

# Studien zur Aktivierung von substituierten Cyclobutanonen mittels *N*-Heterozyklischer Carbene

## NMR-Spektren:

3-(4-Methoxyphenyl)-2-methylaminocyclopent-2-enon:

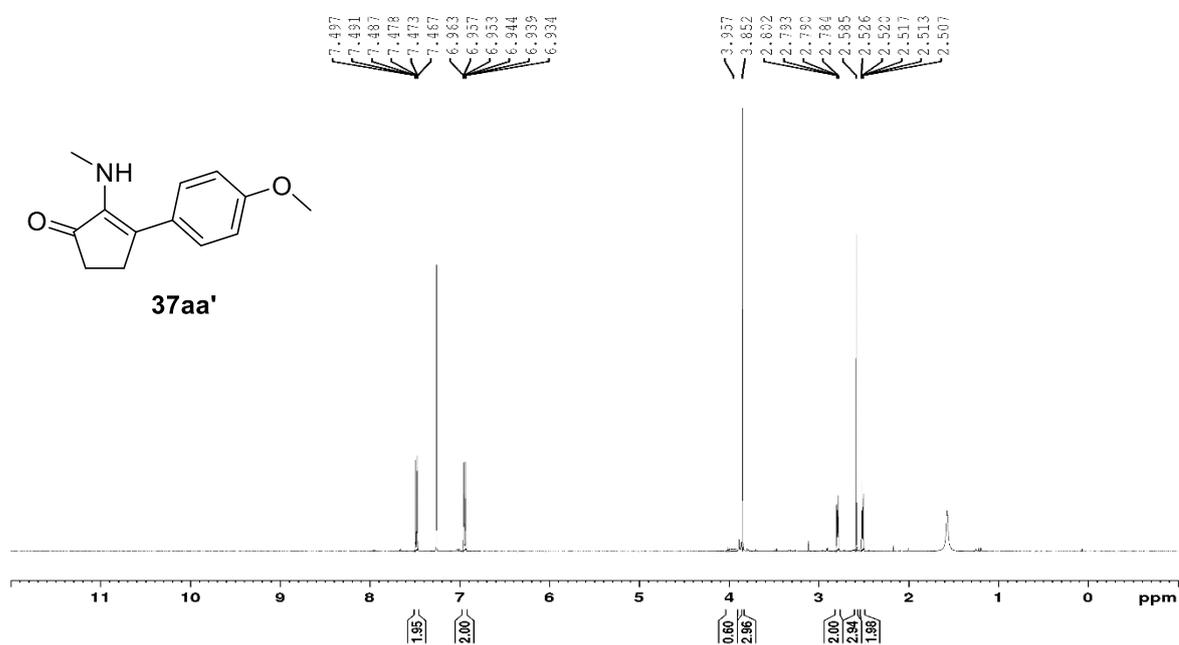


Abbildung A 1: <sup>1</sup>H-NMR-Spektrum von 3-(4-Methoxyphenyl)-2-methylaminocyclopent-2-enon **37aa'**.

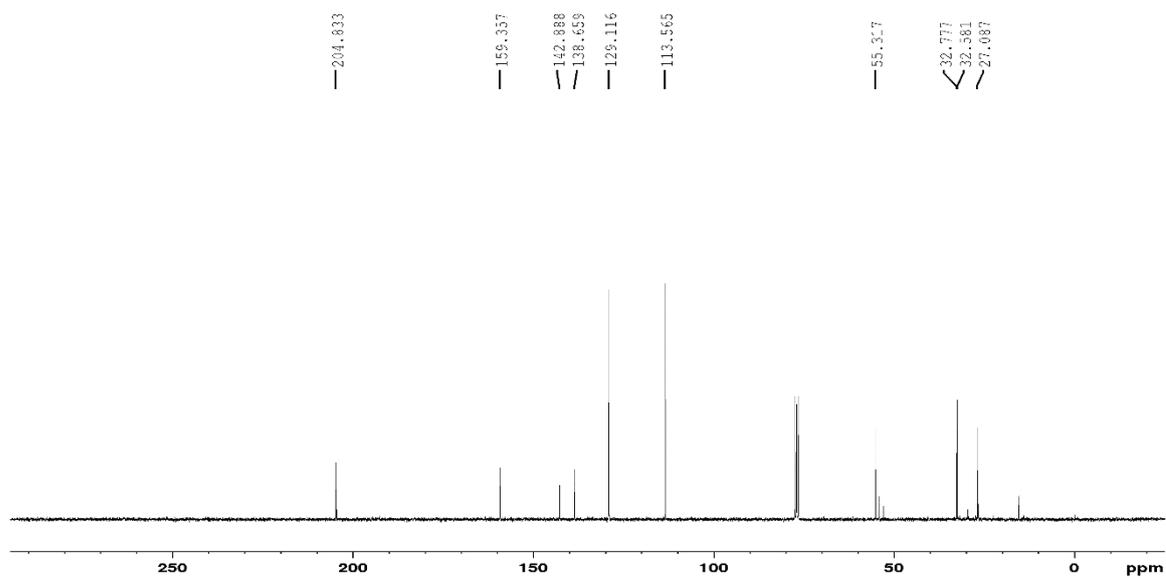


Abbildung A 2:  $^{13}\text{C}$ -NMR-Spektrum von 3-(4-Methoxyphenyl)-2-methylaminocyclopent-2-enon **37aa'**.

3-(4-Methoxyphenyl)-2-benzylaminocyclopent-2-enon:

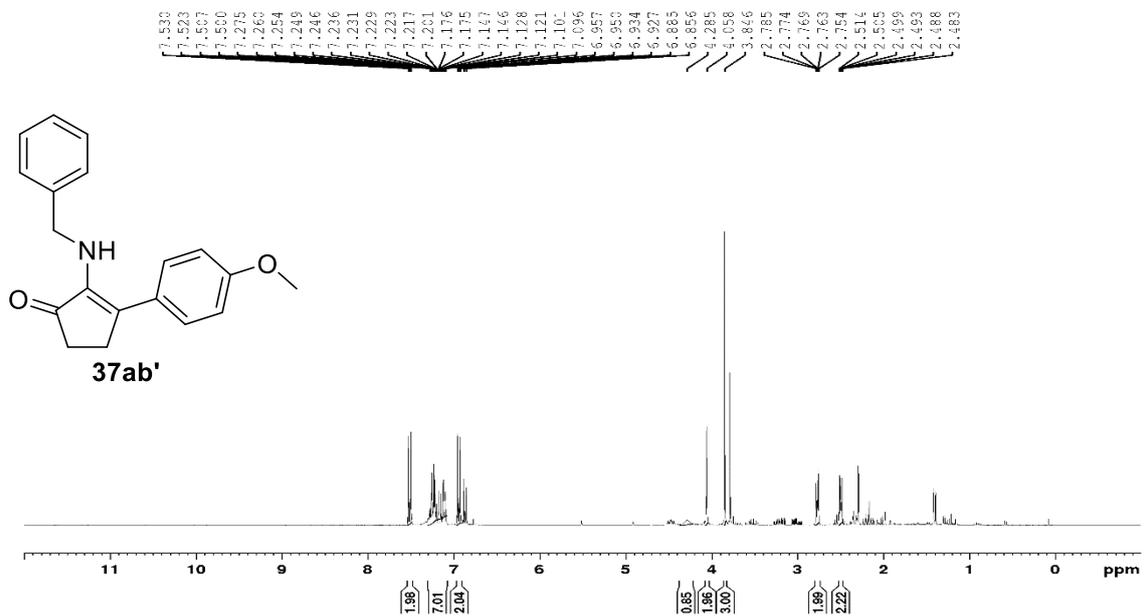


Abbildung A 3: <sup>1</sup>H-NMR-Spektrum von 3-(4-Methoxyphenyl)-2-benzylaminocyclopent-2-enon **37ab'**.

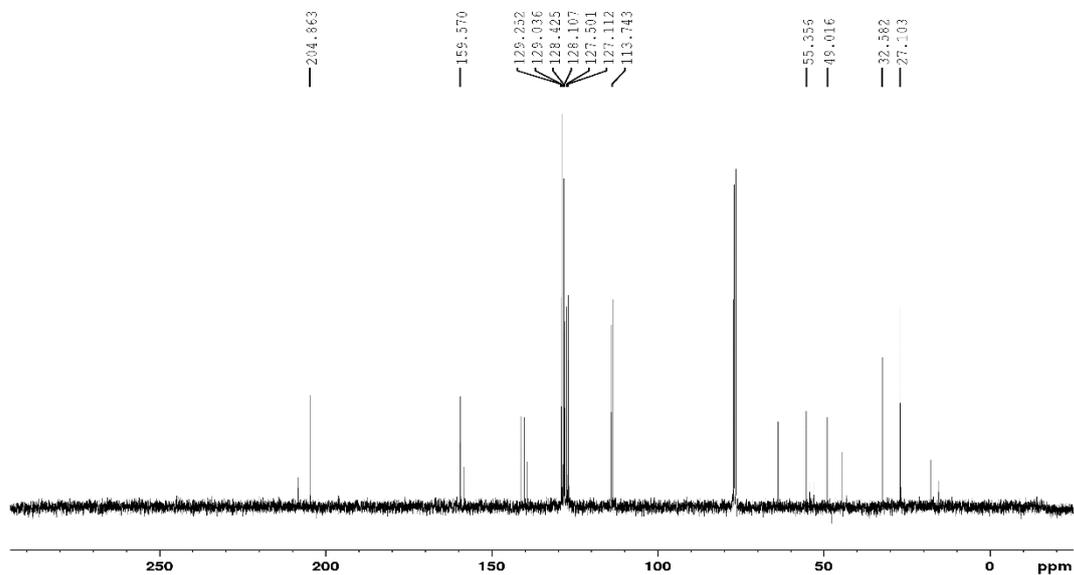


Abbildung A 4: <sup>13</sup>C-NMR-Spektrum von 3-(4-Methoxyphenyl)-2-benzylaminocyclopent-2-enon **37ab'**.

### 3-(4-Methylphenyl)-2-methylaminocyclopent-2-enon:

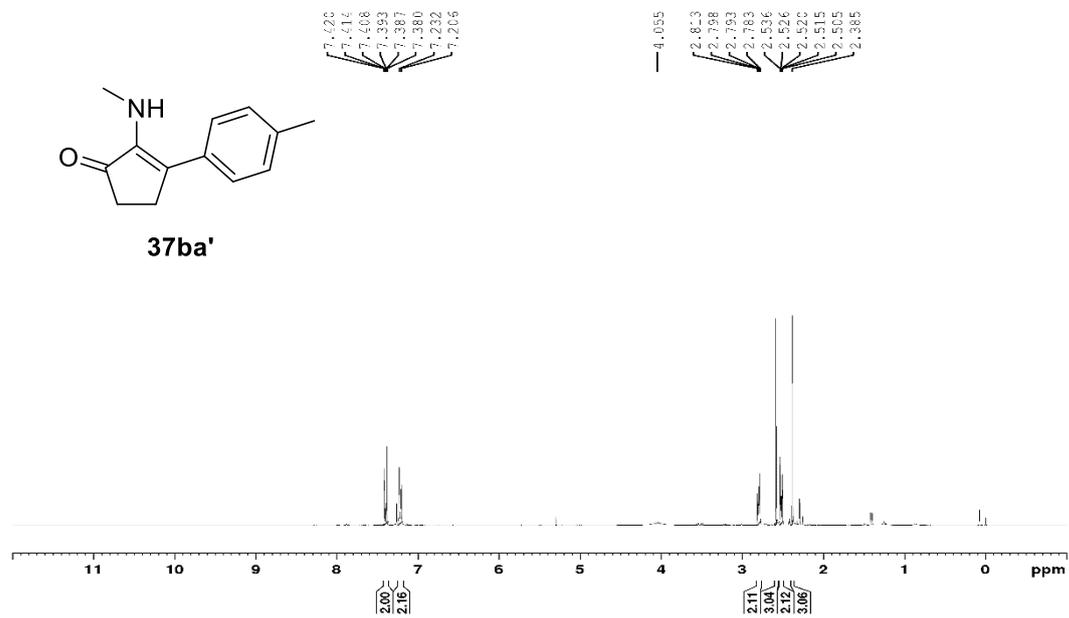


Abbildung A 5: <sup>1</sup>H-NMR-Spektrum von 3-(4-Methylphenyl)-2-methylaminocyclopent-2-enon **37ba'**.

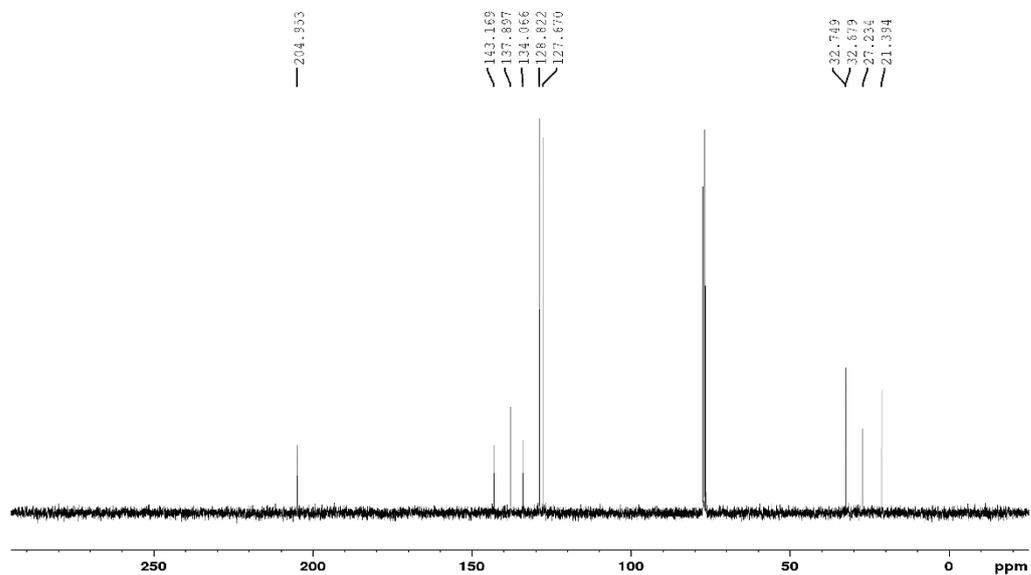


Abbildung A 6: <sup>13</sup>C-NMR-Spektrum von 3-(4-Methylphenyl)-2-methylaminocyclopent-2-enon **37ba'**.

### 3-Phenyl-2-methylaminocyclopent-2-enon:

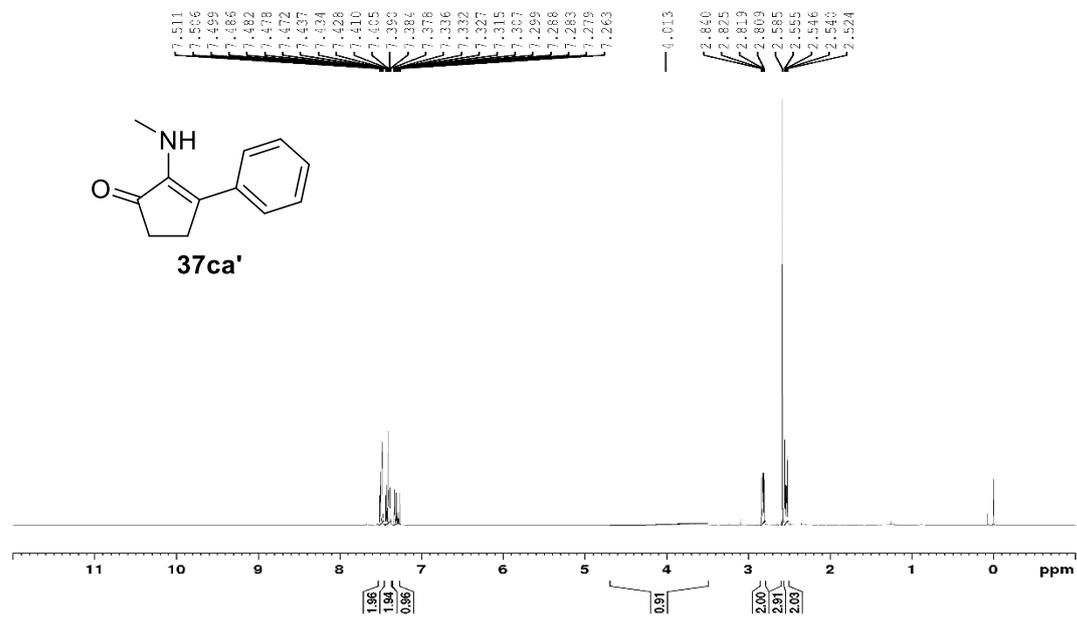


Abbildung A 7: <sup>1</sup>H-NMR-Spektrum von 3-Phenyl-2-methylaminocyclopent-2-enon **37ca'**.

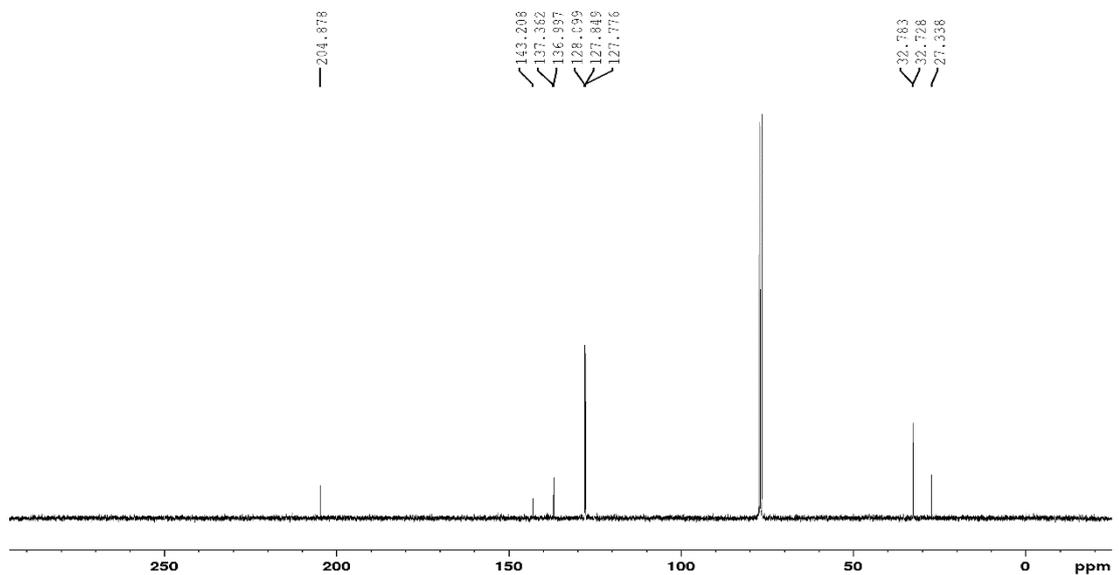


Abbildung A 8: <sup>13</sup>C-NMR-Spektrum von 3-Phenyl-2-methylaminocyclopent-2-enon **37ca'**.

3-(4-Fluorophenyl)-2-methylaminocyclopent-2-enon:

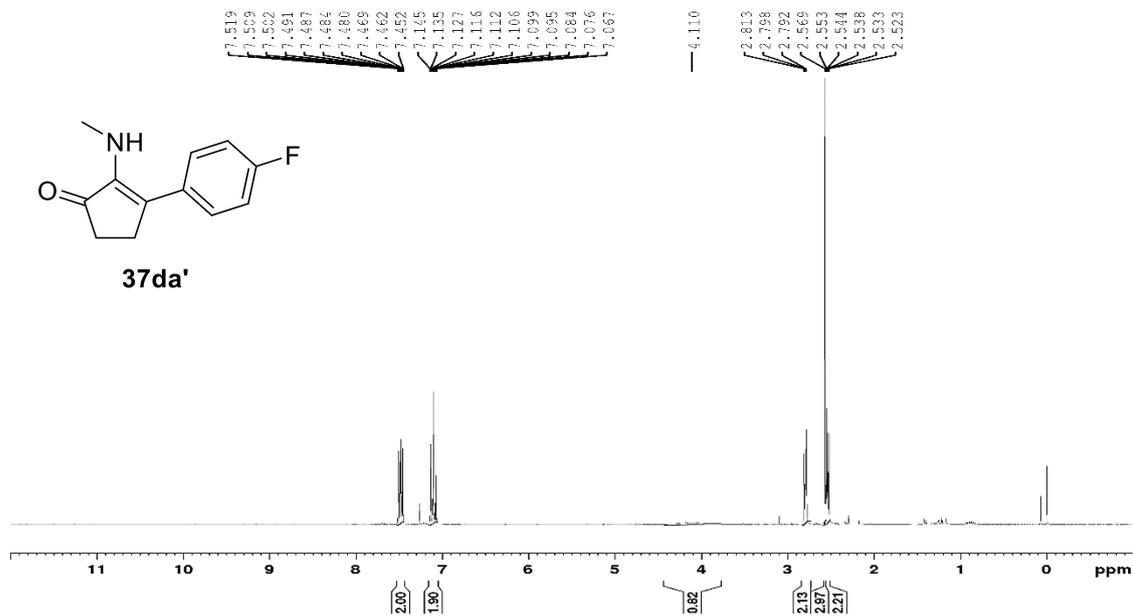


Abbildung A 9: <sup>1</sup>H-NMR-Spektrum von 3-(4-Fluorphenyl)-2-methylaminocyclopent-2-enon **37da'**.

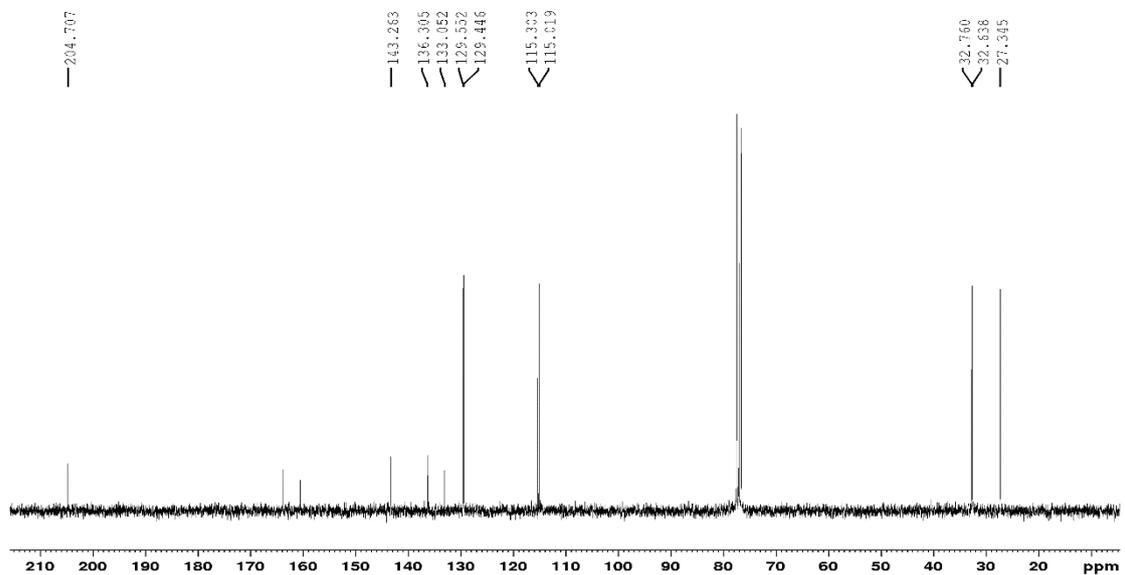


Abbildung A 10: <sup>13</sup>C-NMR-Spektrum von 3-(4-Fluorphenyl)-2-methylaminocyclopent-2-enon **37da'**.

3-(4-Chlorophenyl)-2-methylaminocyclopent-2-enon:

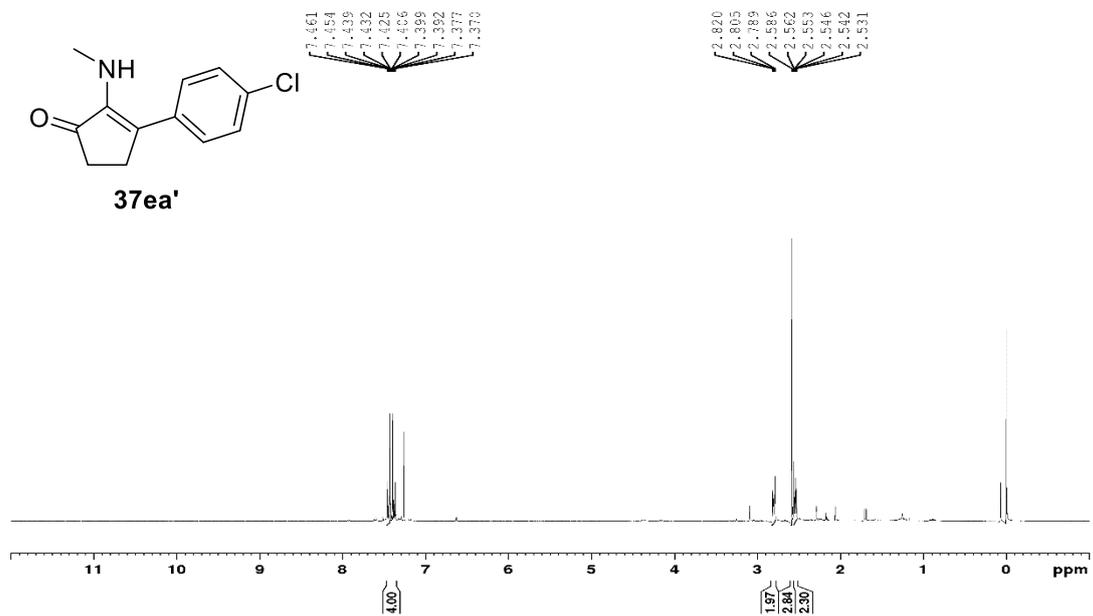


Abbildung A 11: <sup>1</sup>H-NMR-Spektrum von 3-(4-Chlorphenyl)-2-methylaminocyclopent-2-enon **37ea'**.

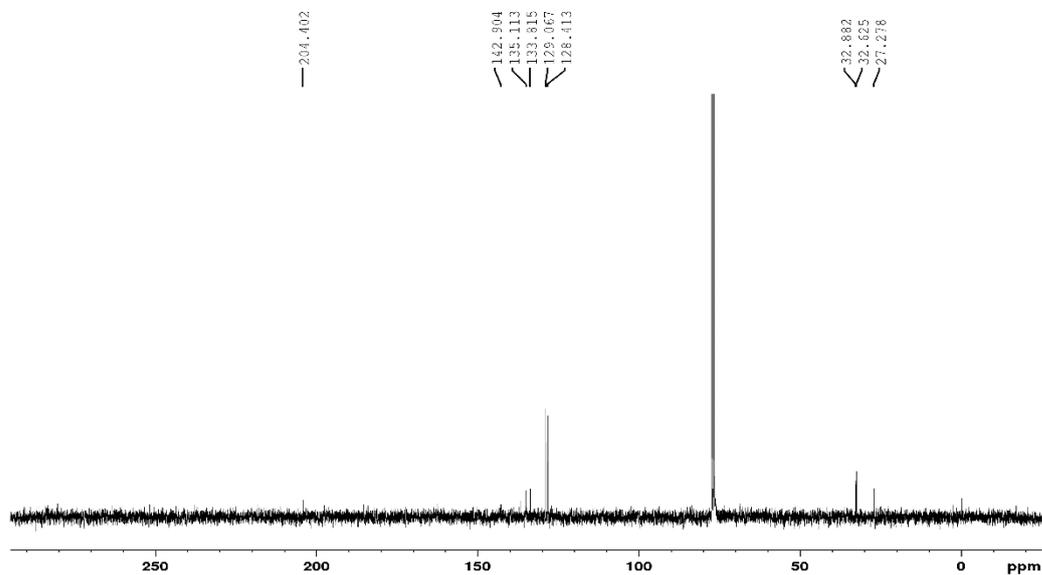


Abbildung A 12: <sup>13</sup>C-NMR-Spektrum von 3-(4-Chlorphenyl)-2-methylaminocyclopent-2-enon **37ea'**.

3-(4-Bromophenyl)-2-methylaminocyclopent-2-enon:

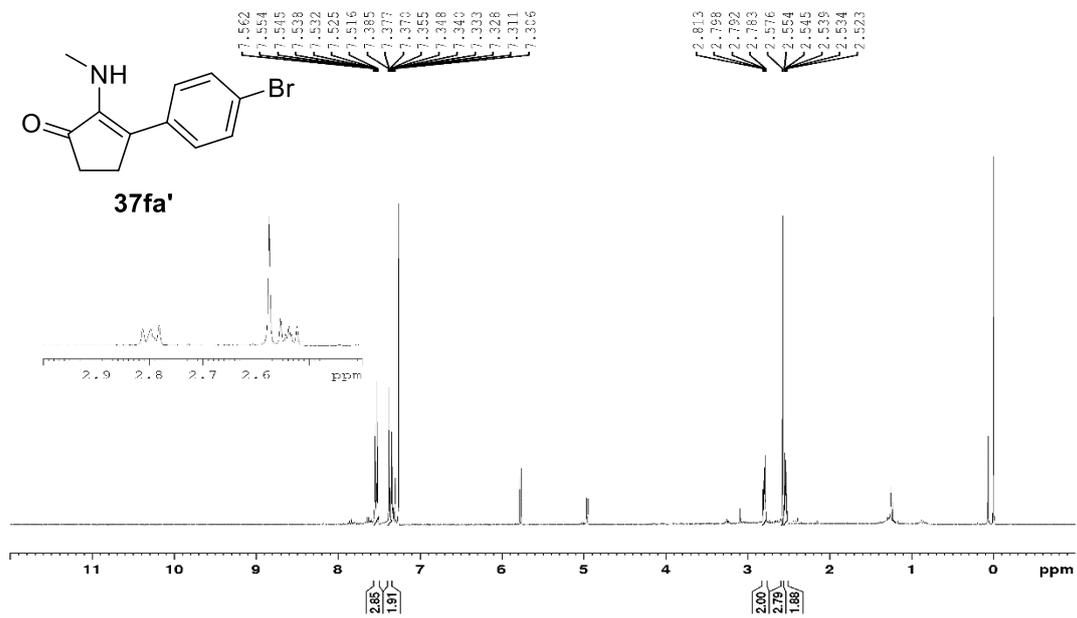


Abbildung A 13: <sup>1</sup>H-NMR-Spektrum von 3-(4-Chlorphenyl)-2-methylaminocyclopent-2-enon **37fa'**.

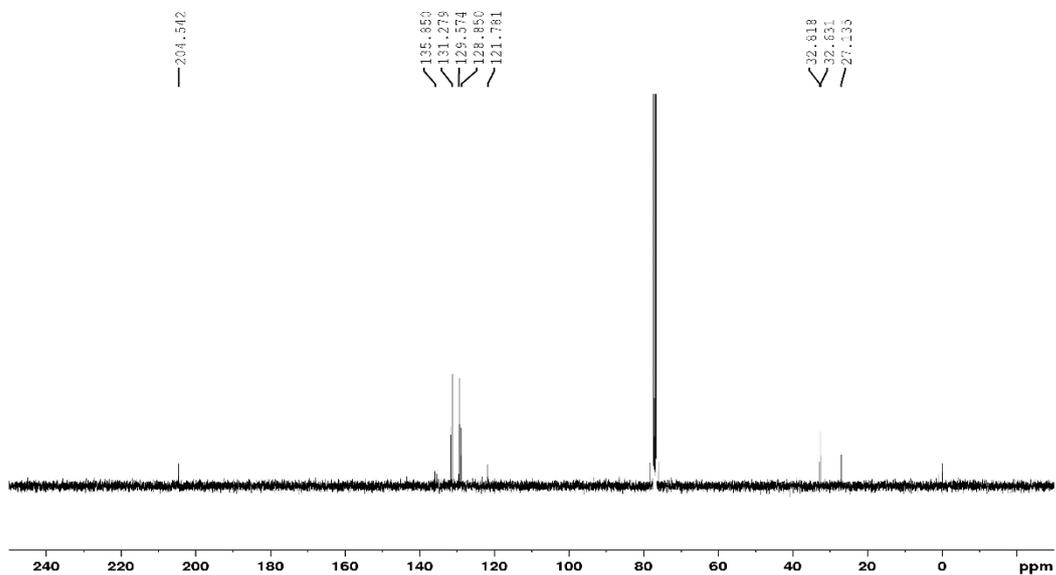


Abbildung A 14: <sup>13</sup>C-NMR-Spektrum von 3-(4-Chlorphenyl)-2-methylaminocyclopent-2-enon **37fa'**.

3-(4-Methoxyphenyl)-2-deuteromethylaminocyclopent-2-enon:

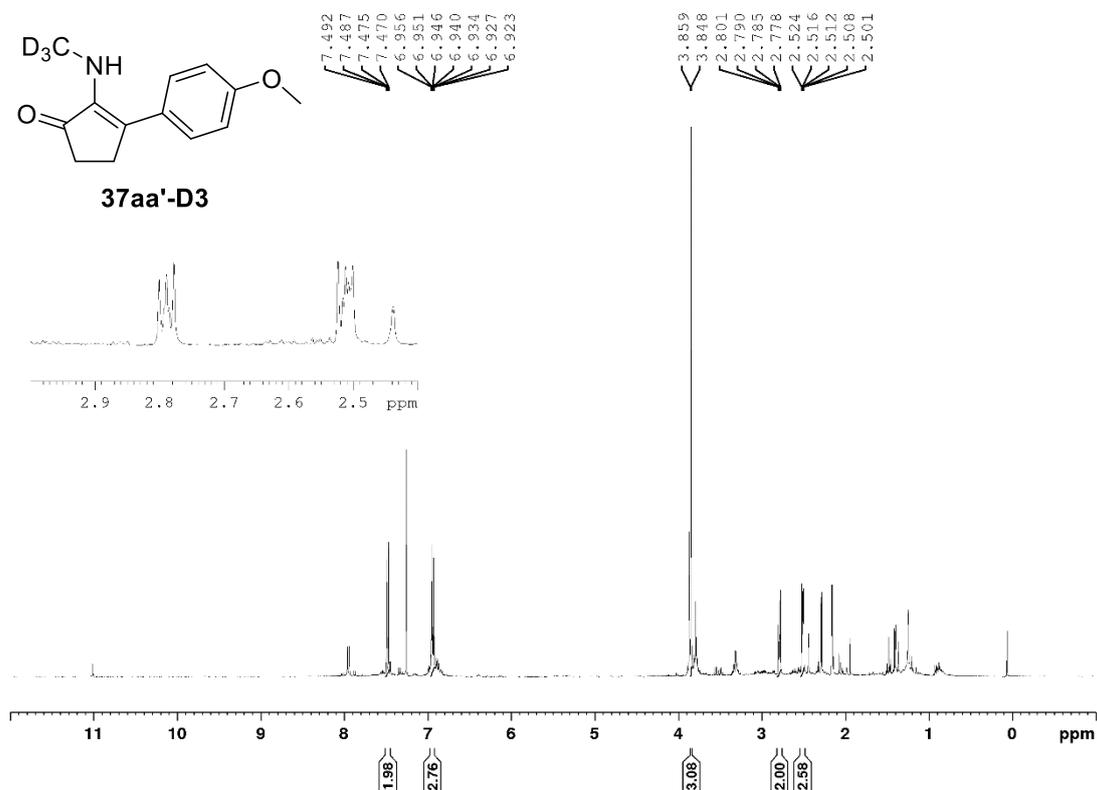


Abbildung A 15: <sup>1</sup>H-NMR-Spektrum von 3-(4-Methoxyphenyl)-2-deuteromethylaminocyclopent-2-enon **37aa'-D3**.

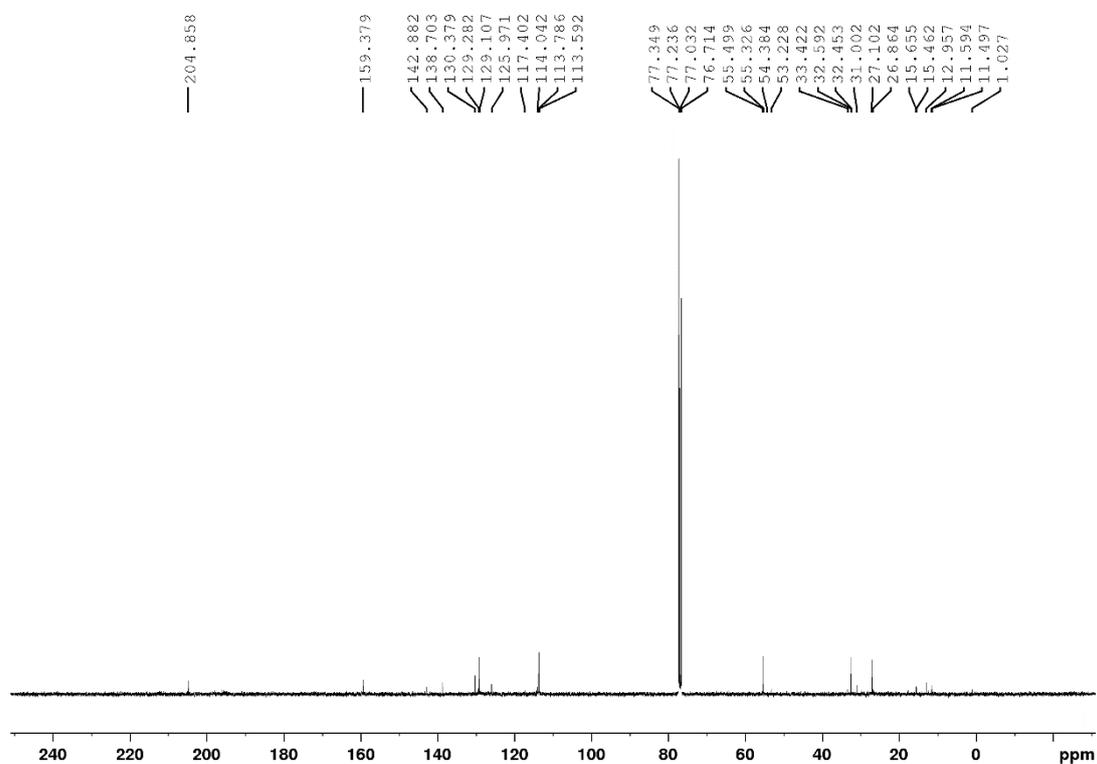


Abbildung A 16: <sup>13</sup>C-NMR-Spektrum von 3-(4-Methoxyphenyl)-2-deuteromethylaminocyclopent-2-enon **37aa'-D3**.

3-(2-Methoxyphenyl)-2-methylaminocyclopent-2-enon:

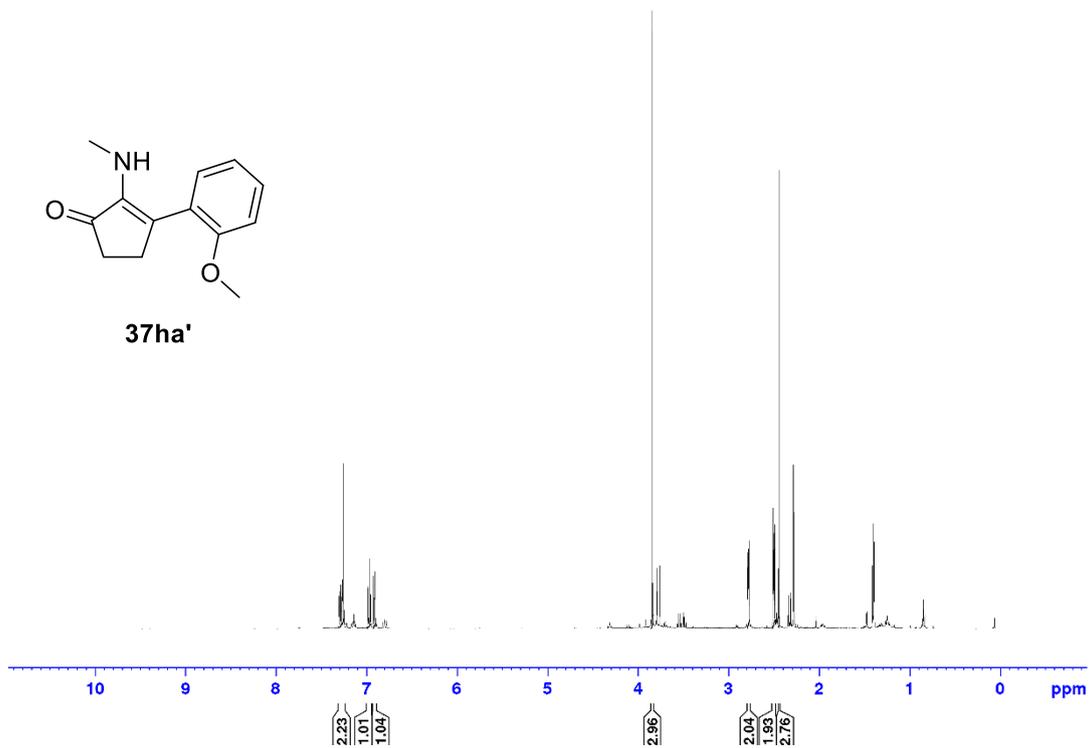


Abbildung A 17: <sup>1</sup>H-NMR-Spektrum von 3-(2-Methoxyphenyl)-2-methylaminocyclopent-2-enon **37ha'**.

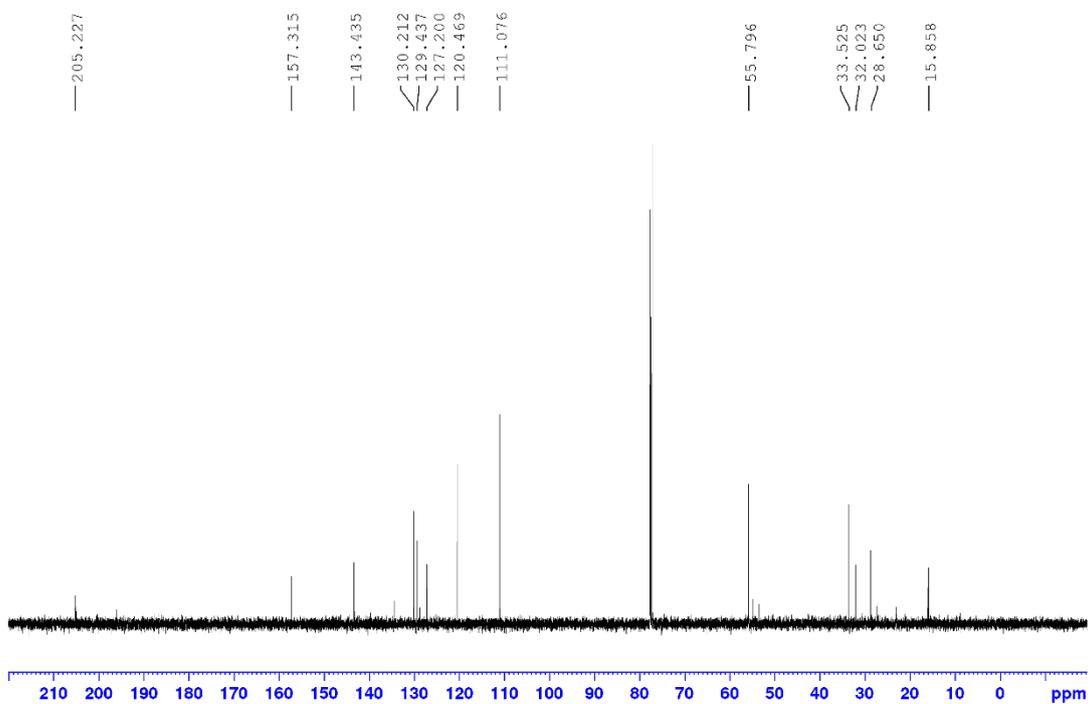


Abbildung A 18: <sup>13</sup>C-NMR-Spektrum von 3-(2-Methoxyphenyl)-2-methylaminocyclopent-2-enon **37ha'**.

2-(4-Methoxyphenyl)cyclobutanon:

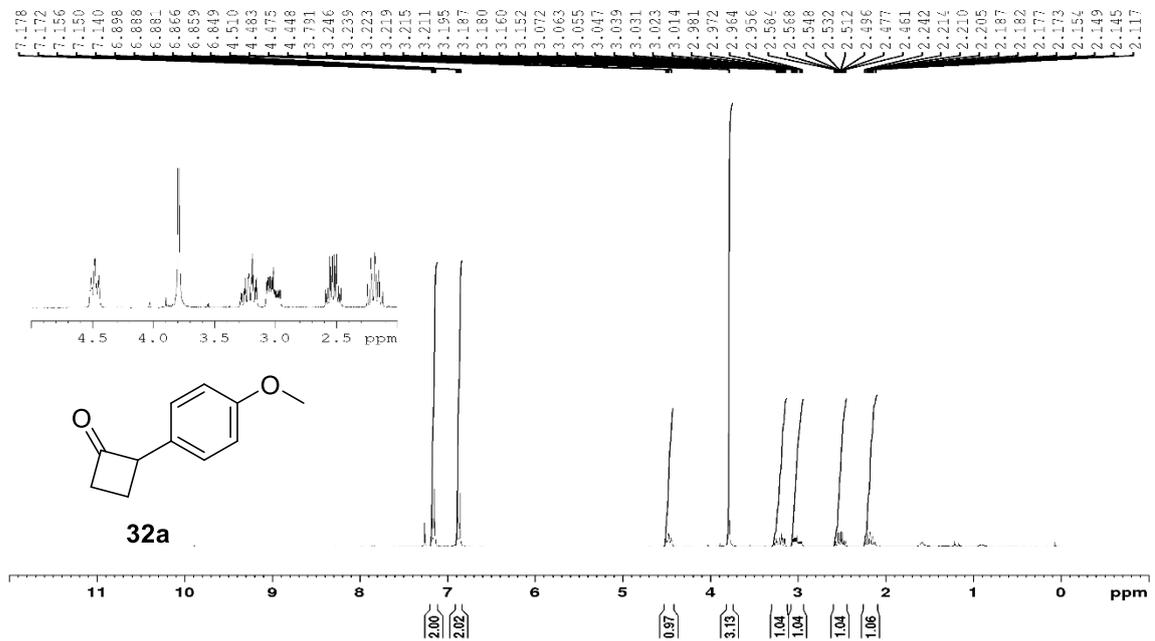


Abbildung A 19: <sup>1</sup>H-NMR-Spektrum von 2-(4-Methoxyphenyl)-cyclobutanon **32a**.

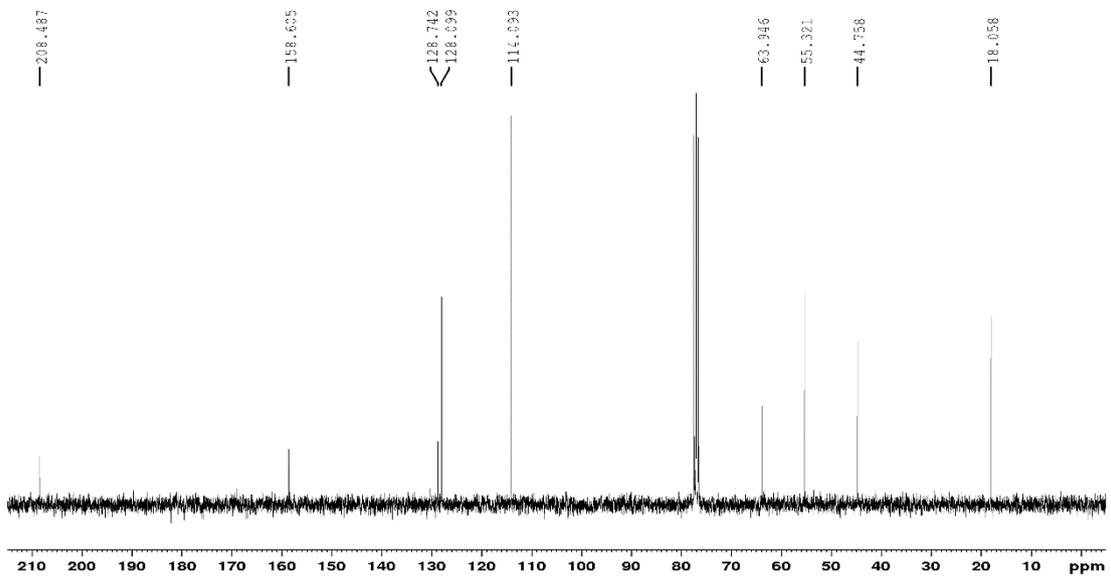


Abbildung A 20: <sup>13</sup>C-NMR-Spektrum von 2-(4-Methoxyphenyl)-cyclobutanon **32a**.



## 2-Phenylcyclobutanon:

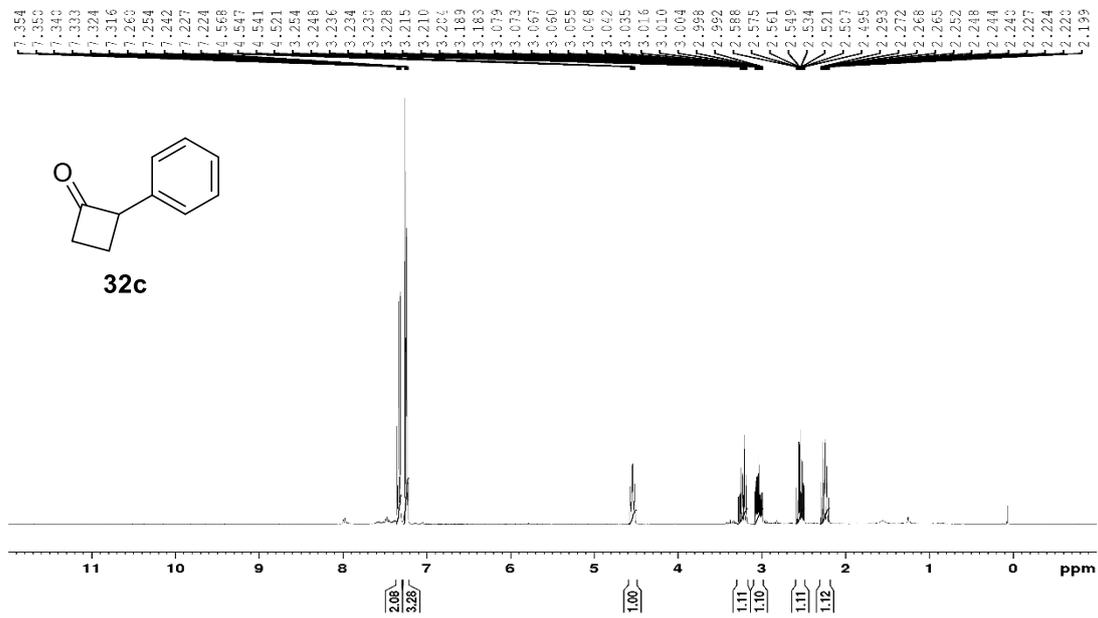


Abbildung A 23: <sup>1</sup>H-NMR-Spektrum von 2-Phenylcyclobutanon **32c**.

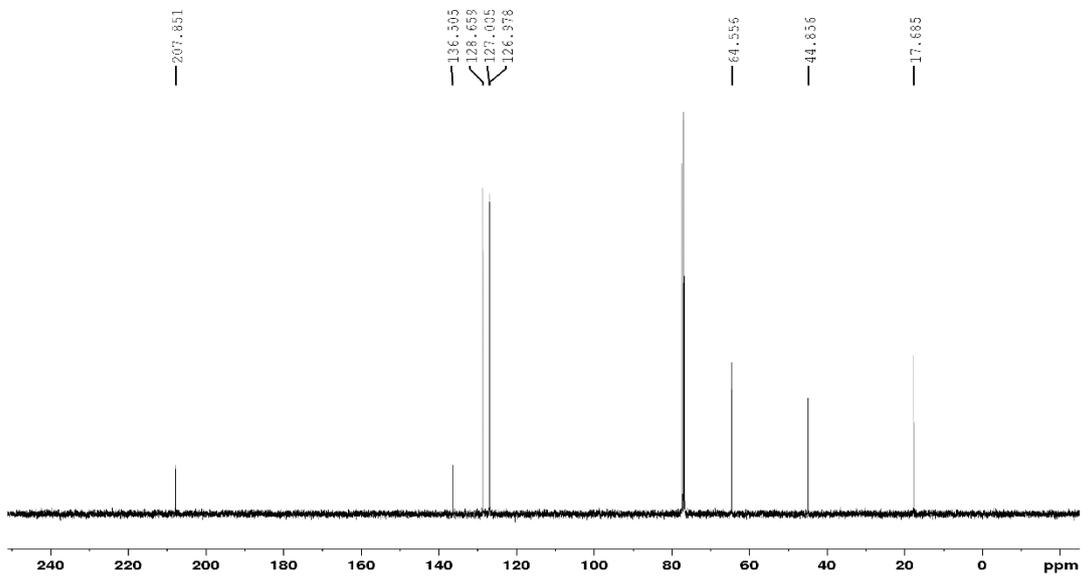


Abbildung A 24: <sup>13</sup>C-NMR-Spektrum von 2-Phenylcyclobutanon **32c**.

## 2-(4-Fluorophenyl)cyclobutanon:

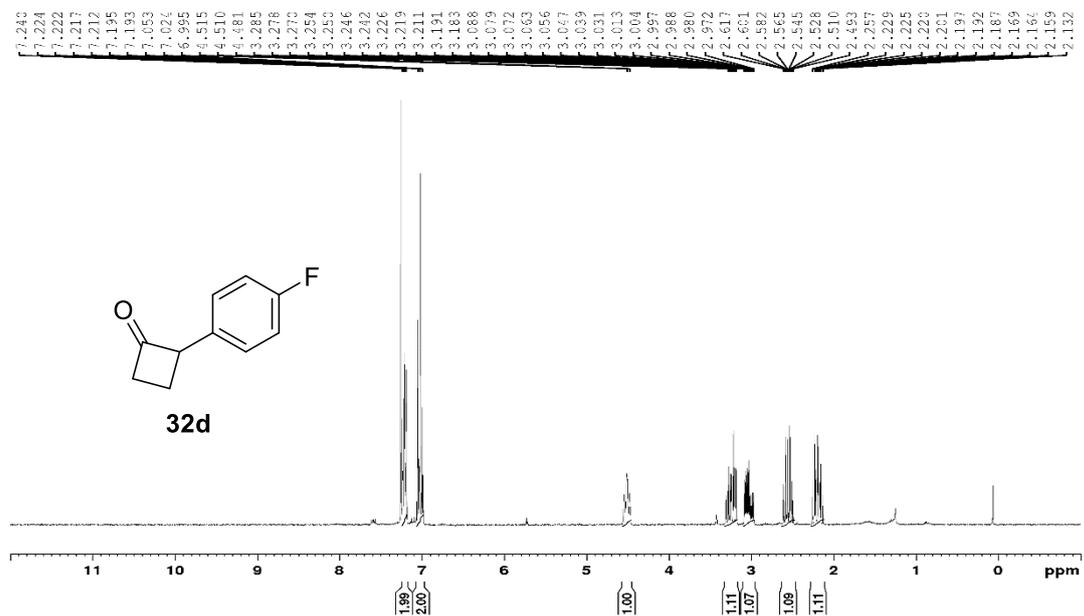


Abbildung A 25: <sup>1</sup>H-NMR-Spektrum von 2-(4-Fluorphenyl)-cyclobutanon **32d**.

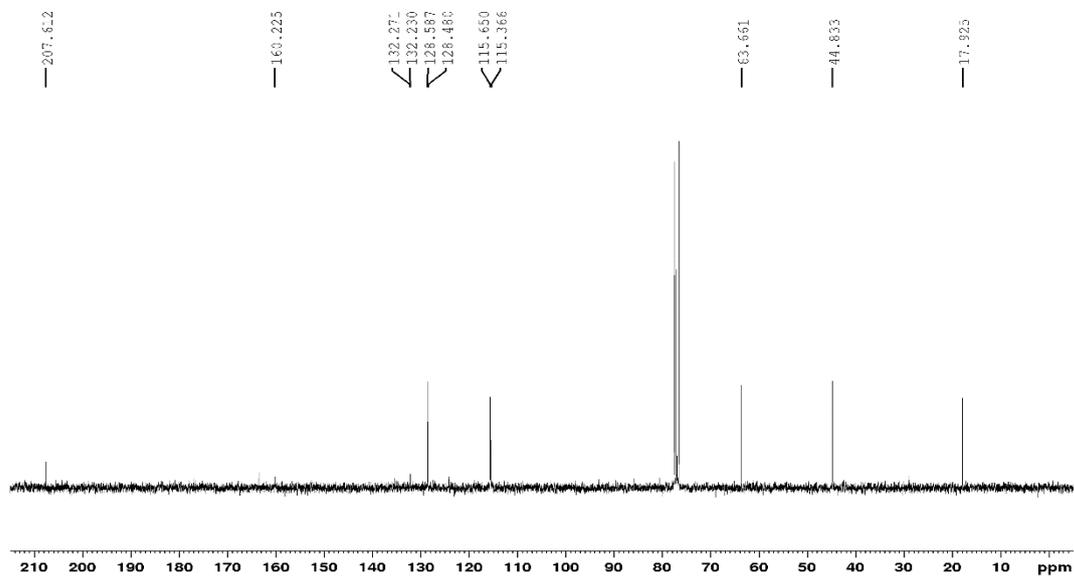


Abbildung A 26: <sup>13</sup>C-NMR-Spektrum von 2-(4-Fluorphenyl)-cyclobutanon **32d**.

## 2-(4-Chlorphenyl)cyclobutanon:

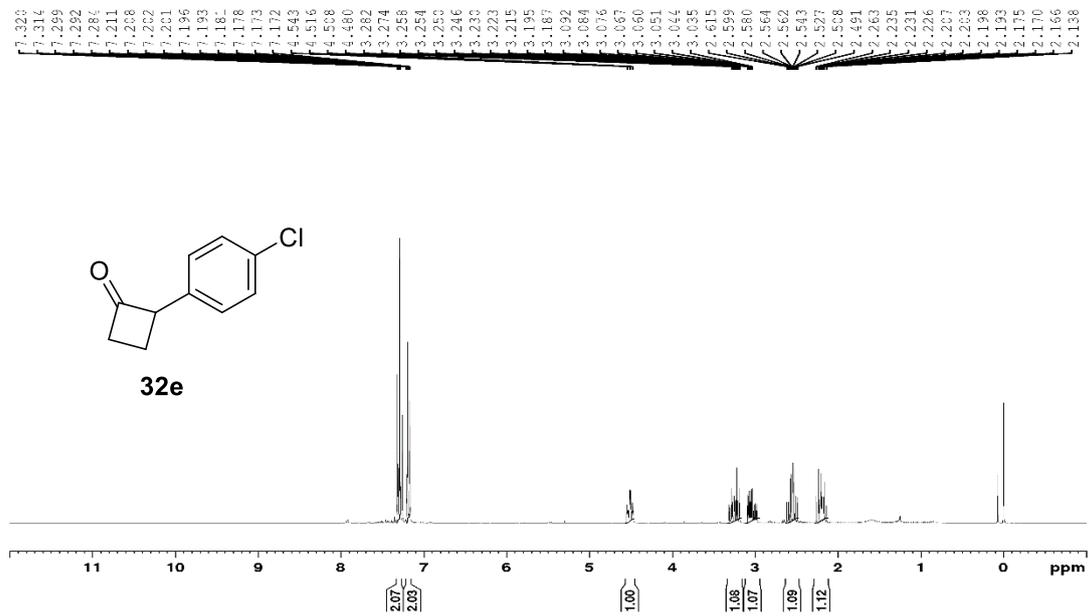


Abbildung A 27: <sup>1</sup>H-NMR-Spektrum von 2-(4-Chlorphenyl)-cyclobutanon **32e**.

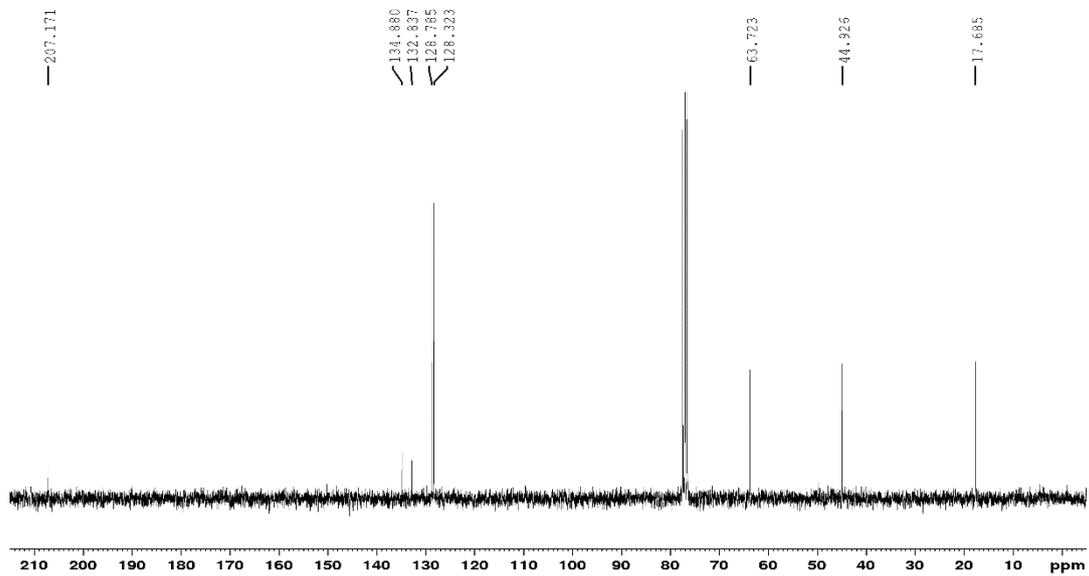


Abbildung A 28: <sup>13</sup>C-NMR-Spektrum von 2-(4-Chlorphenyl)-cyclobutanon **32e**.

2-(4-Bromophenyl)cyclobutanon:

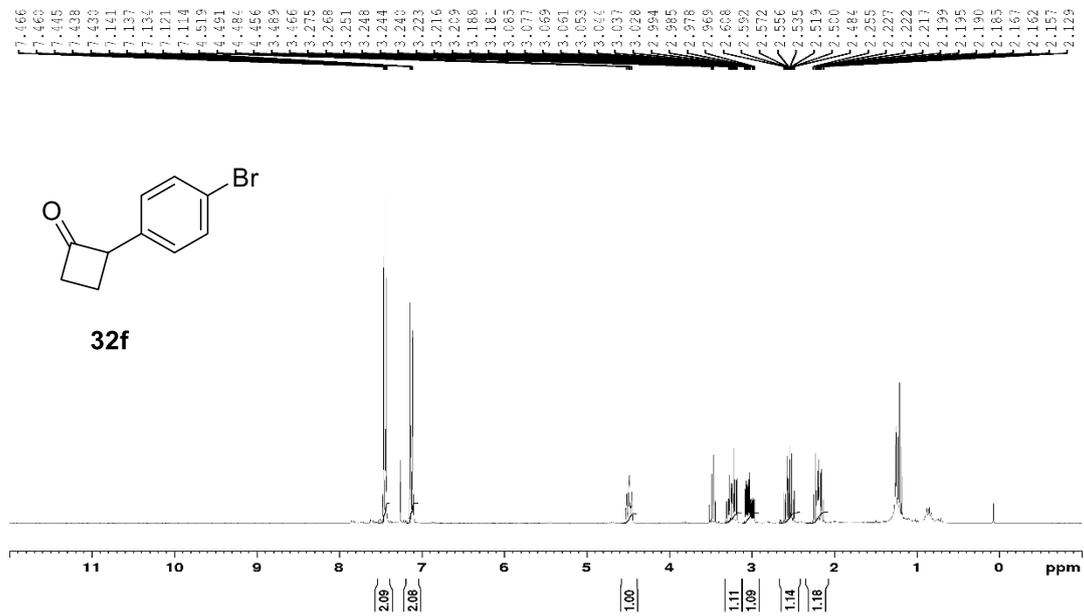


Abbildung A 29: <sup>1</sup>H-NMR-Spektrum von 2-(4-Bromphenyl)-cyclobutanon **32f**.

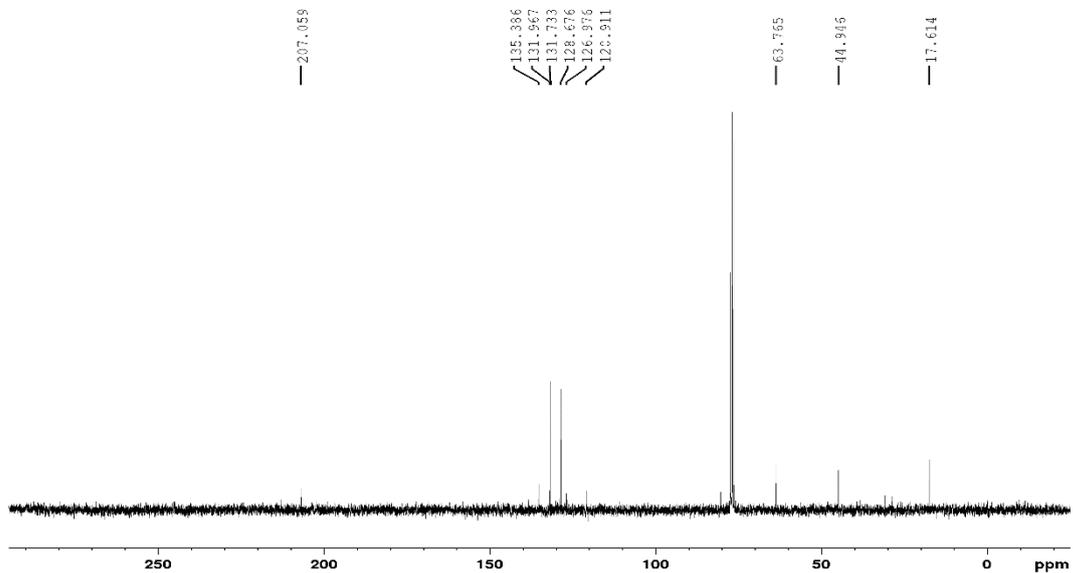


Abbildung A 30: <sup>13</sup>C-NMR-Spektrum von 2-(4-Bromphenyl)-cyclobutanon **32f**.

## 2-(2-Methoxyphenyl)cyclobutanon

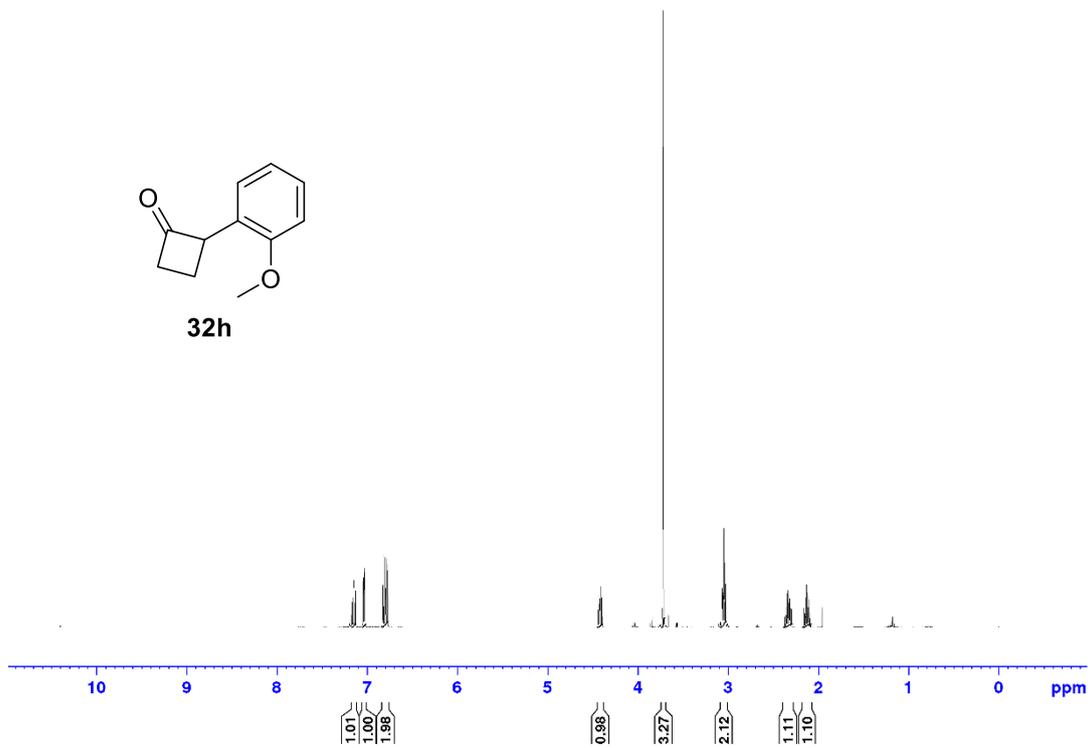


Abbildung A 31: <sup>1</sup>H-NMR-Spektrum von 2-(2-Methoxyphenyl)-cyclobutanon **32h**.

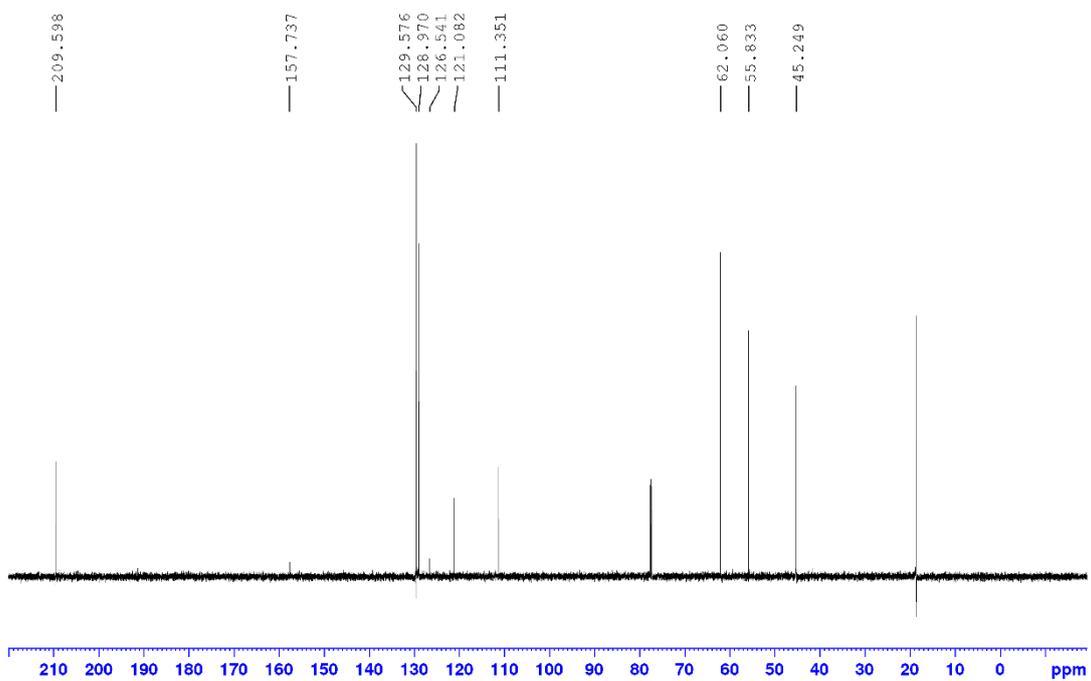


Abbildung A 32: <sup>13</sup>C-NMR-Spektrum von 2-(2-Methoxyphenyl)-cyclobutanon **32h**.

2-Methyl-2-(4-methoxyphenyl)cyclobutanon:

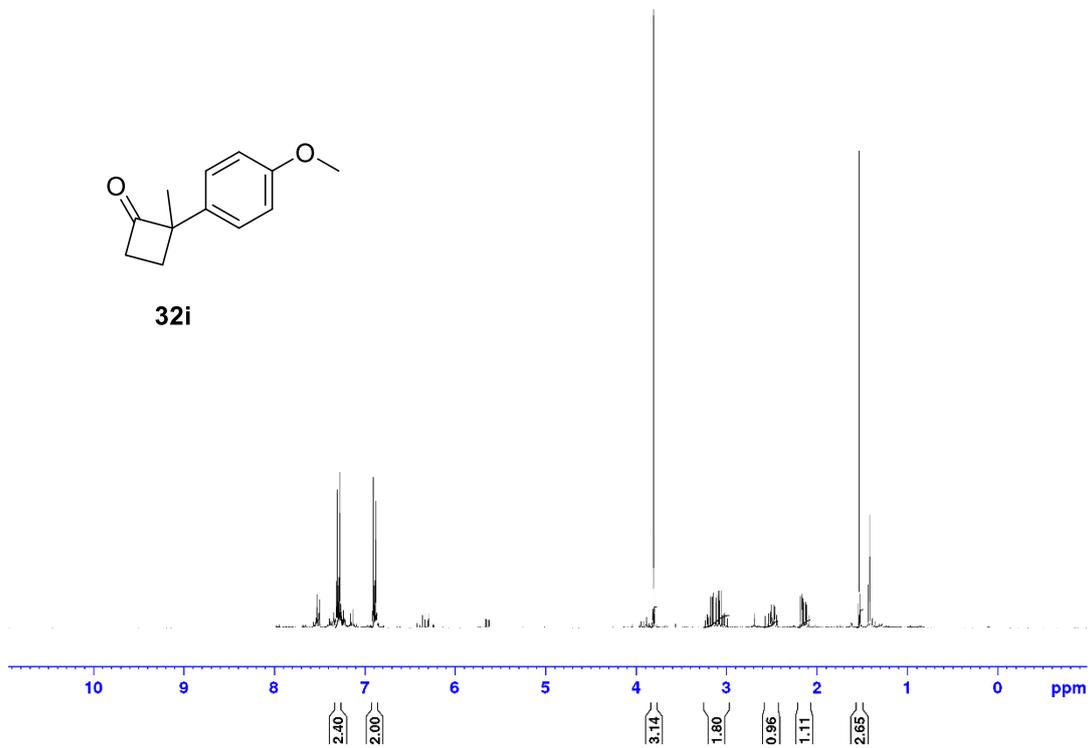


Abbildung A 33: <sup>1</sup>H-NMR-Spektrum von 2-Methyl-2-(4-methoxyphenyl)-cyclobutanon **32i**.

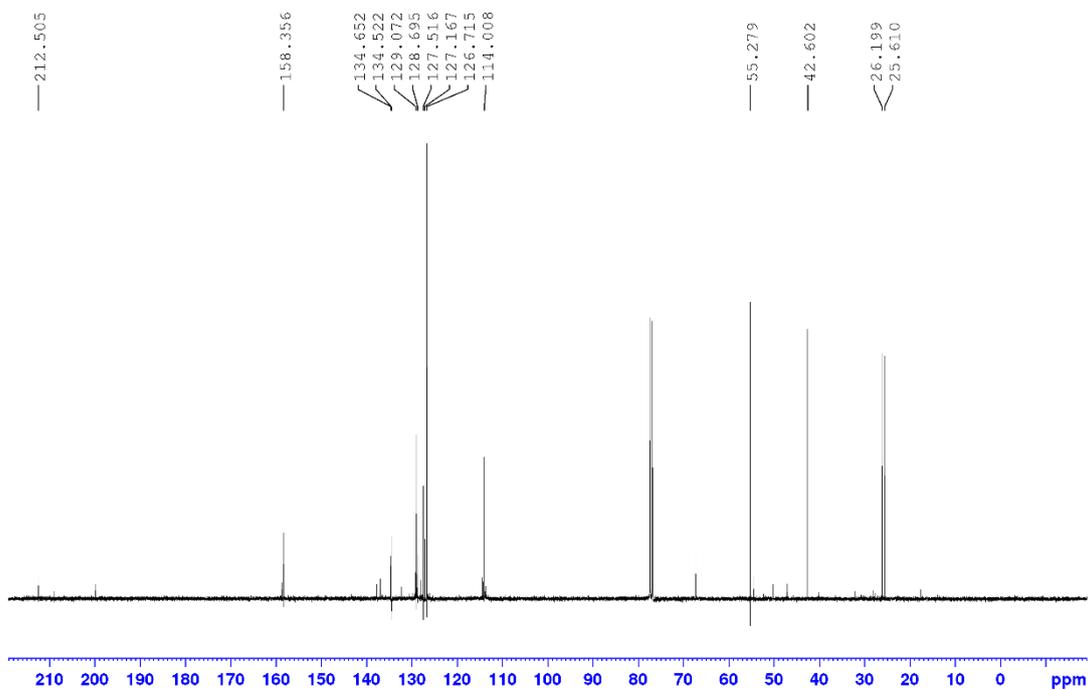


Abbildung A 34: <sup>13</sup>C-NMR-Spektrum von 2-Methyl-2-(4-methoxyphenyl)-cyclobutanon **32i**.

# 1-(4-Methoxyphenyl)-1-cyclopropylmethen:

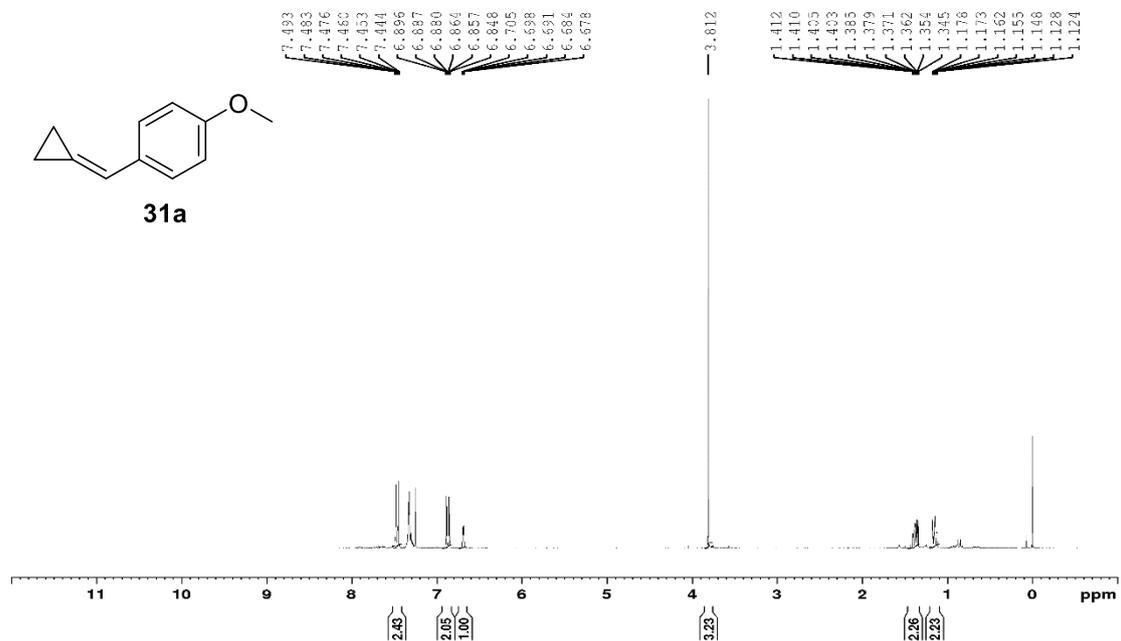


Abbildung A 35: <sup>1</sup>H-NMR-Spektrum von 1-(4-Methoxyphenyl)-1-cyclopropylmethen **31a**.

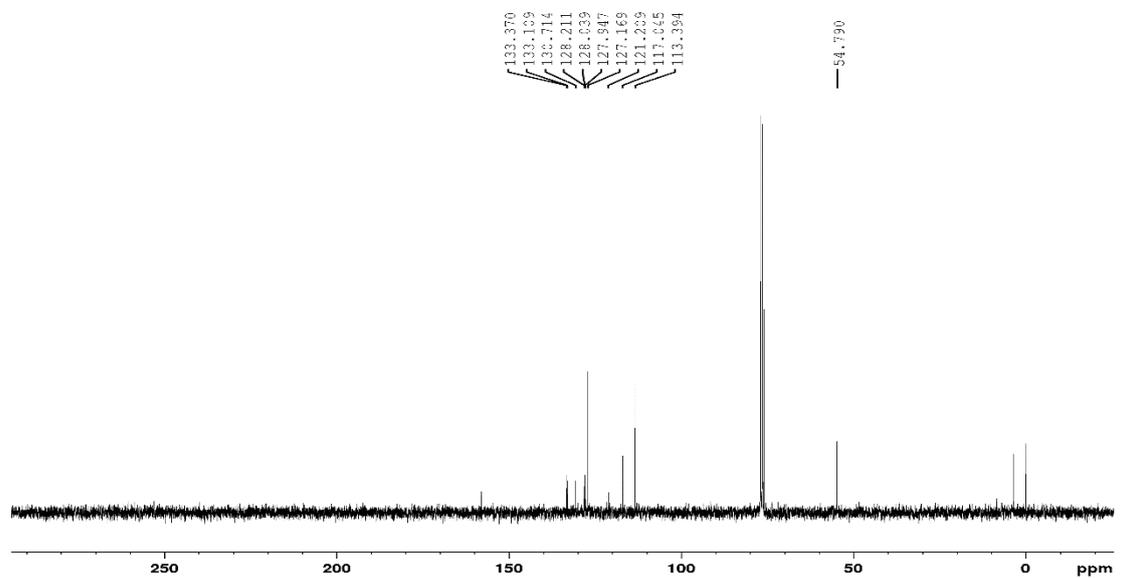


Abbildung A 36: <sup>13</sup>C-NMR-Spektrum von 1-(4-Methoxyphenyl)-1-cyclopropylmethen **31a**.

1-(4-Methylphenyl)-1-cyclopropylmethen:

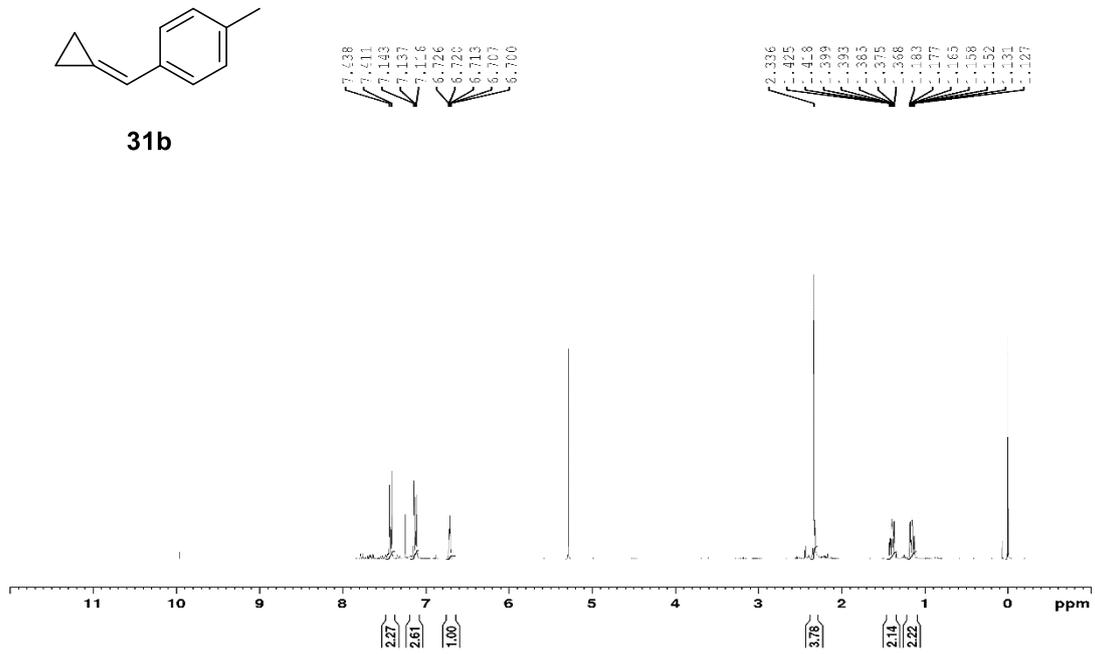


Abbildung A 37: <sup>1</sup>H-NMR-Spektrum von 1-(4-Methylphenyl)-1-cyclopropylmethen **31b**.

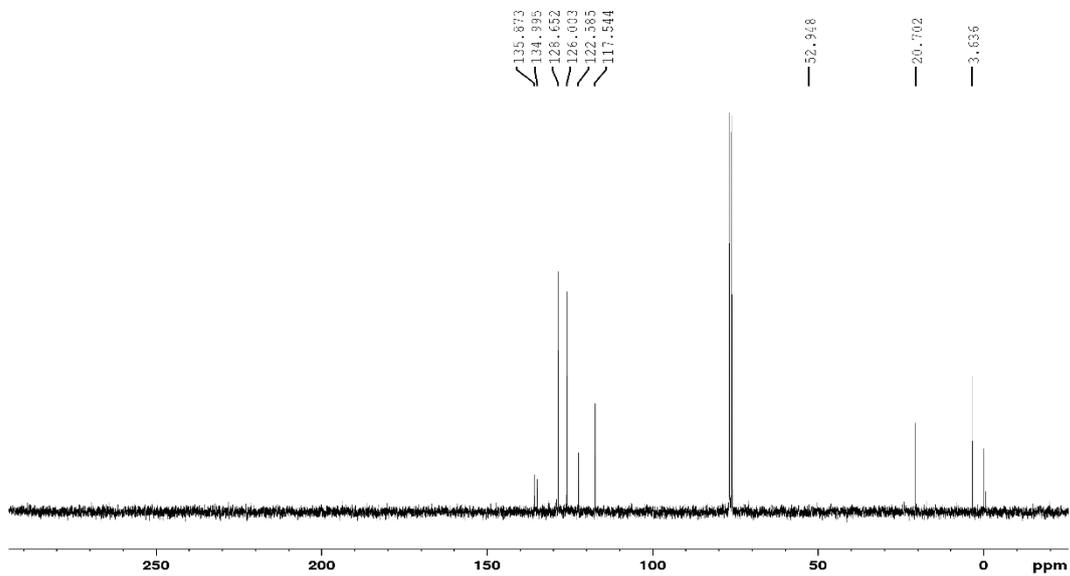


Abbildung A 38: <sup>13</sup>C-NMR-Spektrum von 1-(4-Methylphenyl)-1-cyclopropylmethen **31b**.

## 1-Phenyl-1-cyclopropylmethen:

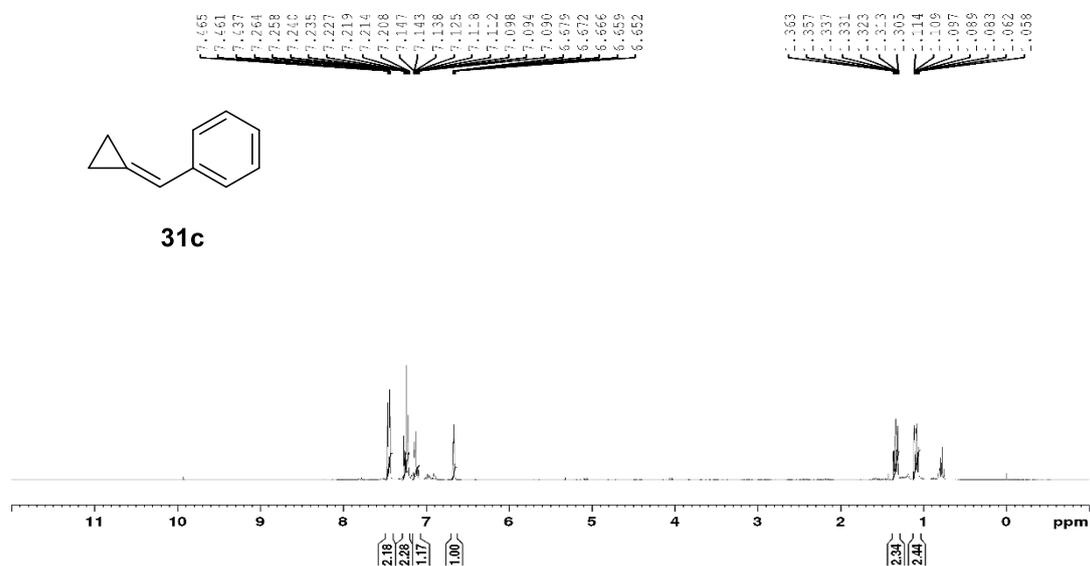


Abbildung A 39: <sup>1</sup>H-NMR-Spektrum von 1-Phenyl-1-cyclopropylmethen **31c**.

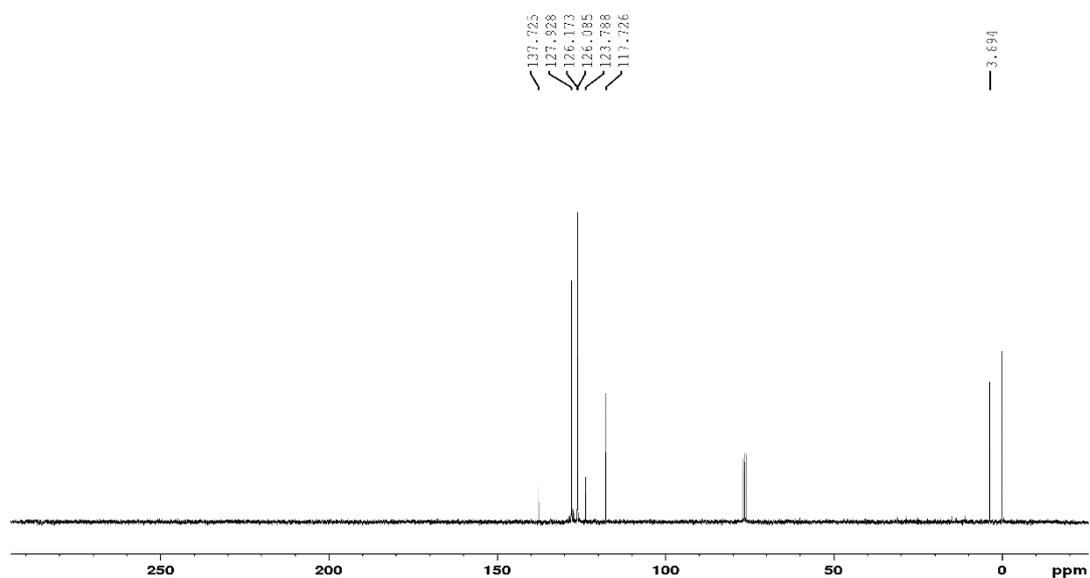


Abbildung A 40: <sup>13</sup>C-NMR-Spektrum von 1-Phenyl-1-cyclopropylmethen **31c**.

# 1-(4-Cyanophenyl)-1-cyclopropylmethen

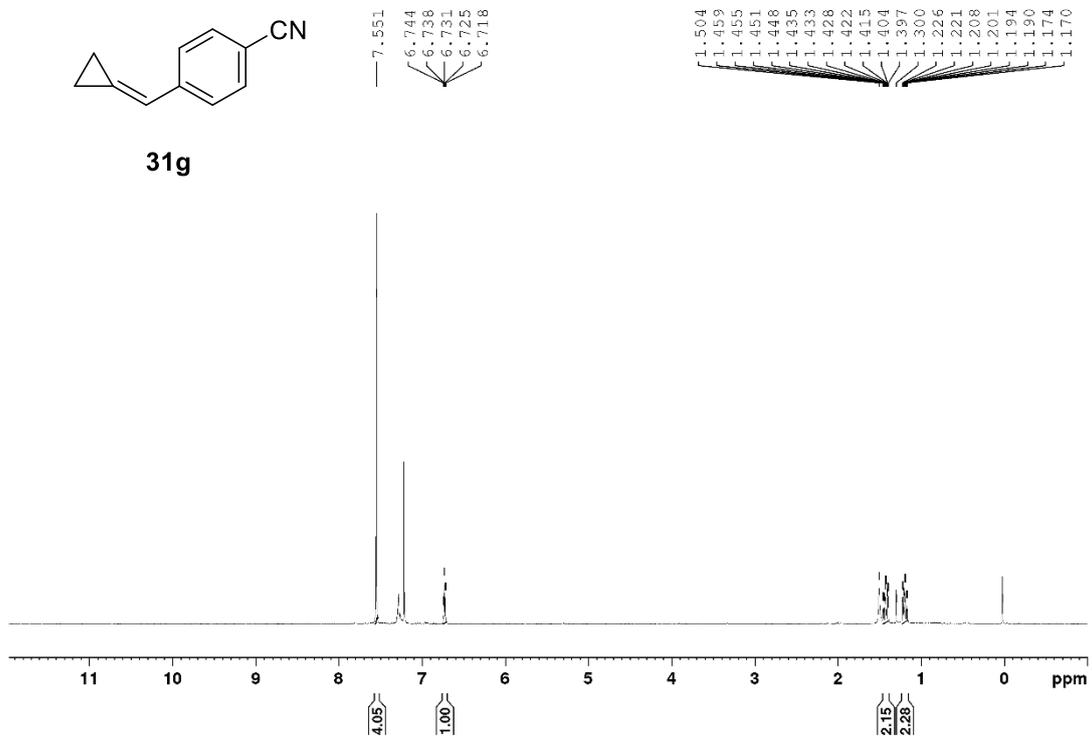


Abbildung A 41: <sup>1</sup>H-NMR-Spektrum von 1-(4-Cyanophenyl)-1-cyclopropylmethen **31g**.

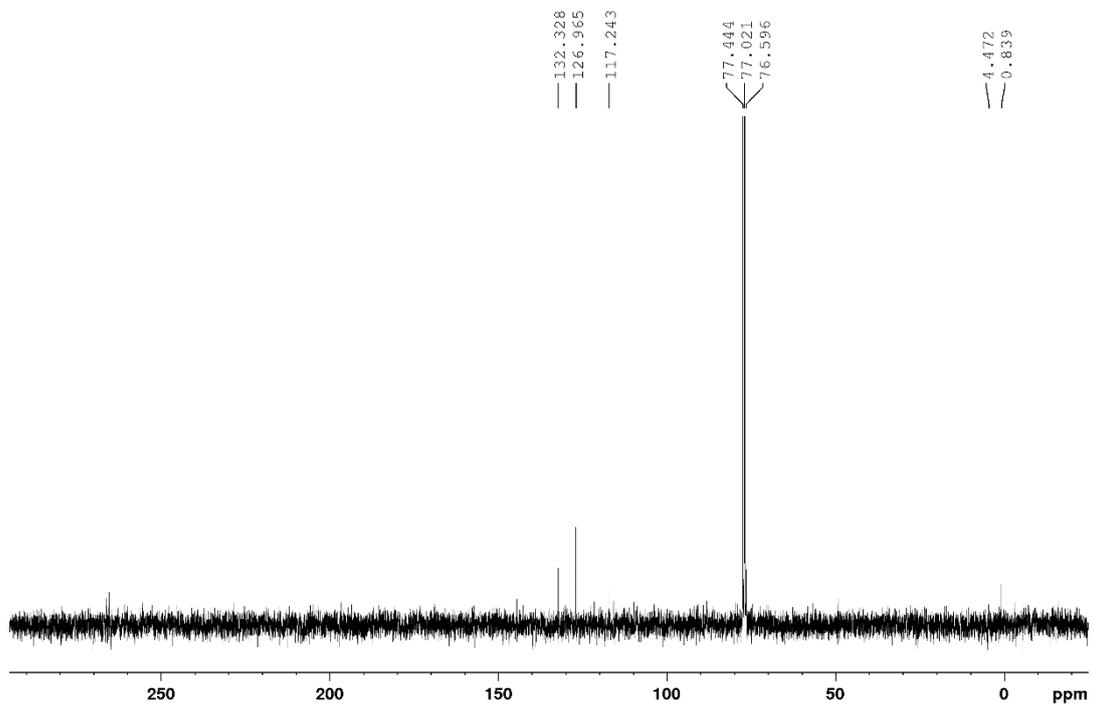


Abbildung A 42: <sup>13</sup>C-NMR-Spektrum von 1-(4-Cyanophenyl)-1-cyclopropylmethen **31g**.

1-(4-Fluorphenyl)-1-(1-(phenylthio)cyclopropyl)methanol:

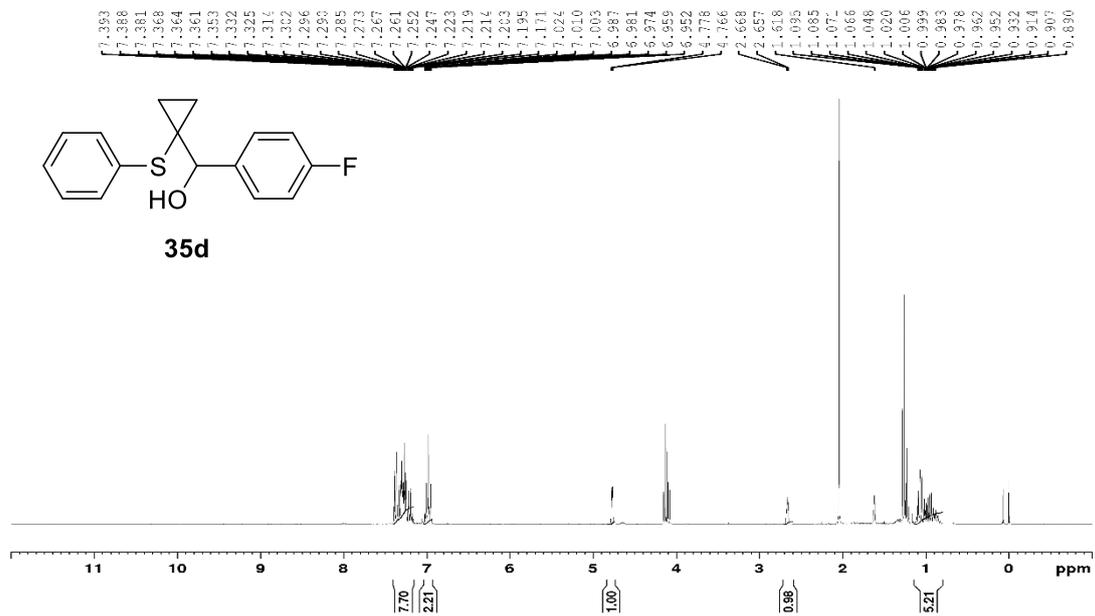


Abbildung A 43: <sup>1</sup>H-NMR-Spektrum von 1-(4-Fluorphenyl)-1-(1-(phenylthio)cyclopropyl)methanol **35d**.

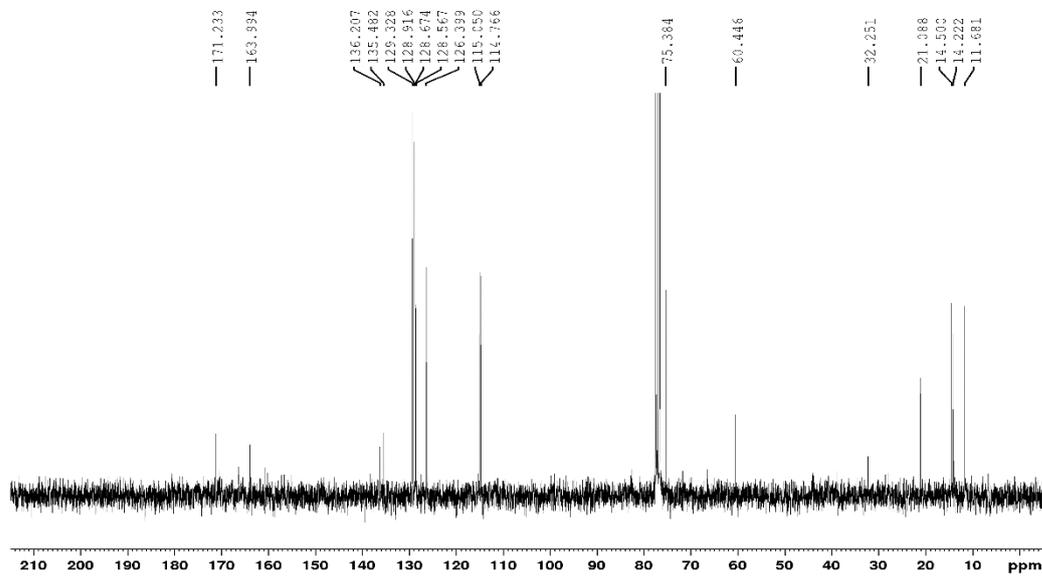


Abbildung A 44: <sup>13</sup>C-NMR-Spektrum von 1-(4-Fluorphenyl)-1-(1-(phenylthio)cyclopropyl)methanol **35d**.

1-(4-Chlorphenyl)-1-(1-(phenylthio)cyclopropyl)methanol:

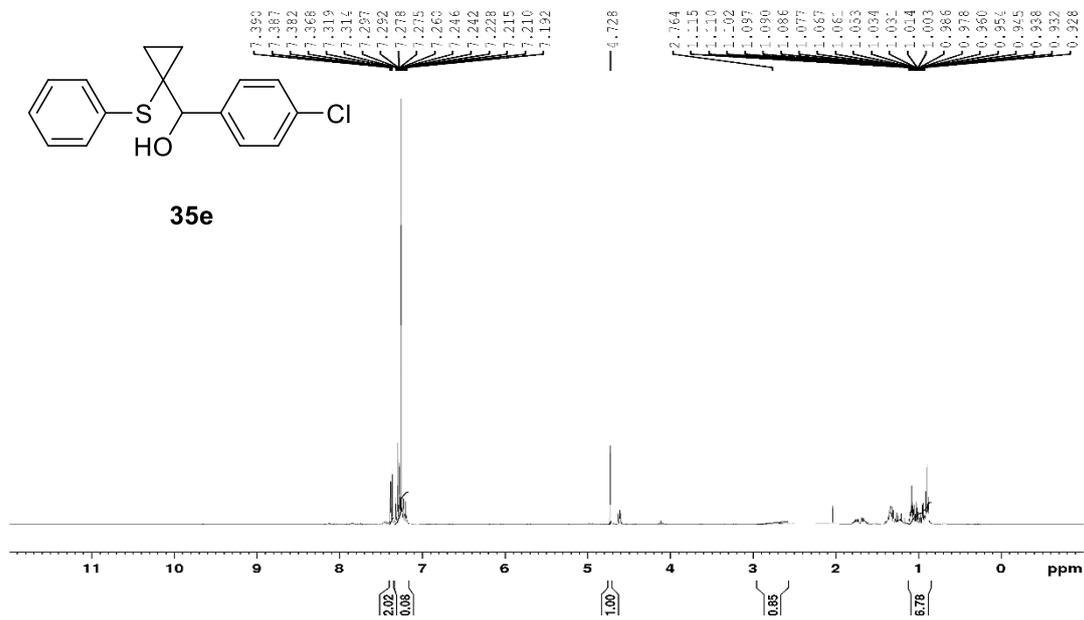


Abbildung A 45: <sup>1</sup>H-NMR-Spektrum von 1-(4-Chlorphenyl)-1-(1-(phenylthio)cyclopropyl)methanol **35e**.

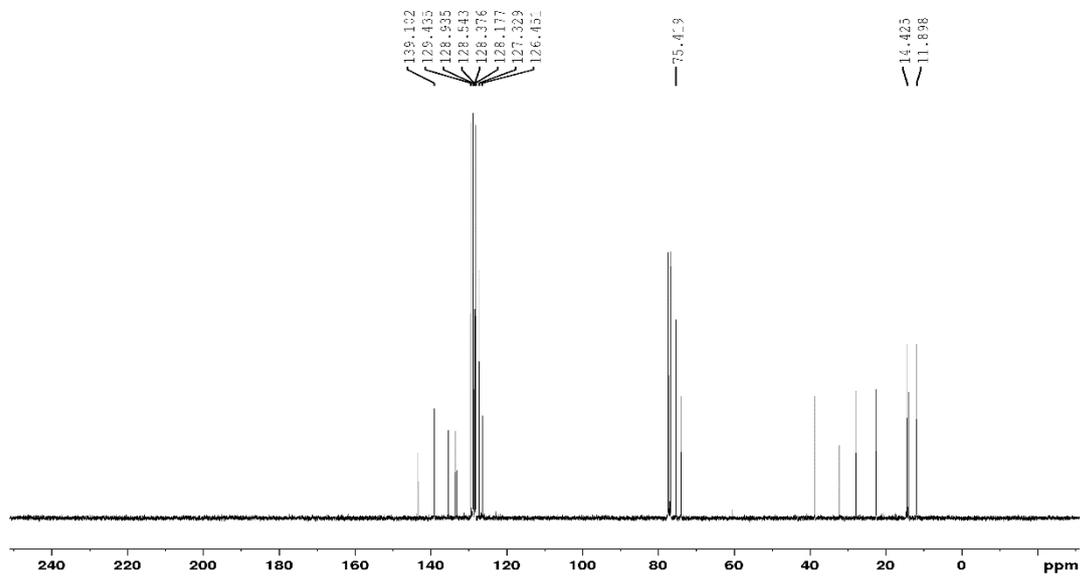


Abbildung A 46: <sup>13</sup>C-NMR-Spektrum von 1-(4-Chlorphenyl)-1-(1-(phenylthio)cyclopropyl)methanol **35e**.

1-(4-Bromophenyl)-1-(1-(phenylthio)cyclopropyl)methanol:

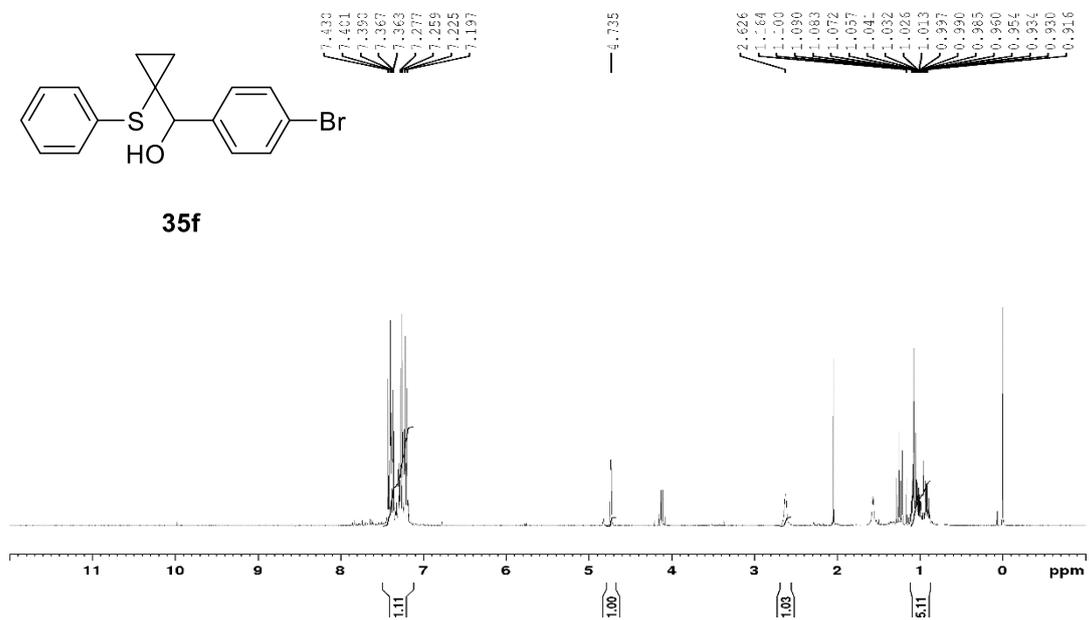


Abbildung A 47: <sup>1</sup>H-NMR-Spektrum von 1-(4-Bromphenyl)-1-(1-(phenylthio)cyclopropyl)methanol **35f**.

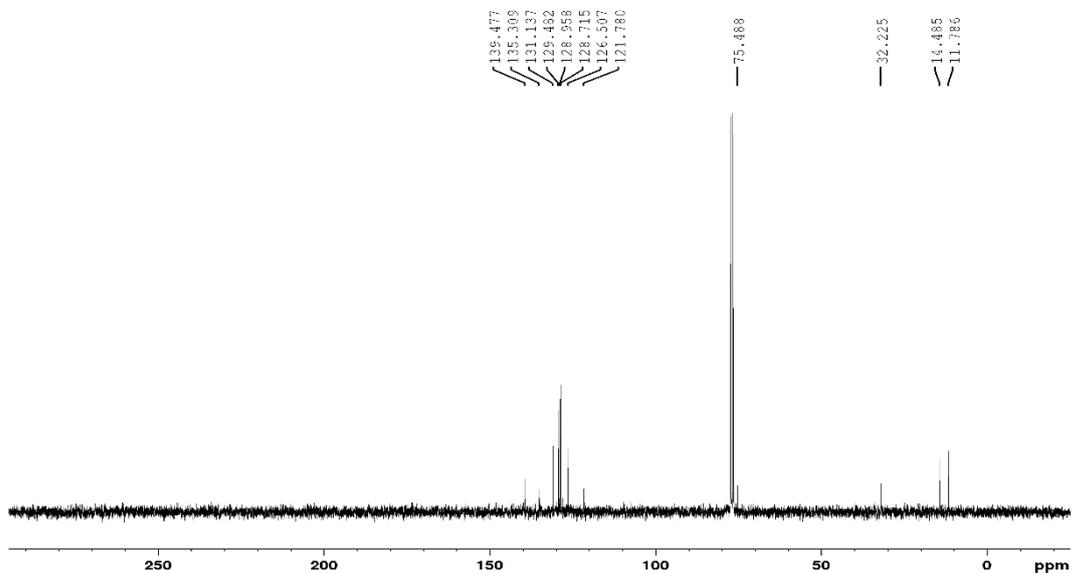


Abbildung A 48: <sup>13</sup>C-NMR-Spektrum von 1-(4-Bromphenyl)-1-(1-(phenylthio)cyclopropyl)methanol **35f**.

1-(2-Methoxyphenyl)-1-(1-(phenylthio)cyclopropyl)methanol:

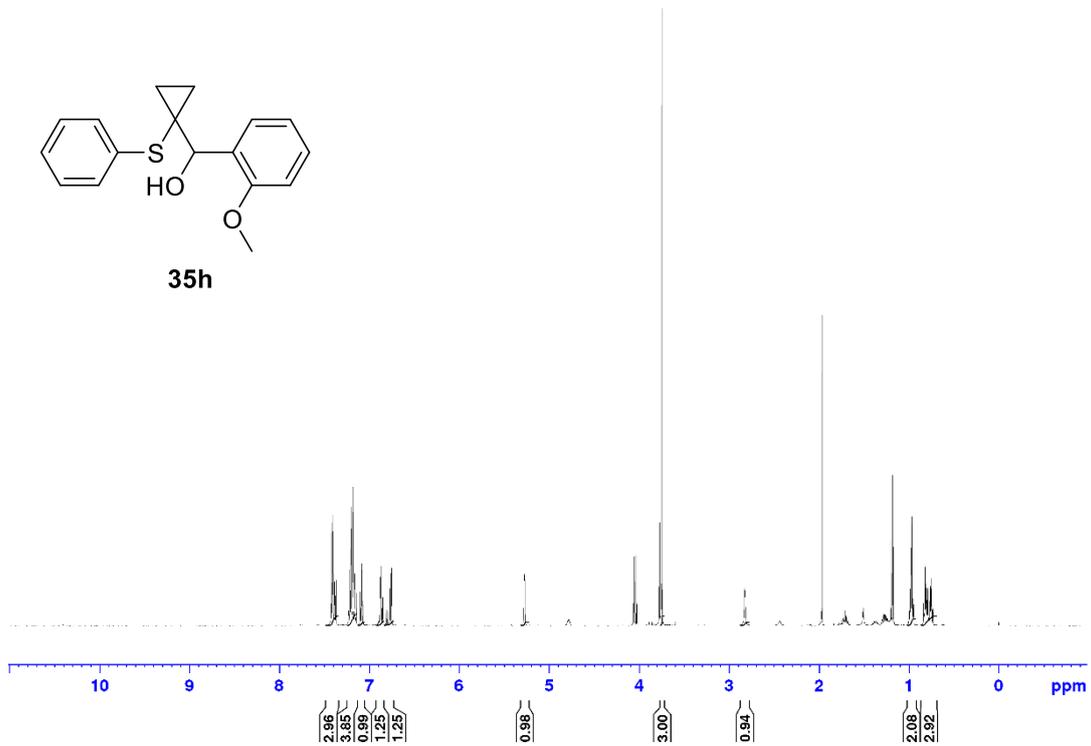


Abbildung A 49: <sup>1</sup>H-NMR-Spektrum von 1-(2-Methoxyphenyl)-1-(1-(phenylthio)cyclopropyl)methanol **35h**.

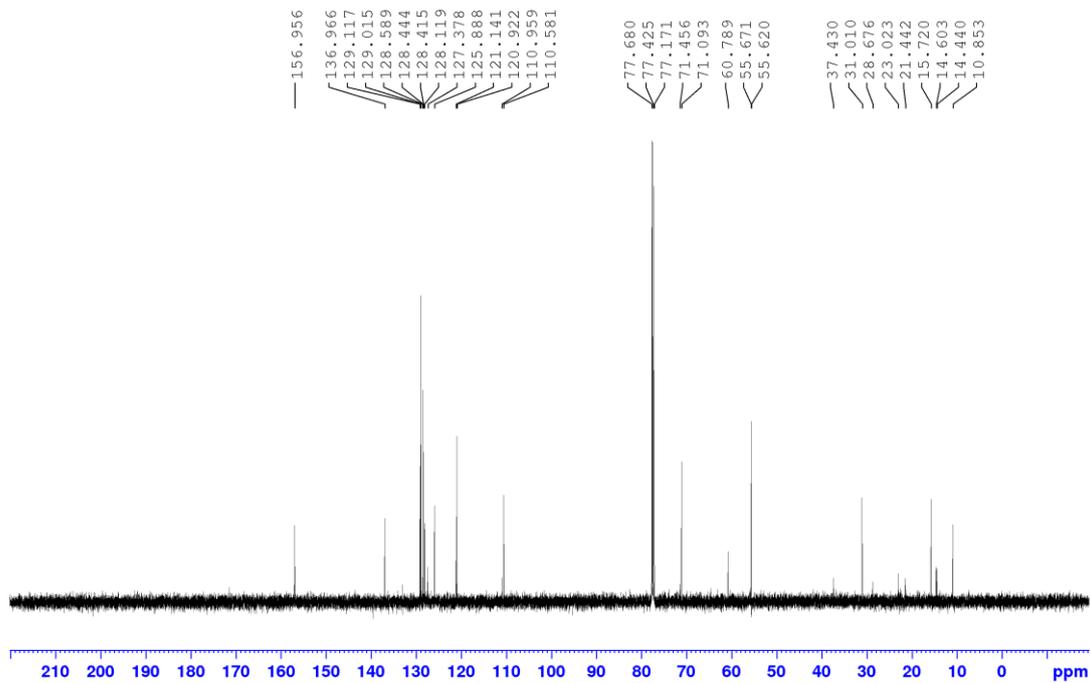


Abbildung A 50: <sup>13</sup>C-NMR-Spektrum von 1-(2-Methoxyphenyl)-1-(1-(phenylthio)cyclopropyl)methanol **35h**.

1-(4-Methoxyphenyl)-1-(1-(phenylthio)cyclopropyl)ethanol:

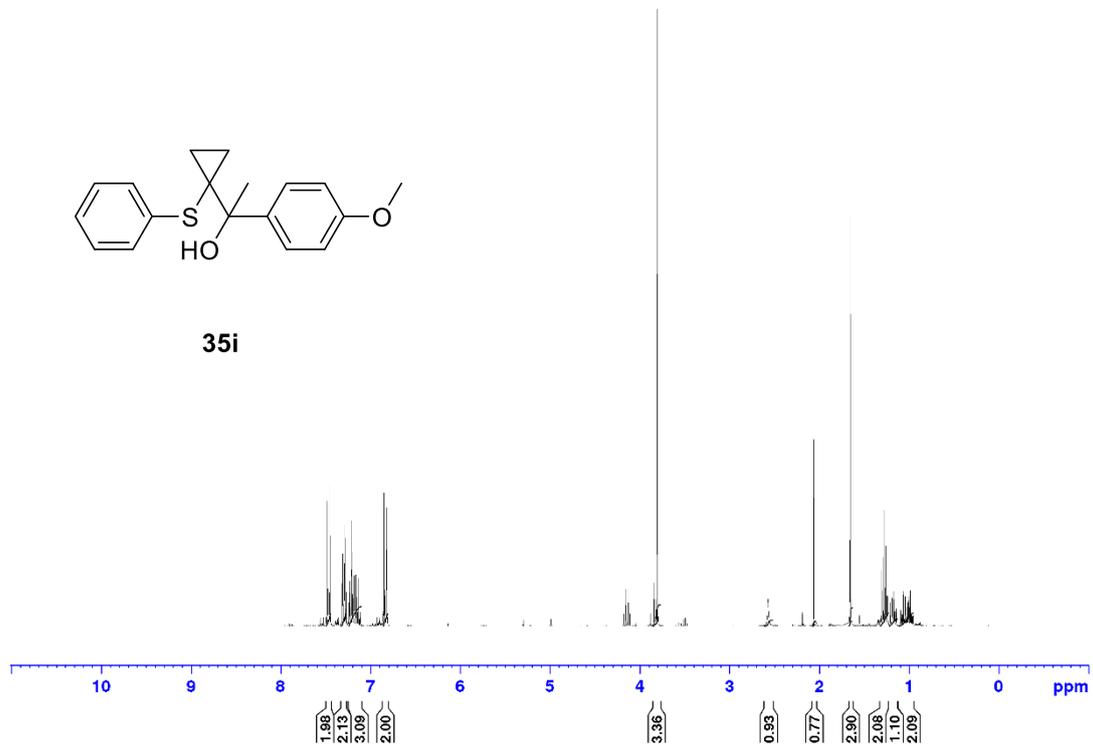


Abbildung A 51: <sup>1</sup>H-NMR-Spektrum von 1-(4-Methoxyphenyl)-1-(1-(phenylthio)cyclopropyl)ethanol **35i**.

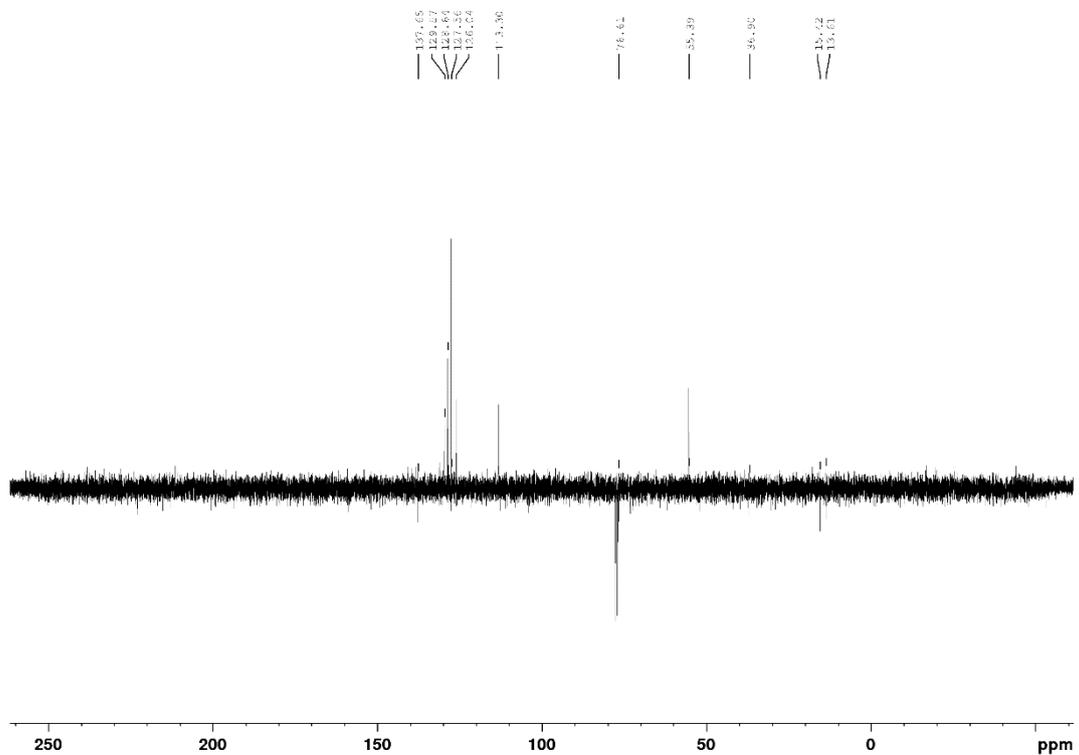


Abbildung A 52: <sup>13</sup>C-NMR-Spektrum von 1-(4-Methoxyphenyl)-1-(1-(phenylthio)cyclopropyl)ethanol **35i**.

2,3,4-Trimethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on:

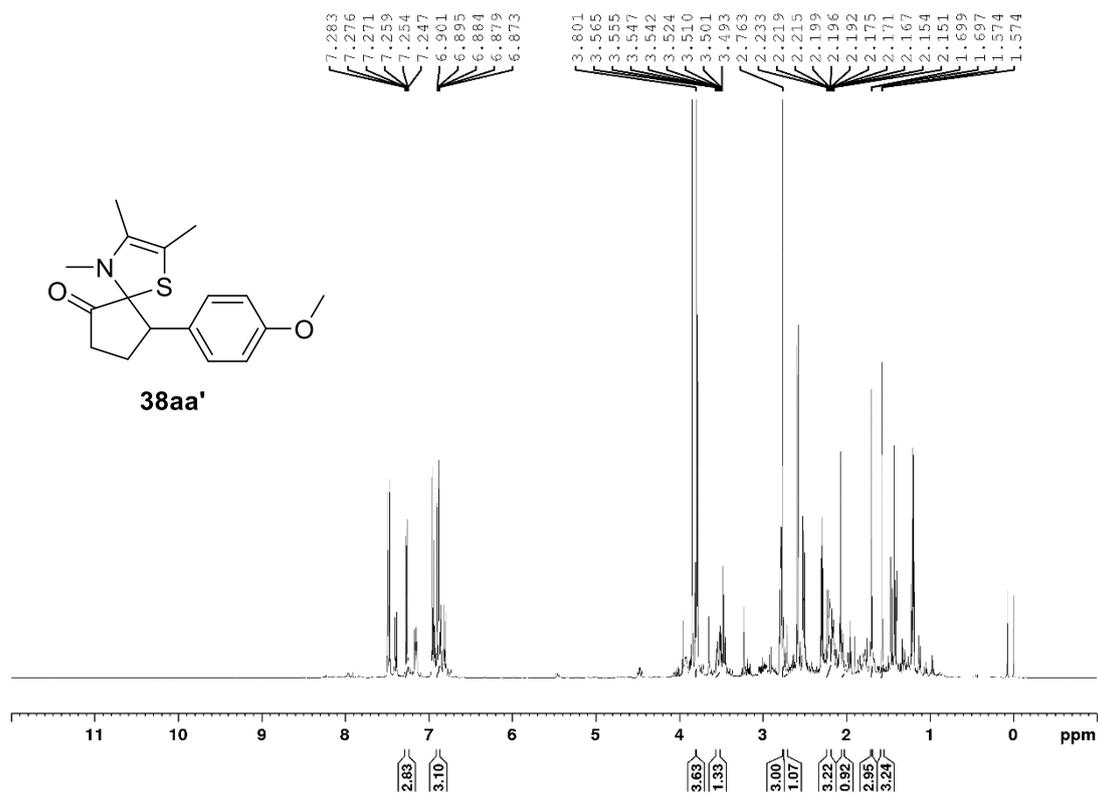


Abbildung A 53: <sup>1</sup>H-NMR-Spektrum von 2,3,4-Trimethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on **38aa'**.

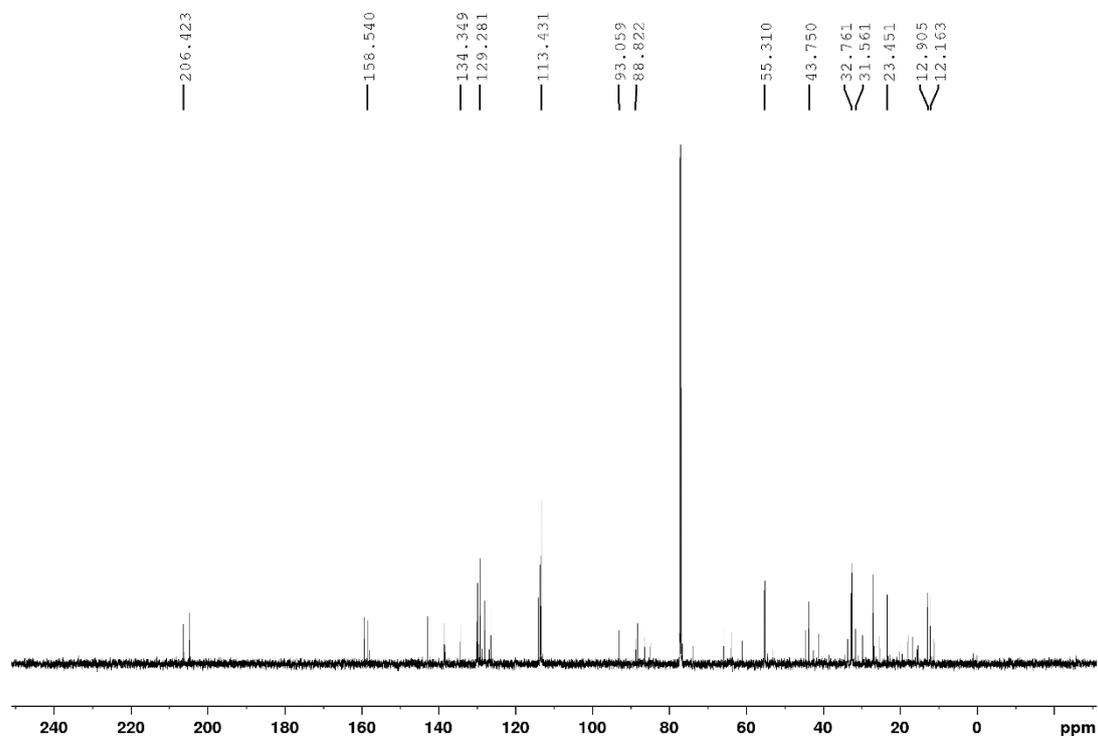


Abbildung A 54: <sup>13</sup>C-NMR-Spektrum von 2,3,4-Trimethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on **38aa'**.

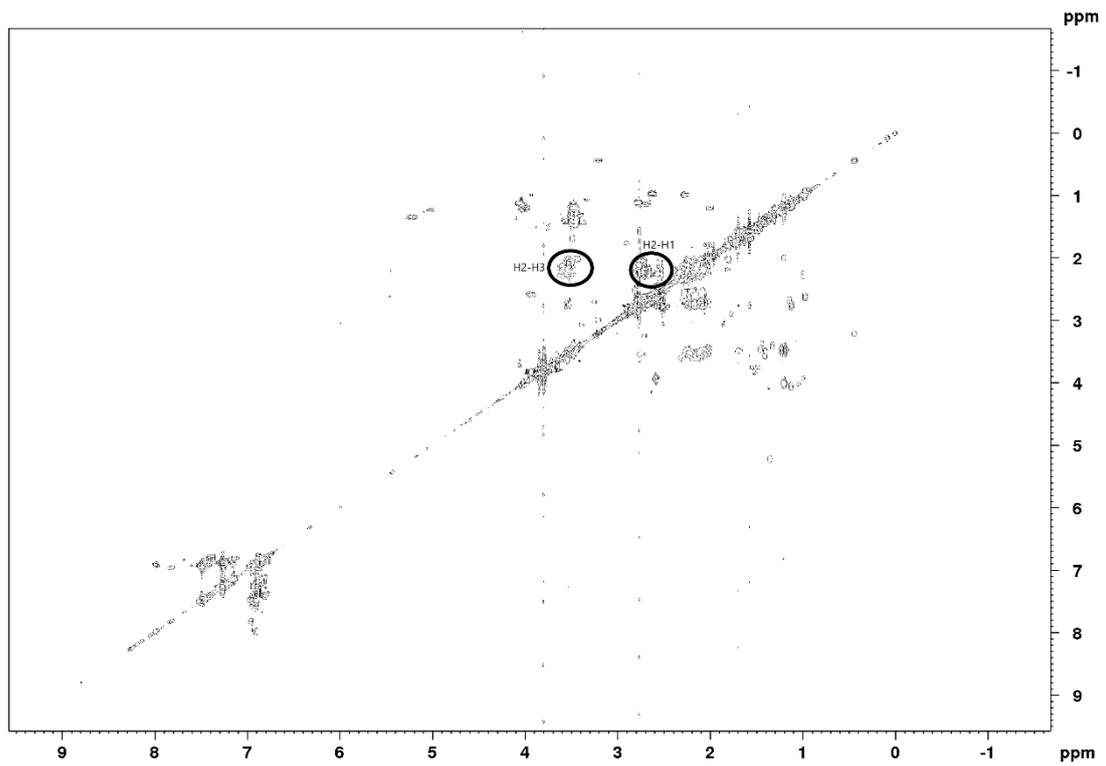


Abbildung A 55: H,H-Cosy-NMR-Spektrum von 2,3,4-Trimethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on **38aa'**.

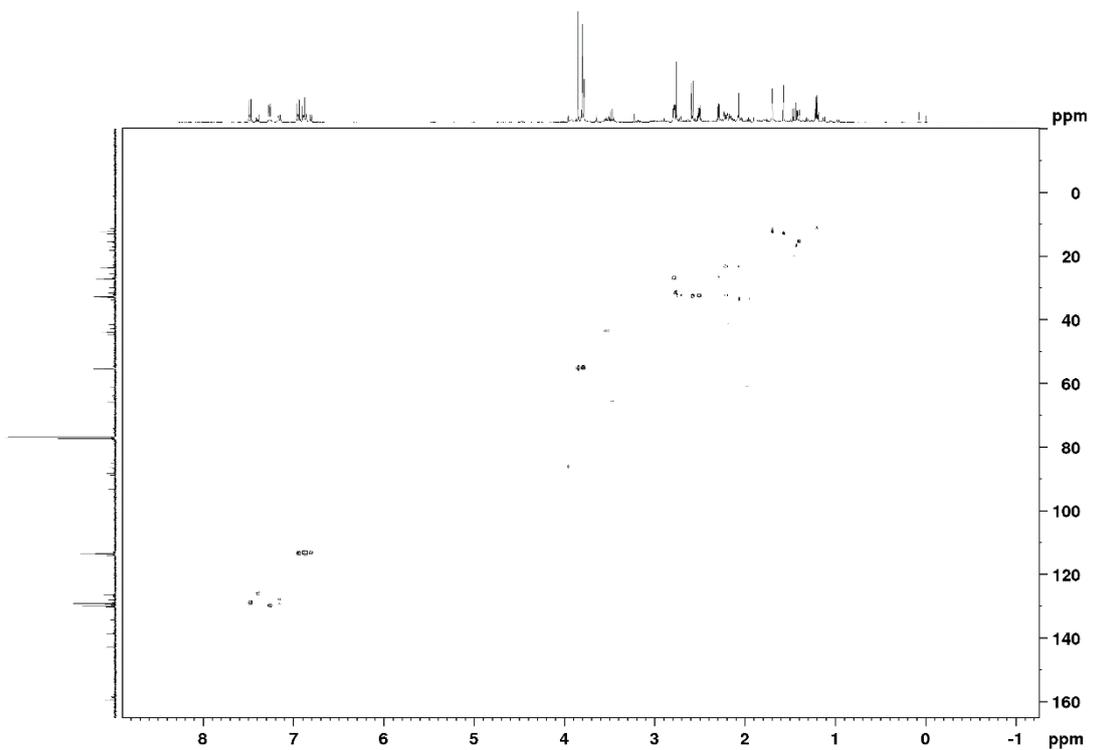


Abbildung A 56: HSQC-NMR-Spektrum von 2,3,4-Trimethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on **38aa'**.

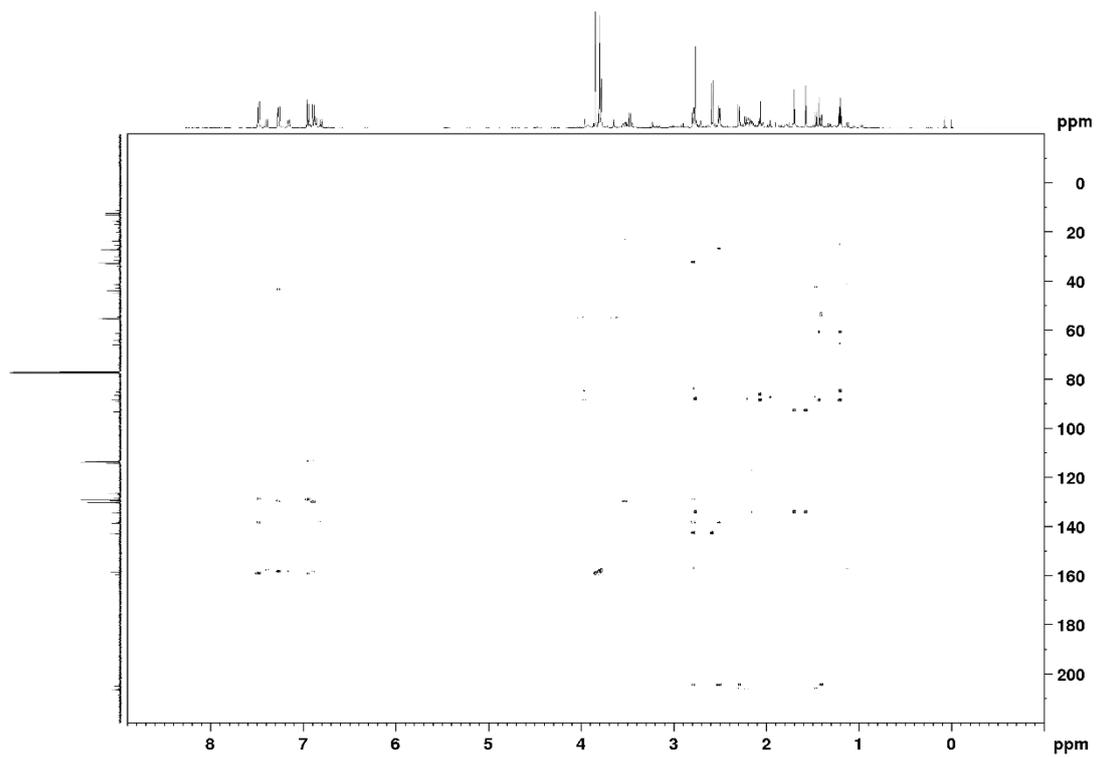


Abbildung A 57: HMBC-NMR-Spektrum von 2,3,4-Trimethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on **38aa'**.

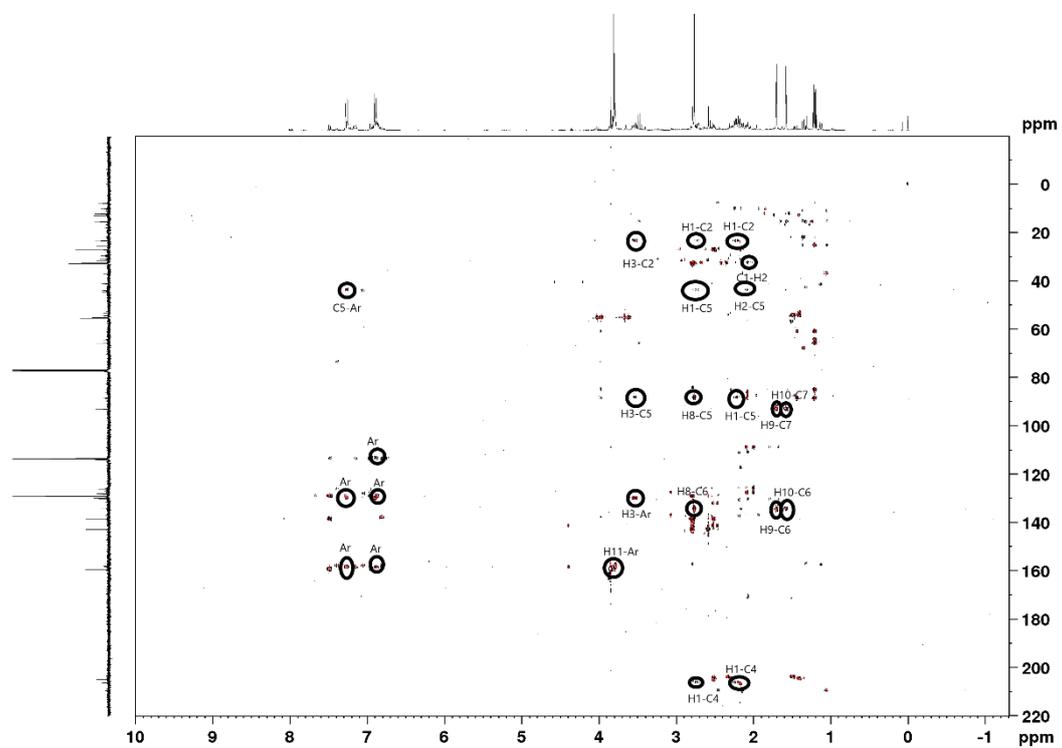


Abbildung A 58:  $^1\text{H}$ HMBC-NMR-Spektrum von 2,3,4-Trimethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on **38aa'** mit Signalzuordnung.

2,3-Dimethyl-4-hydroxyethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on:

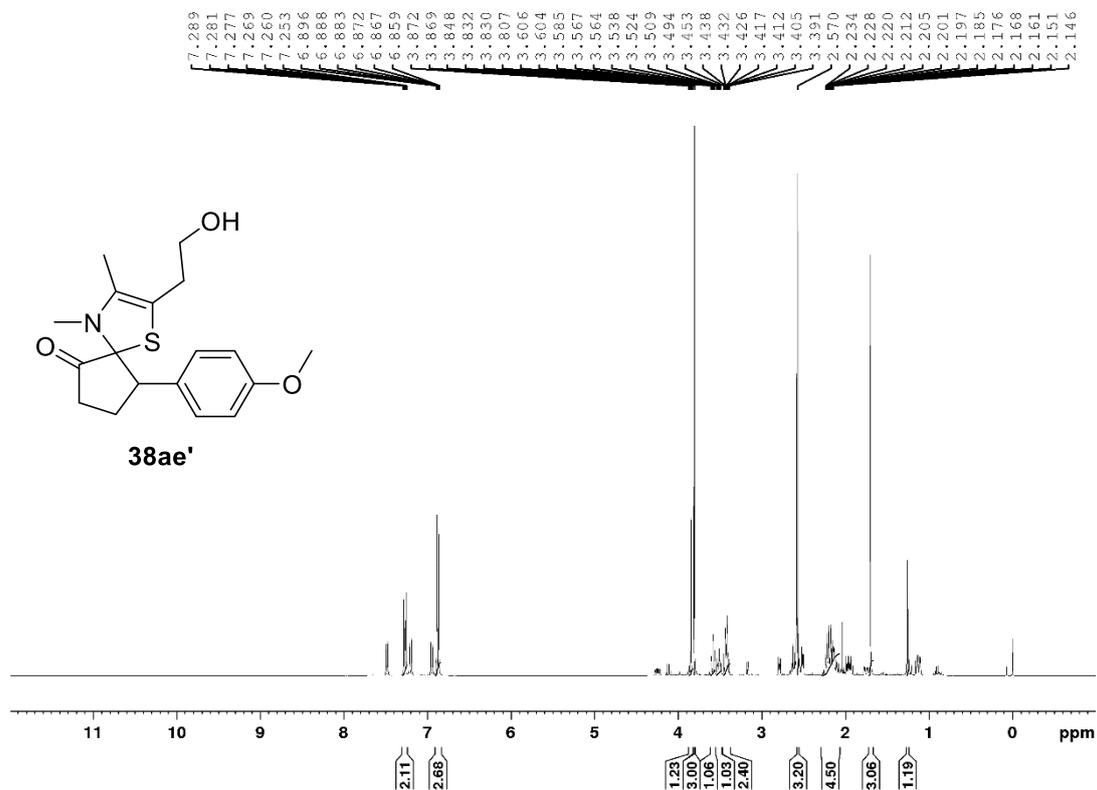


Abbildung A 59: <sup>1</sup>H-NMR-Spektrum von 2,3-Dimethyl-4-hydroxyethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on **38ae'**.

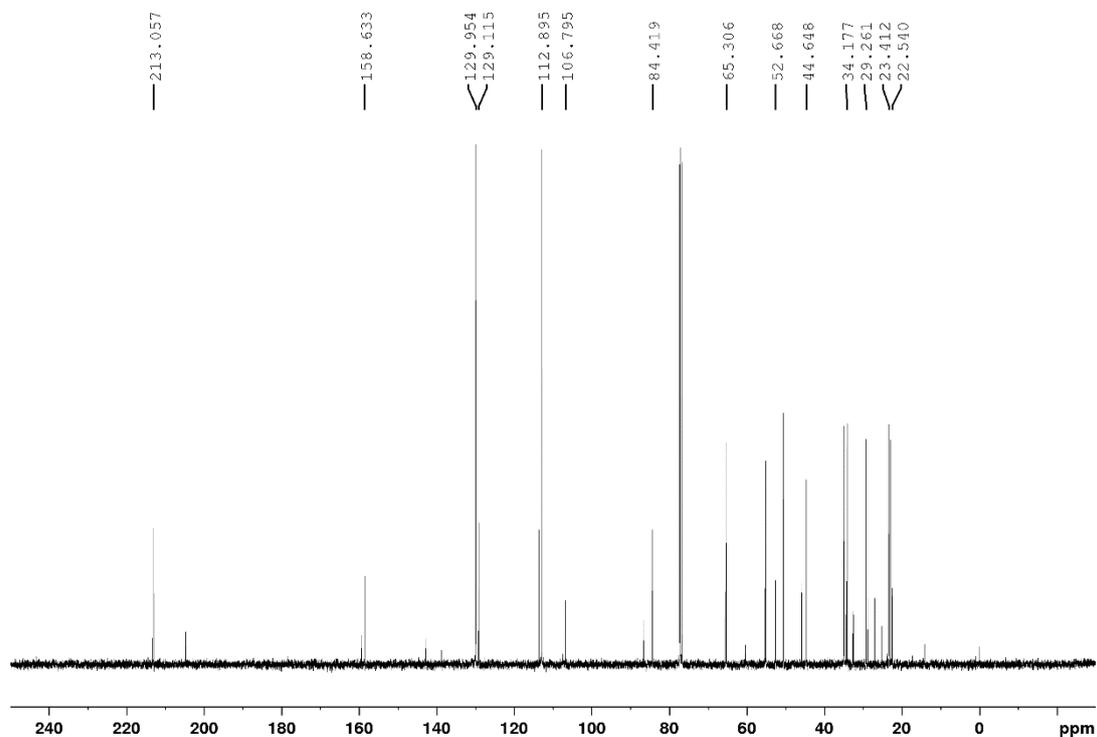


Abbildung A 60: <sup>13</sup>C-NMR-Spektrum von 2,3-Dimethyl-4-hydroxyethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on **38ae'**.

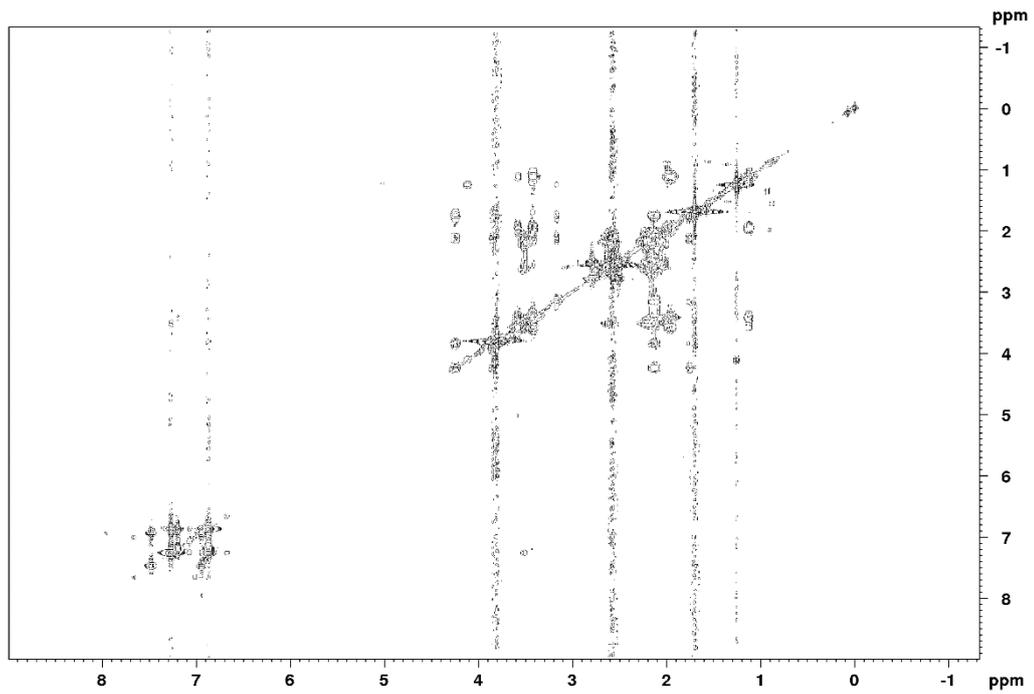


Abbildung A 61: H,H-COSY-NMR-Spektrum von 2,3-Dimethyl-4-hydroxyethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on **38ae'**.

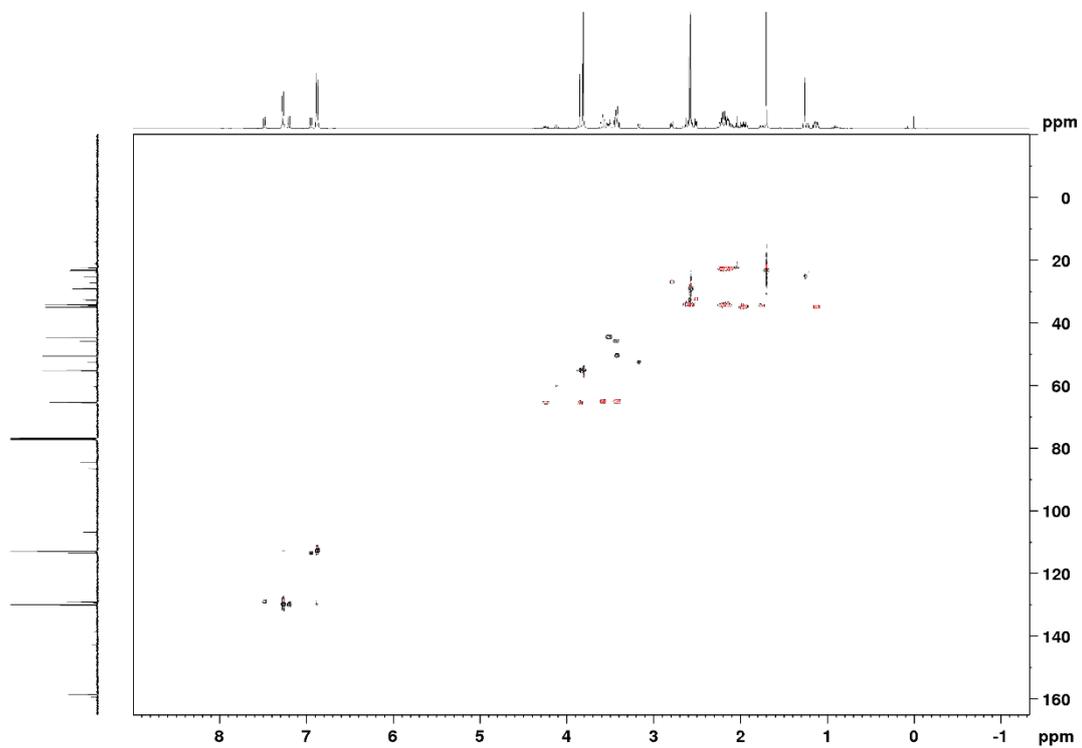


Abbildung A 62: HSQC-NMR-Spektrum von 2,3-Dimethyl-4-hydroxyethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on **38ae'**.

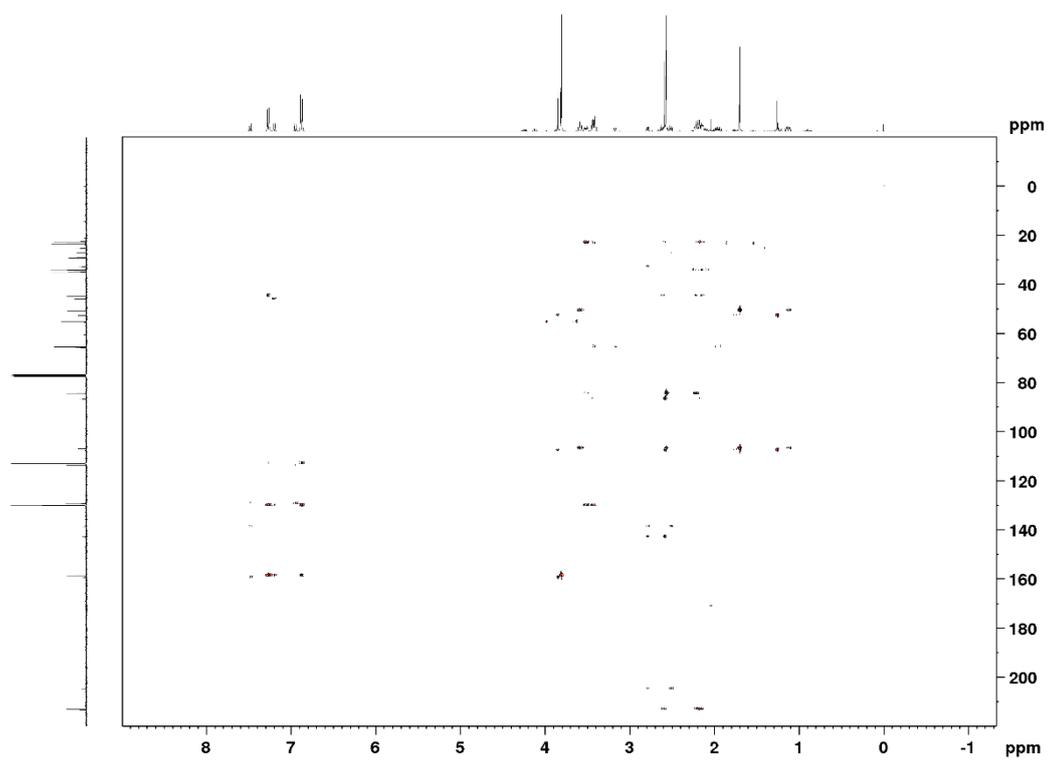


Abbildung A 63: HMBC-NMR-Spektrum von 2,3-Dimethyl-4-hydroxyethyl-9-(4-methoxyphenyl)-1-thia-4-azaspiro[4.4]non-2-en-6-on **38ae**.

1-(4-Methoxyphenyl)-1-cyclobutylmethen:

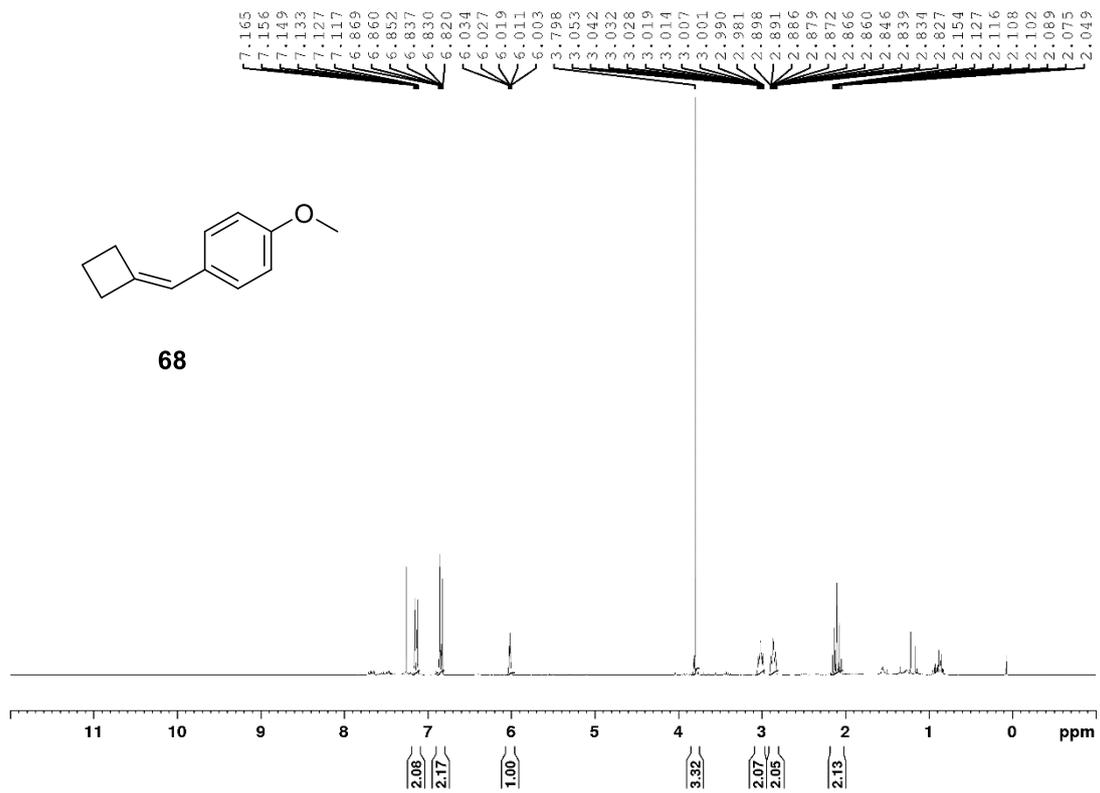


Abbildung A 64: <sup>1</sup>H-NMR-Spektrum 1-(4-Methoxyphenyl)-1-cyclobutylmethen **68**.

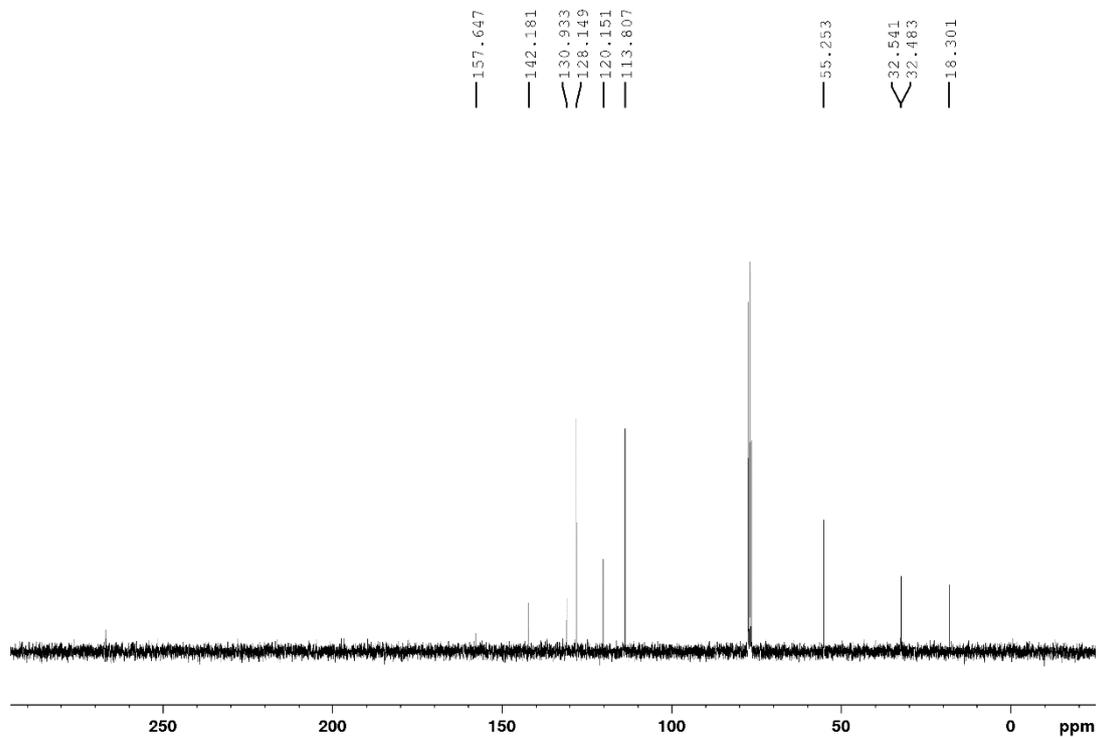


Abbildung A 65: <sup>13</sup>C-NMR-Spektrum 1-(4-Methoxyphenyl)-1-cyclobutylmethen **68**.

2-(4-Methoxyphenyl)cyclopentanon:

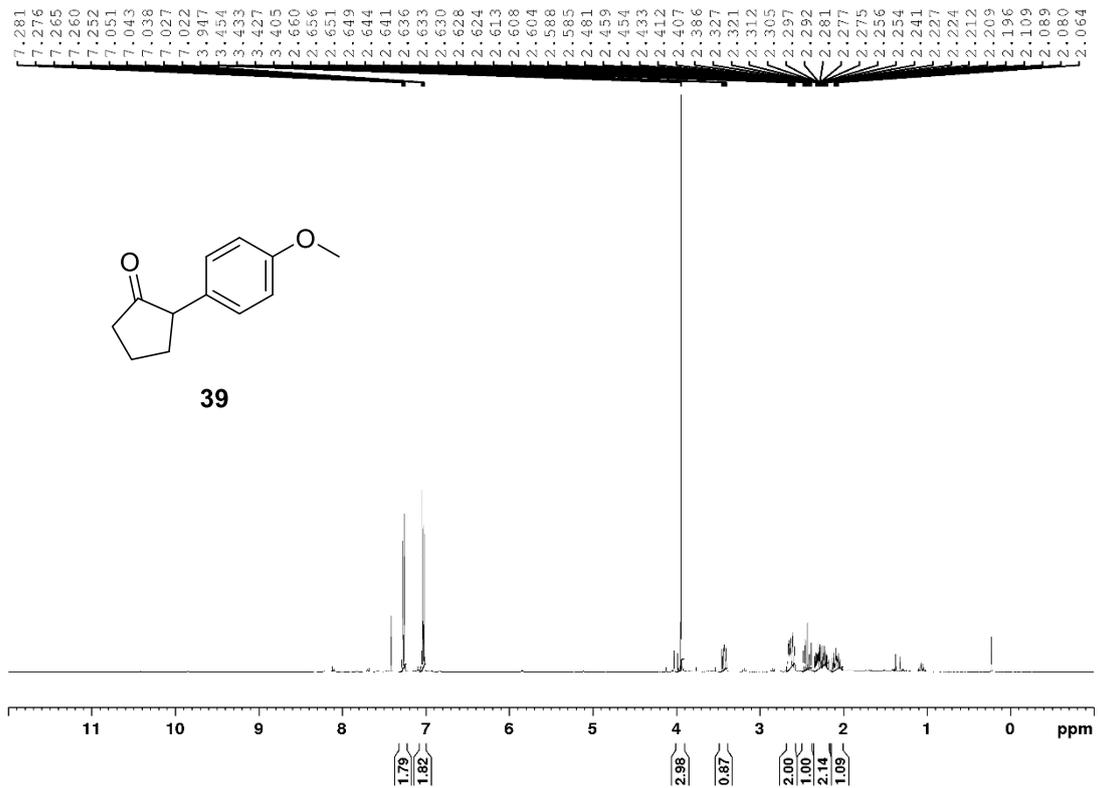


Abbildung A 66: <sup>1</sup>H-NMR-Spektrum 2-(4-Methoxyphenyl)cyclopentanon **39**.

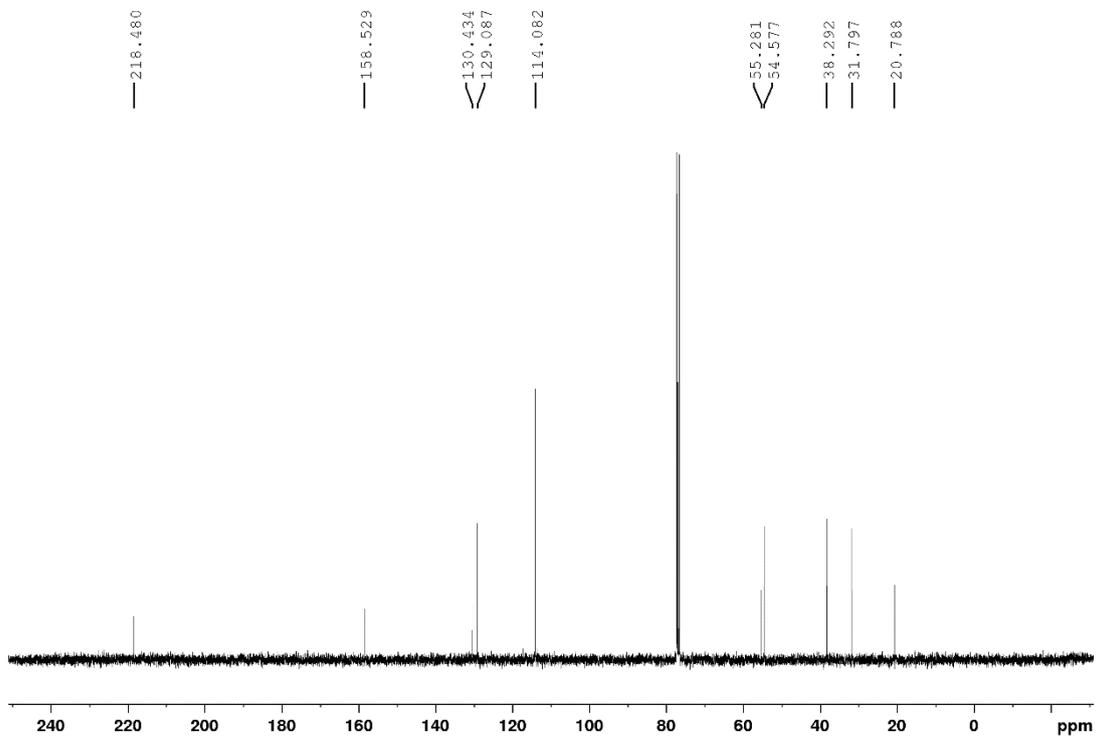


Abbildung A 67: <sup>13</sup>C-NMR-Spektrum 2-(4-Methoxyphenyl)cyclopentanon **39**.

### 3,4,5-Trimethylthiazoliumiodid

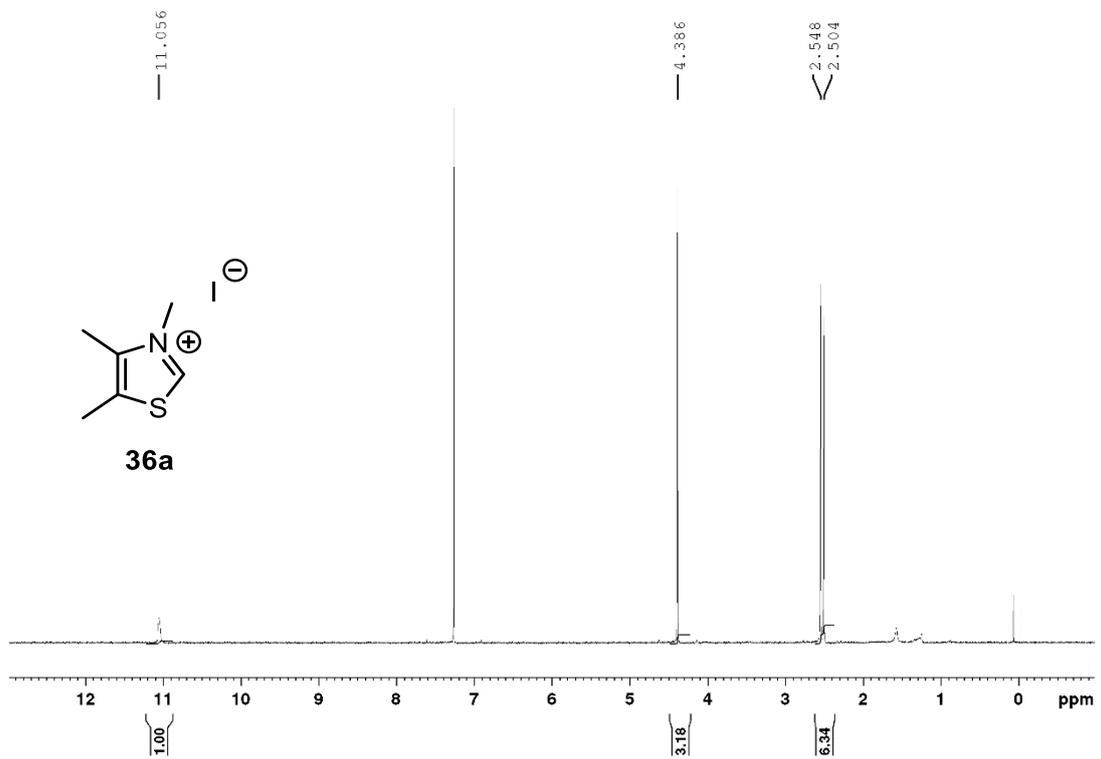


Abbildung A 68:  $^1\text{H}$ -NMR-Spektrum 3,4,5-Trimethylthiazoliumiodid **36a**.

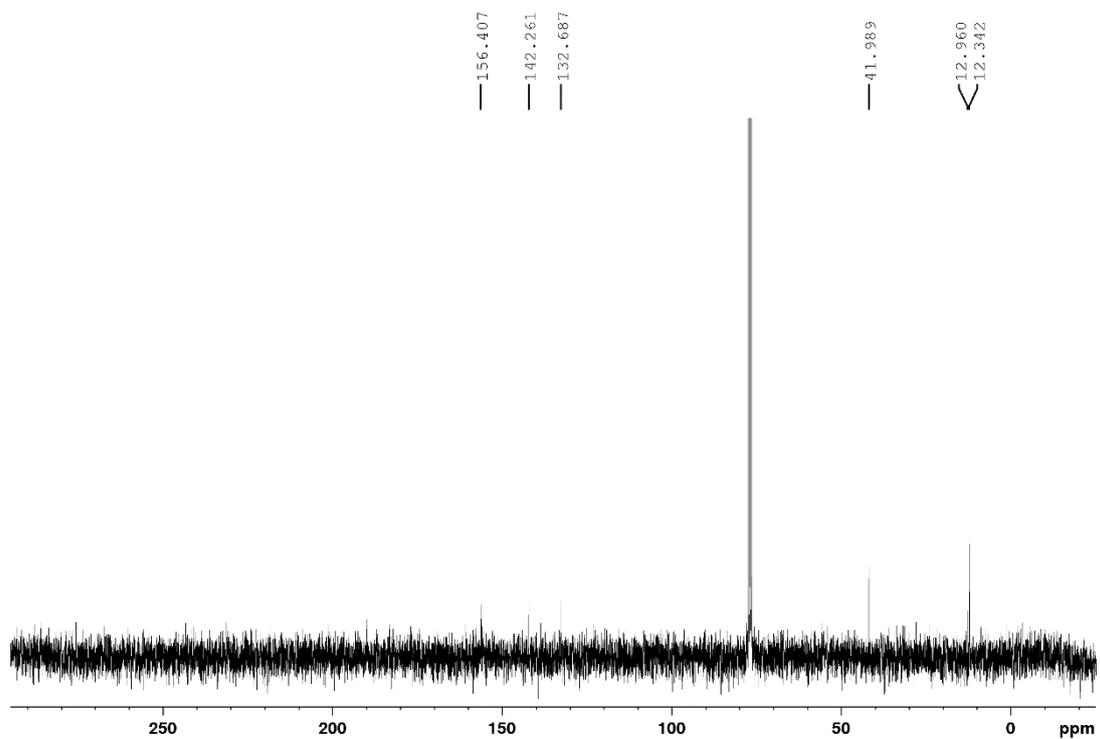


Abbildung A 69:  $^{13}\text{C}$ -NMR-Spektrum 3,4,5-Trimethylthiazoliumiodid **36a**.

### 3-Deuteromethyl-4,5-dimethylthiazoliumiodid

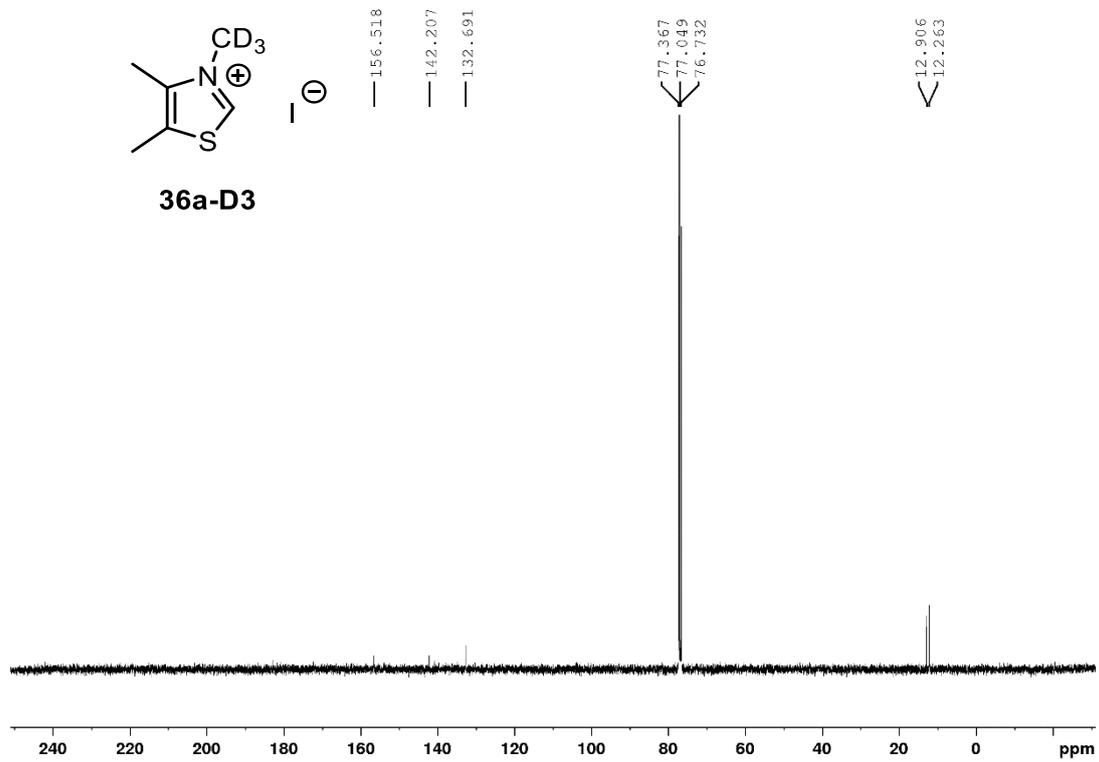


Abbildung A 70: <sup>1</sup>H-NMR-Spektrum 3-Deuteomethyl-4,5-dimethylthiazoliumiodid **36a-D3**.

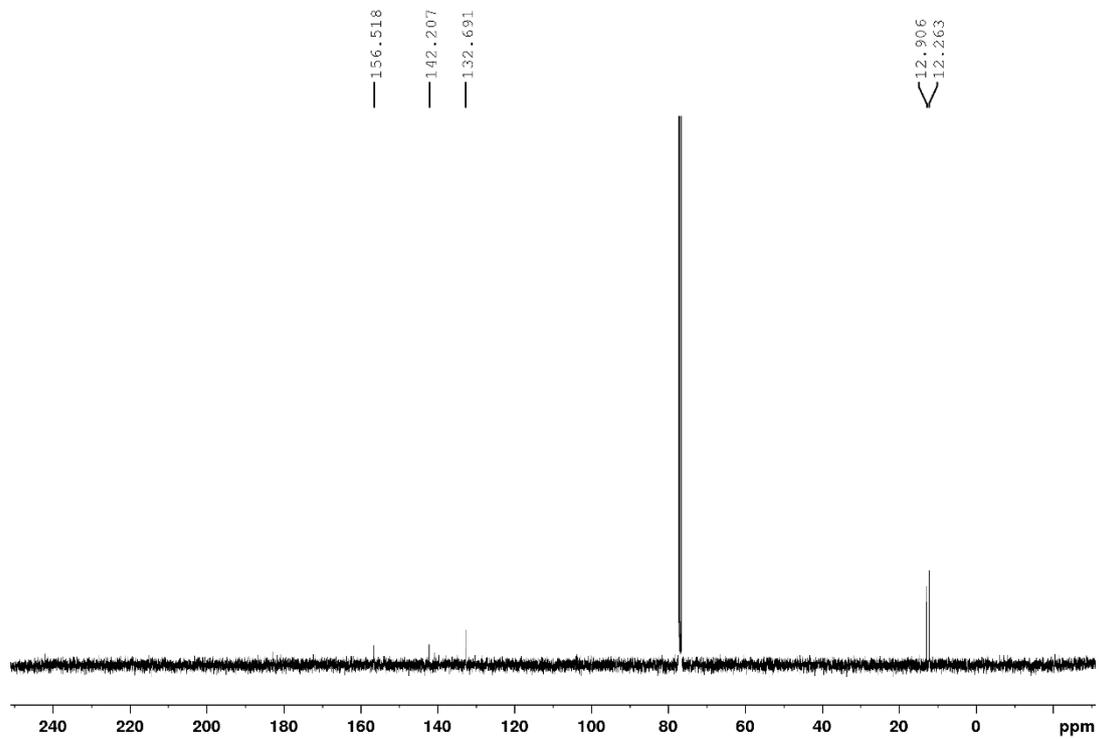


Abbildung A 71: <sup>13</sup>C-NMR-Spektrum 3-Deuteromethyl-4,5-dimethylthiazoliumiodid **36a-D3**.

### 3-Benzyl-4,5-dimethylthiazoliumbromid

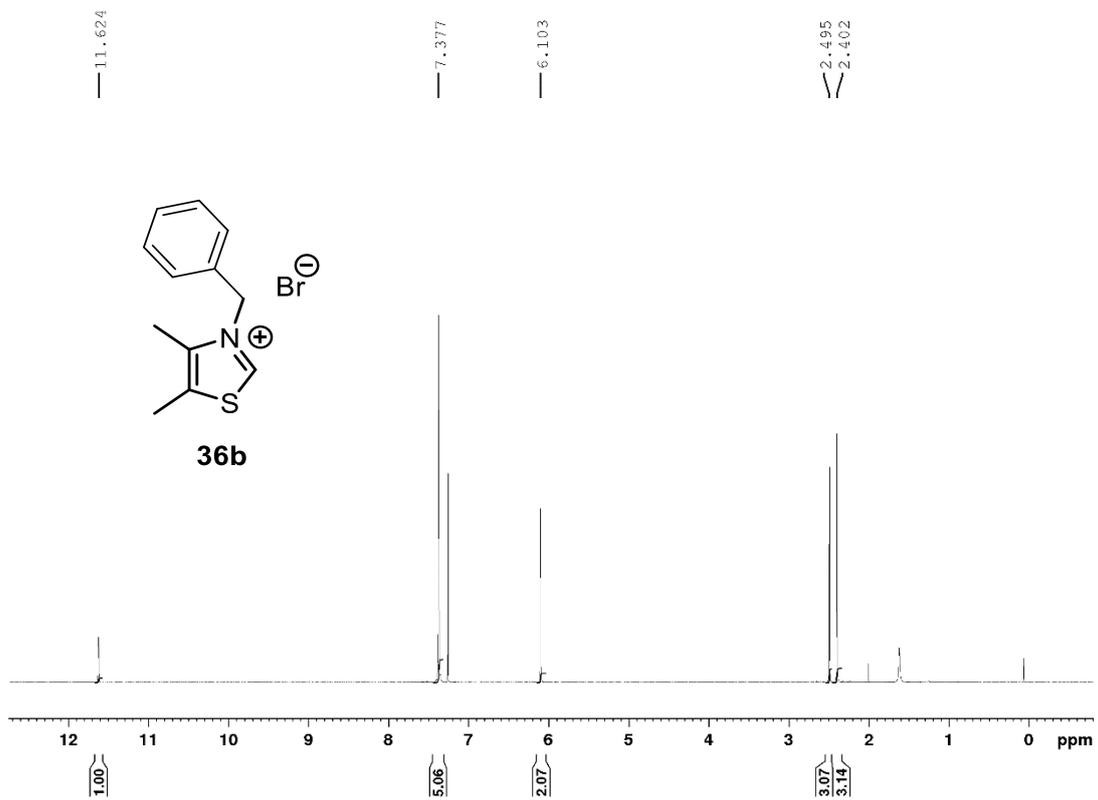


Abbildung A 72: <sup>1</sup>H-NMR-Spektrum 3-Benzyl-4,5-dimethylthiazoliumbromid **36b**.

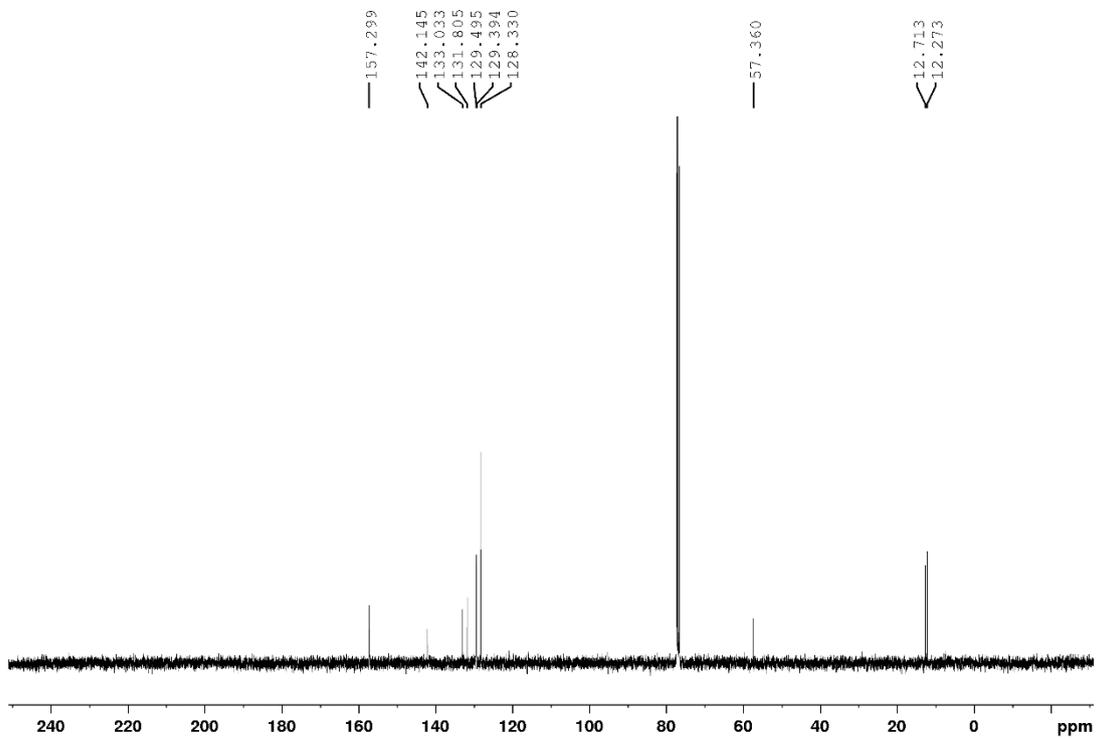


Abbildung A 73: <sup>13</sup>C-NMR-Spektrum 3-Benzyl-4,5-dimethylthiazoliumbromid **36b**.

### 3-Methylbenzothiazoliumiodid:

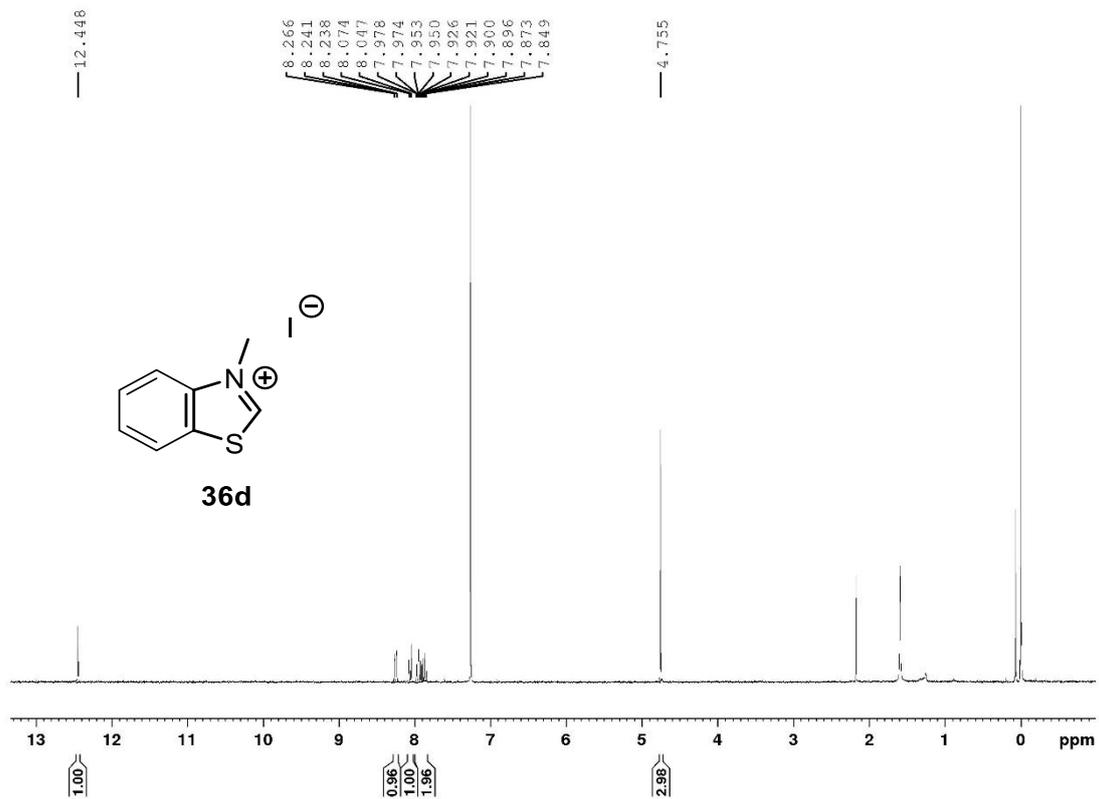


Abbildung A 74:  $^1\text{H}$ -NMR-Spektrum 3-Methylbenzothiazoliumiodid **36d**.

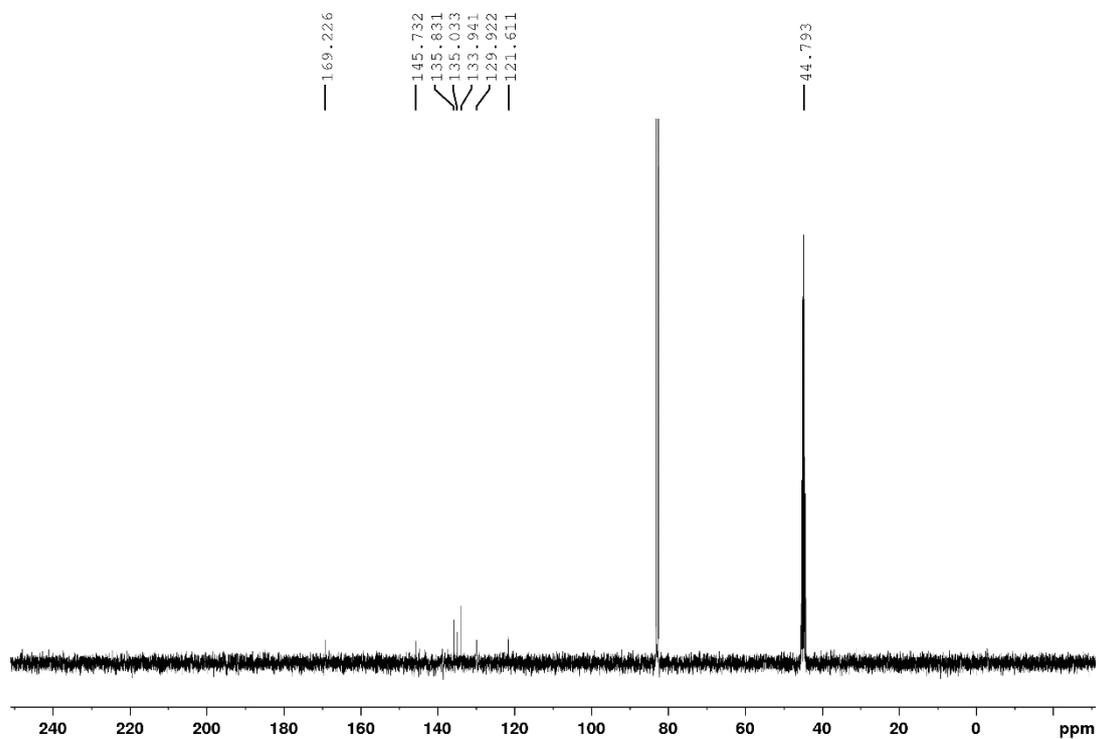


Abbildung A 75:  $^{13}\text{C}$ -NMR-Spektrum 3-Methylbenzothiazoliumiodid **36d**.

### 3,4-Dimethyl-5-hydroxyethylthiazoliumiodid:

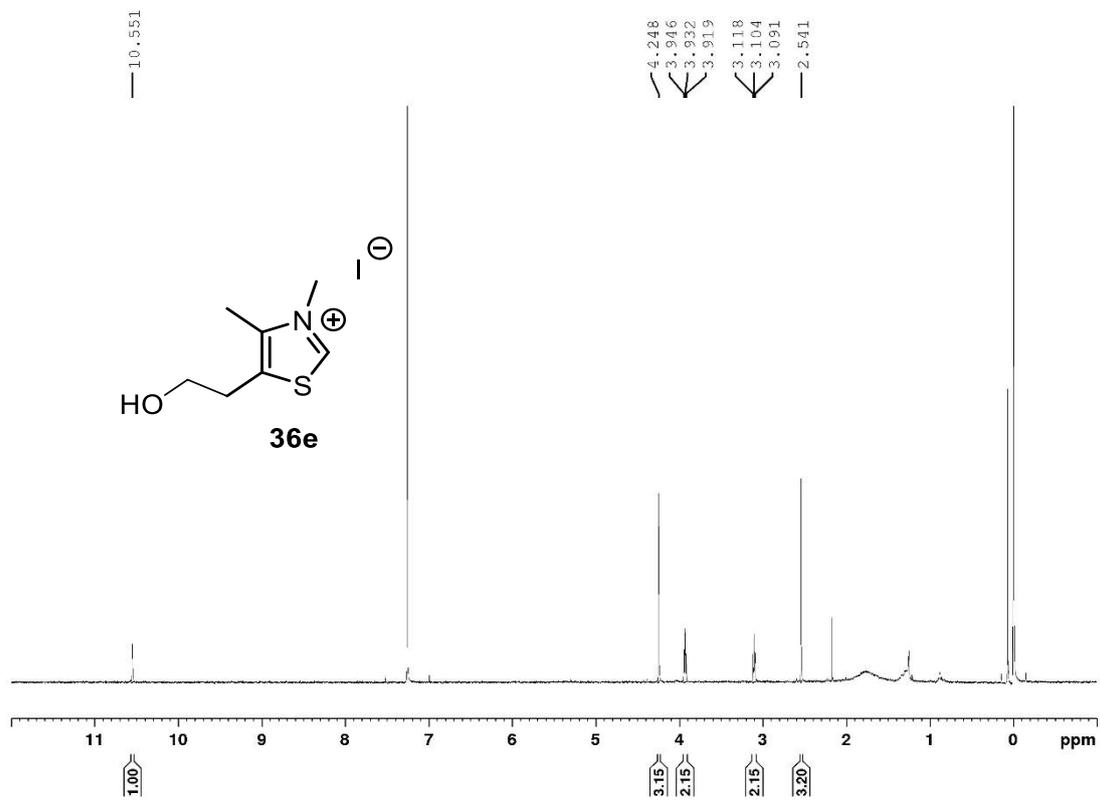


Abbildung A 76: <sup>1</sup>H-NMR-Spektrum 3,4-Dimethyl-5-hydroxyethylthiazoliumiodid **36e**.

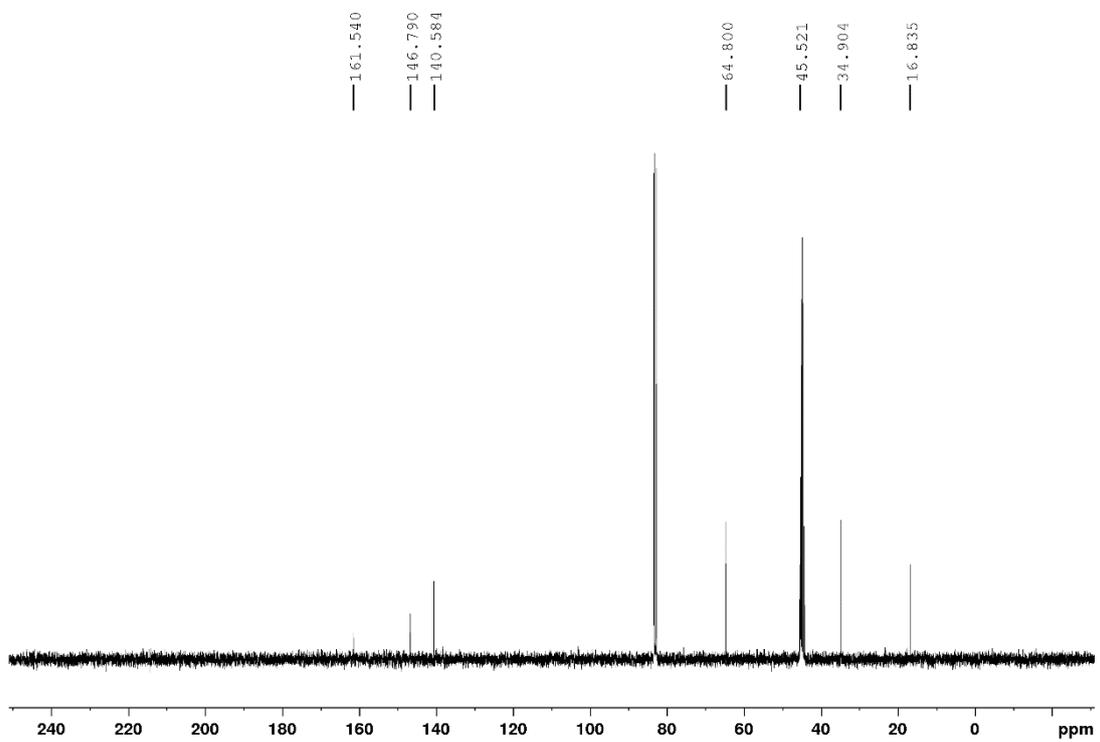


Abbildung A 77: <sup>13</sup>C-NMR-Spektrum 3,4-Dimethyl-5-hydroxyethylthiazoliumiodid **36e**

## NMR-Kinetiken:

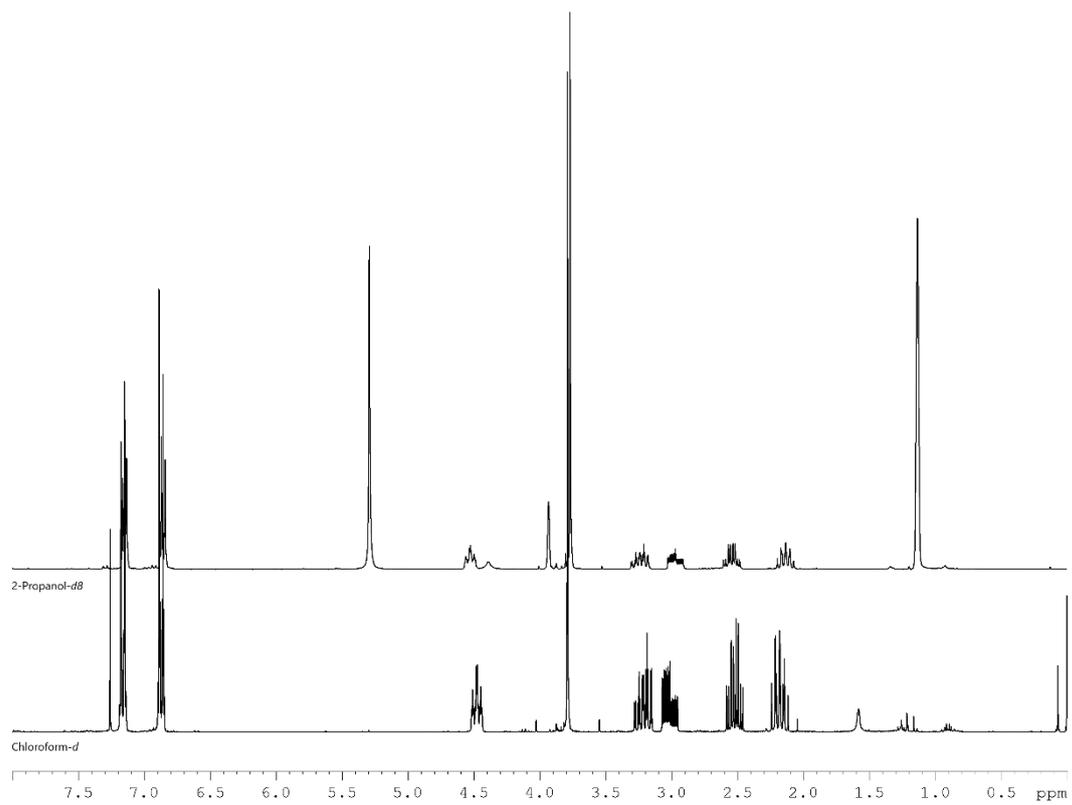
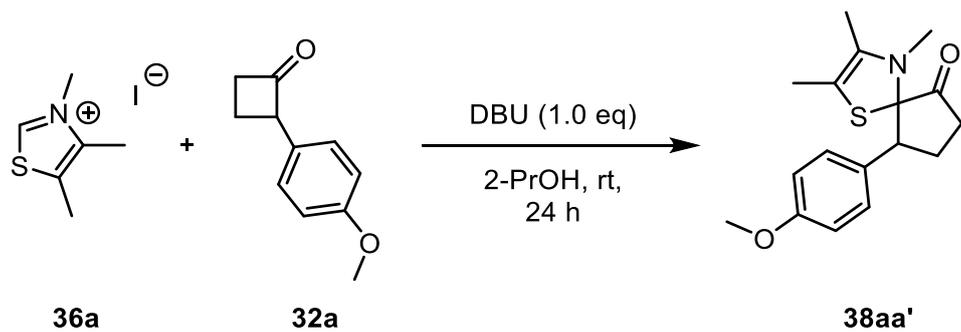


Abbildung A 78: Vergleich der <sup>1</sup>H-NMR-Spektren von 2-(4-Methoxyphenyl)cyclobutanon **32a** in 2-Propanol-*d*<sub>8</sub> (oben) und Chloroform-*d* (unten).



Schema A 1: Reaktionsschema der mittels zeitaufgelöster NMR-Spektroskopie untersuchten Reaktion von Thiazoliumsalz **36a**, Cyclobutanon **32a** und DBU.

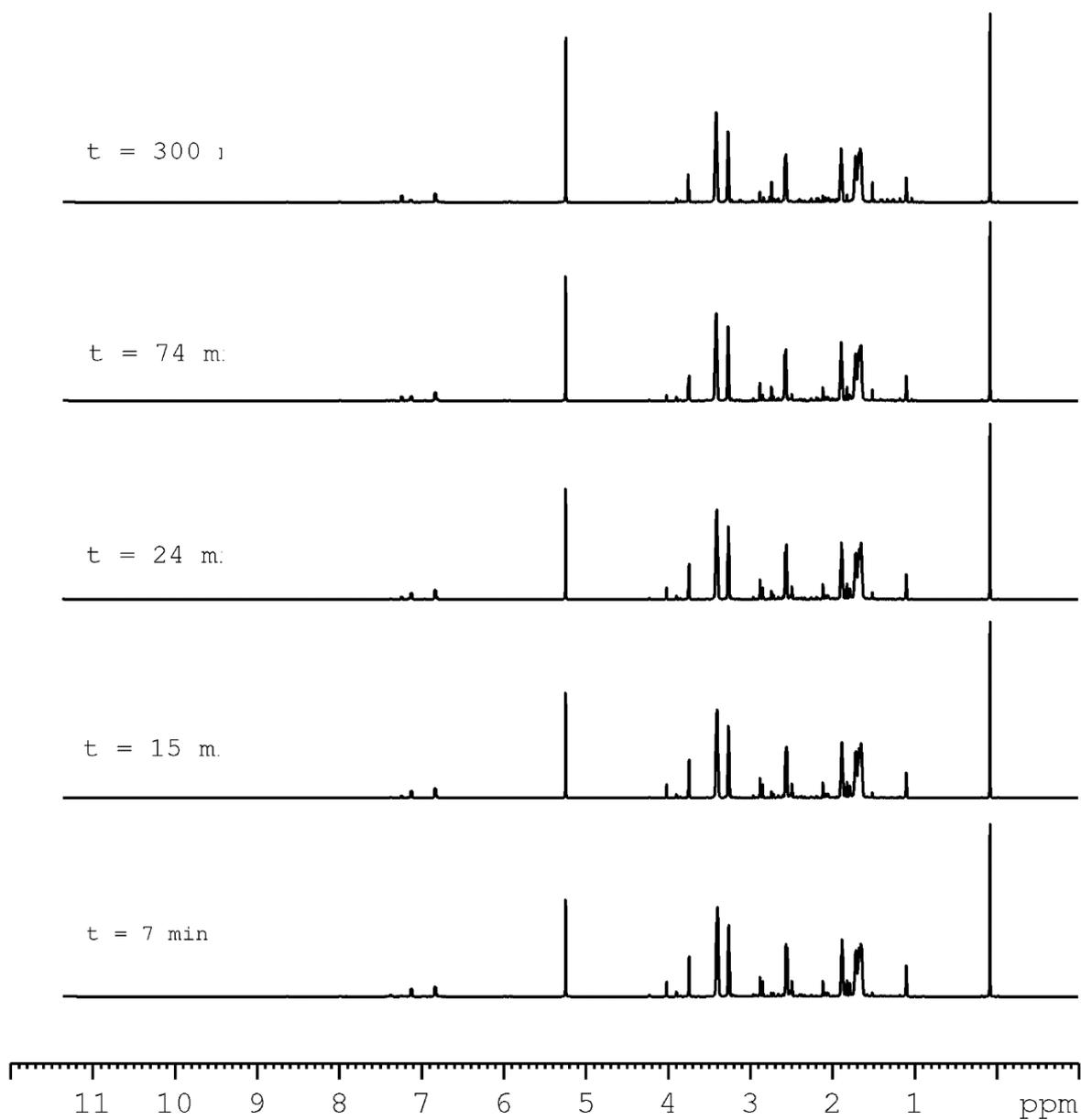


Abbildung A 79: Ausgewählte <sup>1</sup>H-NMR-Spektren des Kinetikexperiments 1 mit Cyclobutanon **32a** zu angegebenen Zeitpunkten.

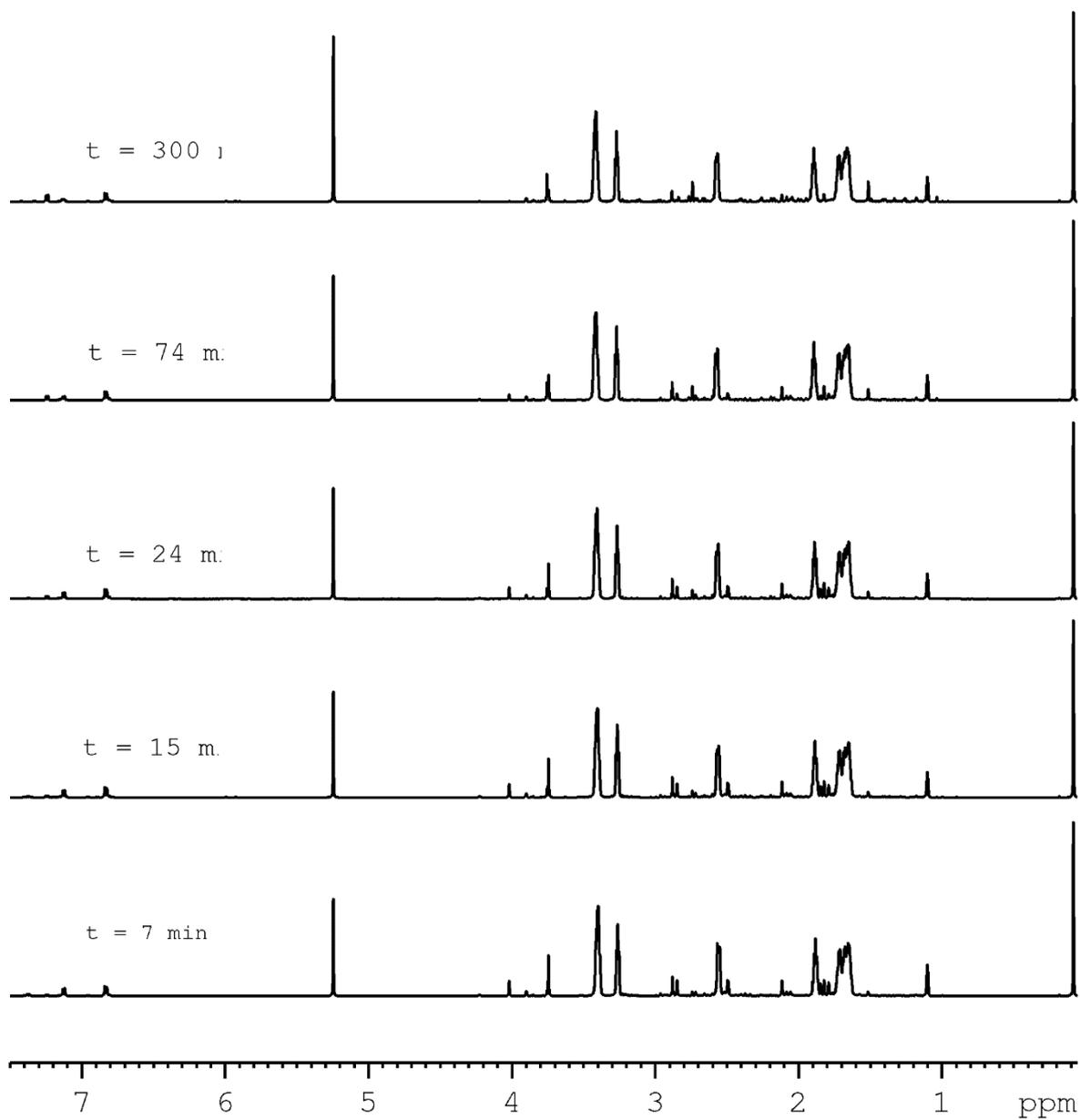


Abbildung A 80: Ausschnitt der ausgewählten  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 1 mit Cyclobutanon **32a** zu angegebenen Zeitpunkten.

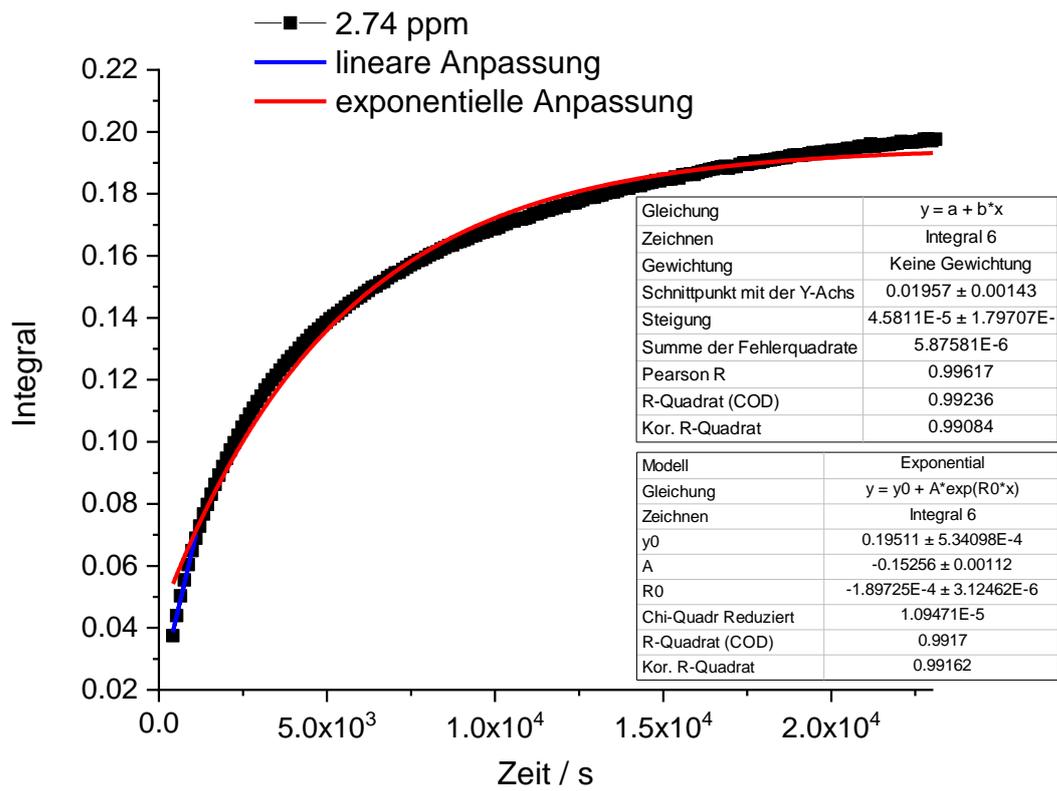
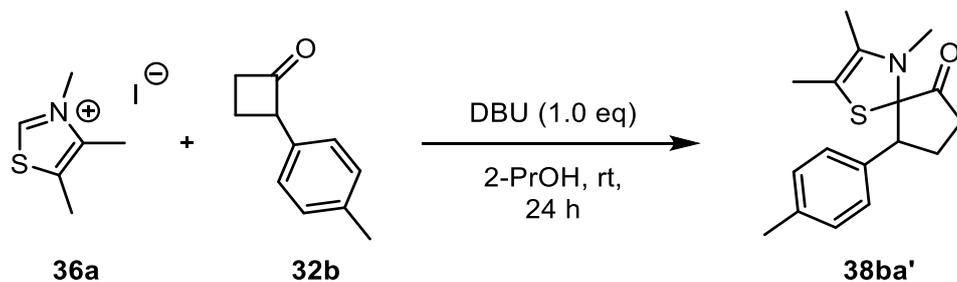


Abbildung A 81: Auftragung der zeitlichen Veränderung des Integrals des Singulett bei 2.74 ppm des Kinetikexperiments 1 mit Cyclobutanon **32a** mit linearer Anpassung des Anfangsbereichs (blaue Linie) und exponentieller Anpassung (rote Linie).



Schema A 2: Reaktionsschema der mittels zeitaufgelöster NMR-Spektroskopie untersuchten Reaktion von Thiazoliumsalz **36a**, Cyclobutanon **32b** und DBU.

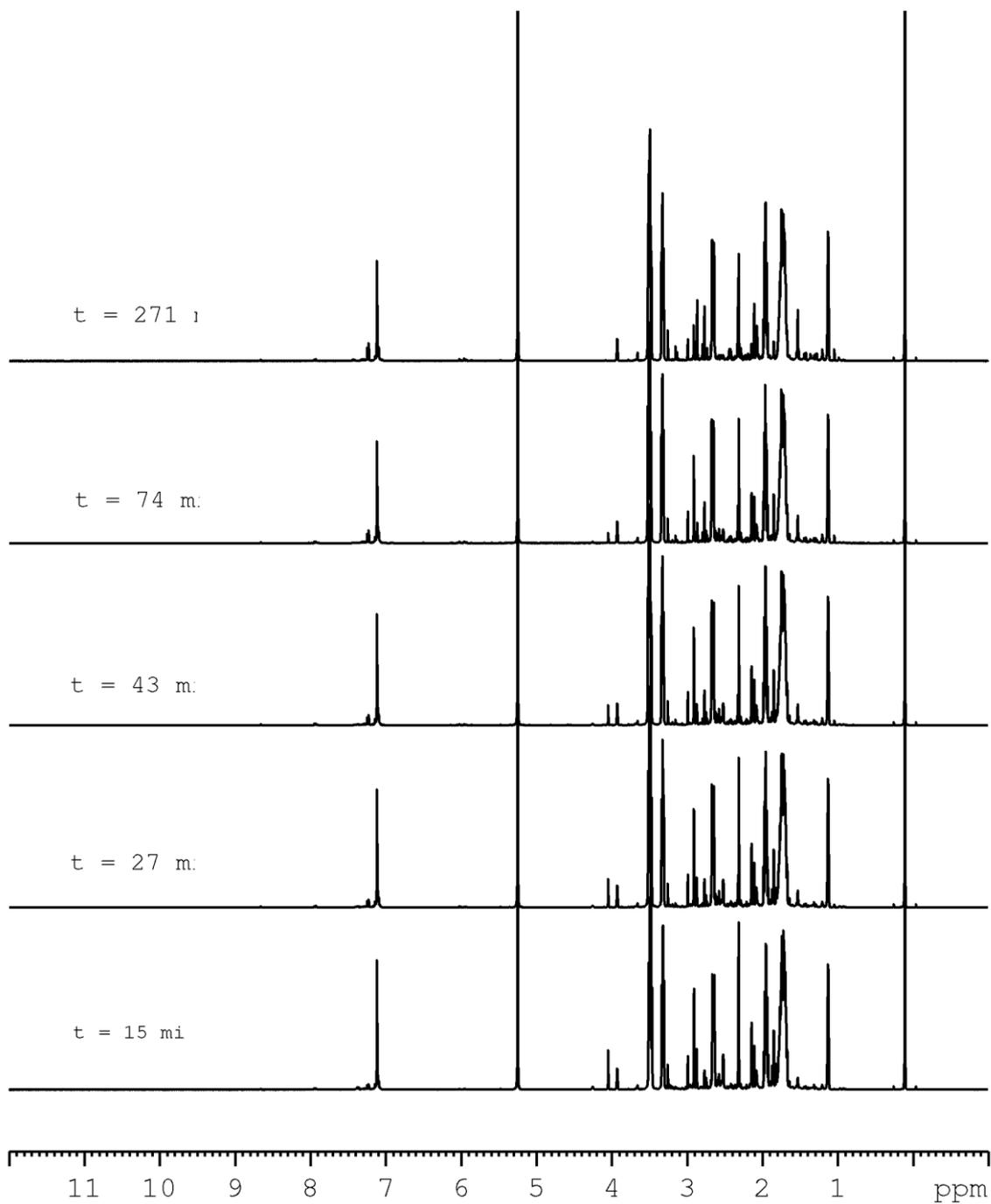


Abbildung A 82: Ausgewählte  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 1 mit Cyclobutanon **32b** zu angegebenen Zeitpunkten.

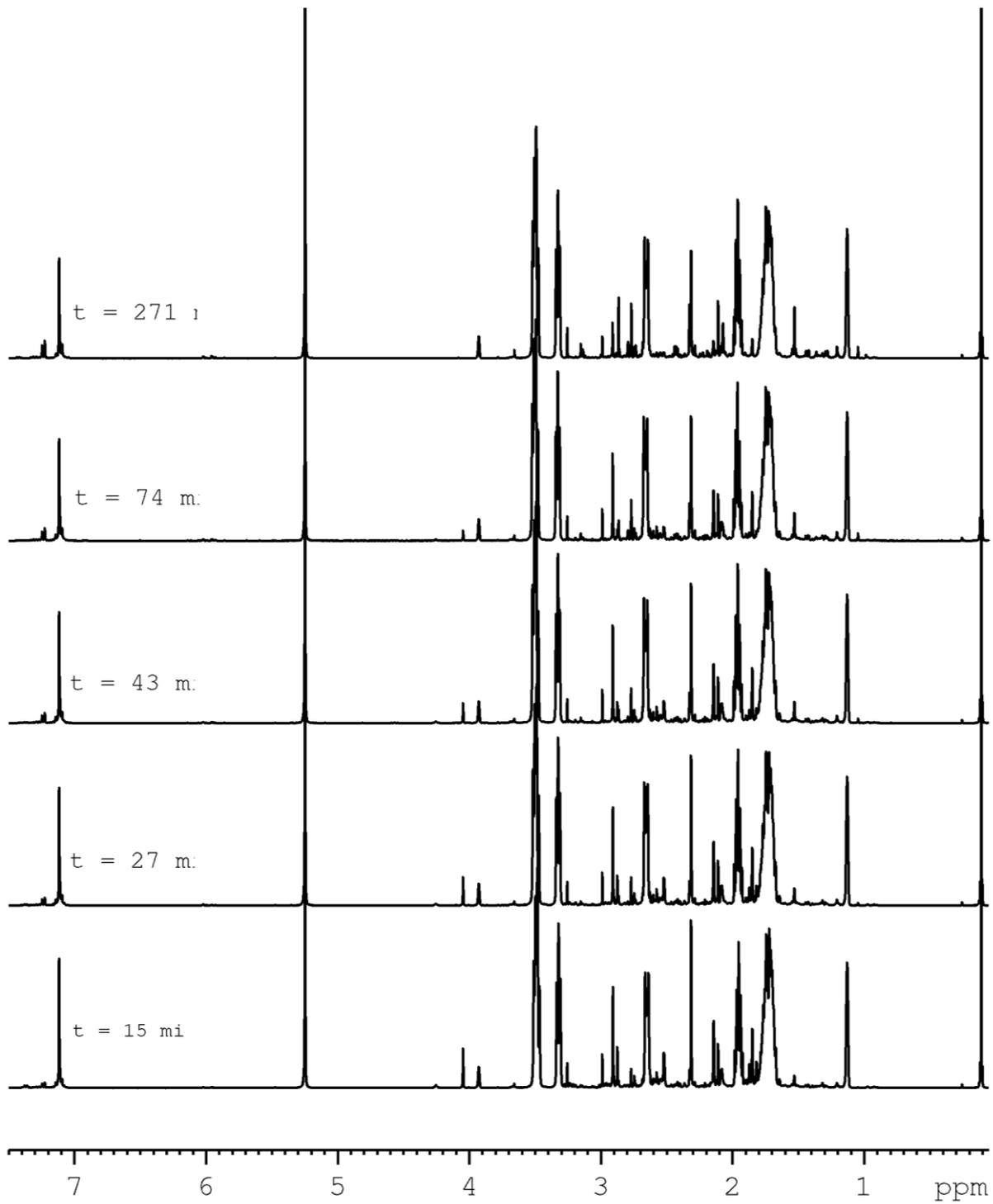


Abbildung A 83: Ausschnitt der ausgewählten  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 1 mit Cyclobutanon **32b** zu angegebenen Zeitpunkten.

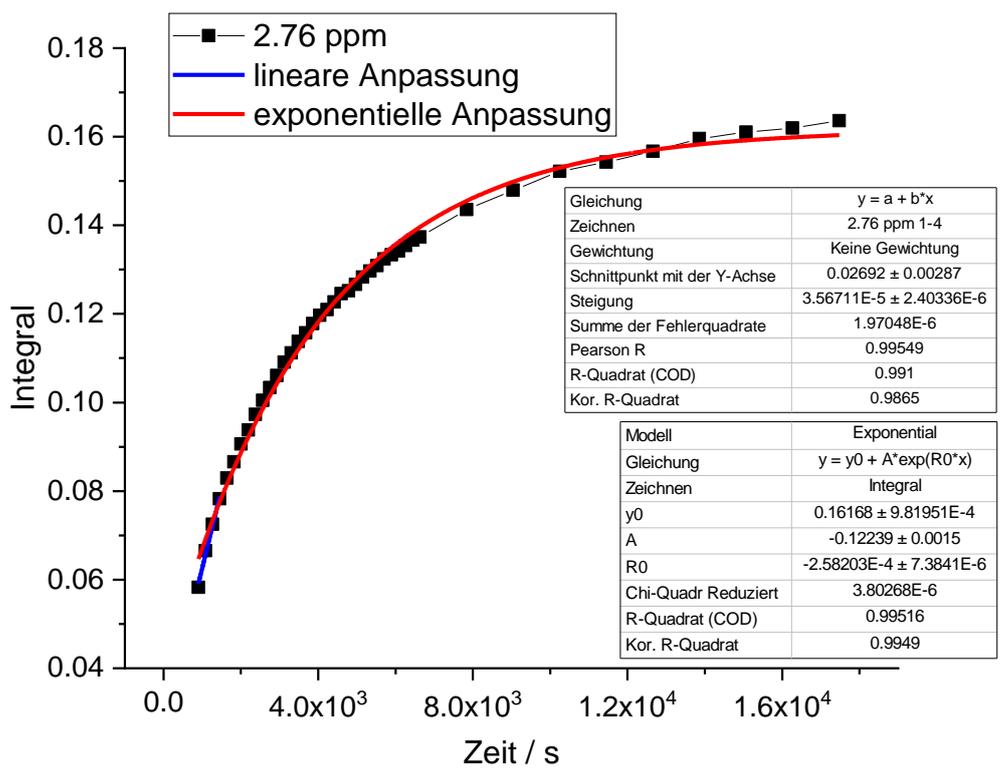


Abbildung A 84: Auftragung der zeitlichen Veränderung des Integrals des Singulett bei 2.76 ppm des Kinetikexperiments 1 mit Cyclobutanon **32b** mit linearer Anpassung des Anfangsbereichs (blaue Linie) und exponentieller Anpassung (rote Linie).

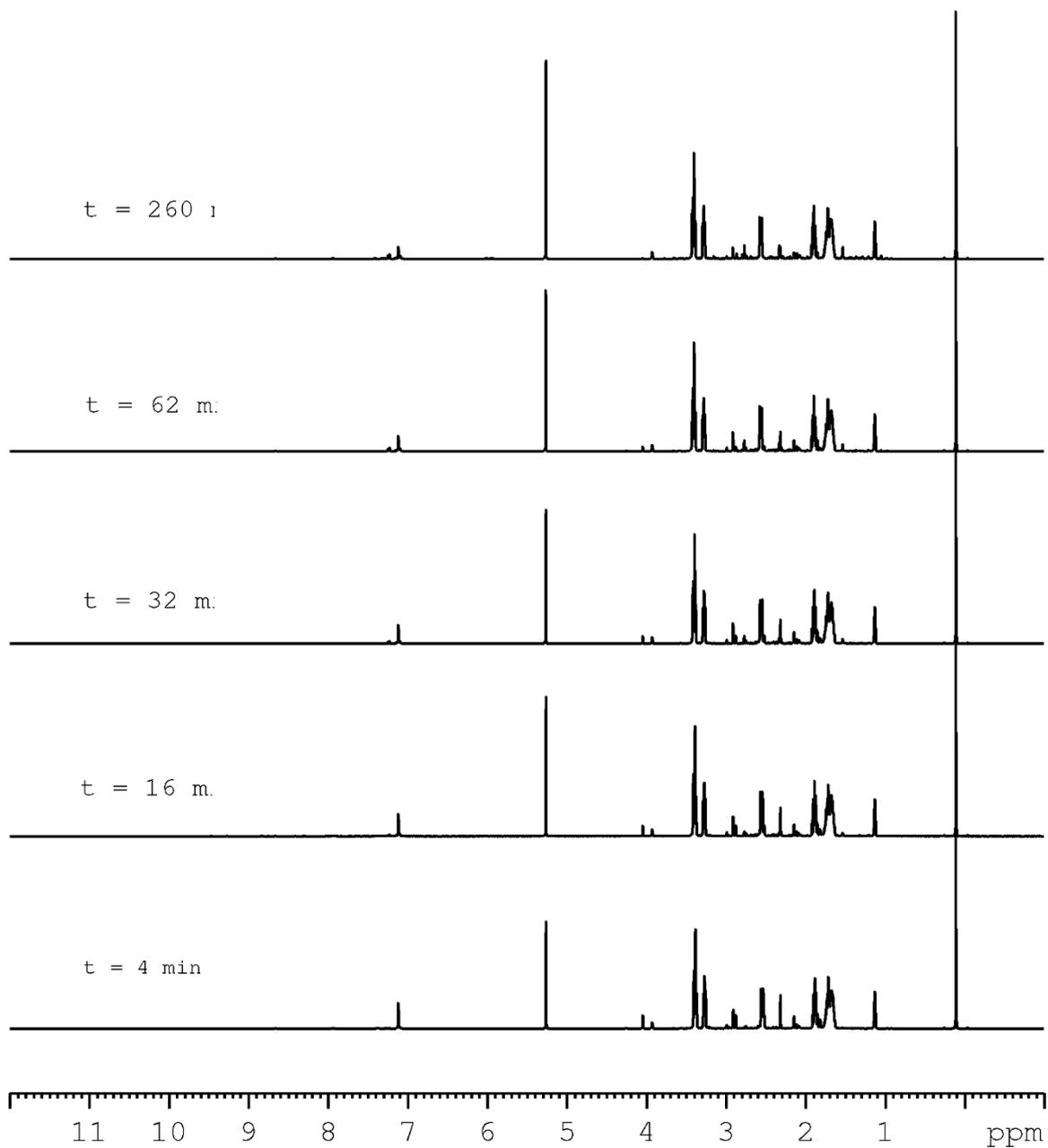


Abbildung A 85: Ausgewählte  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 2 mit Cyclobutanon **32b** zu angegebenen Zeitpunkten.

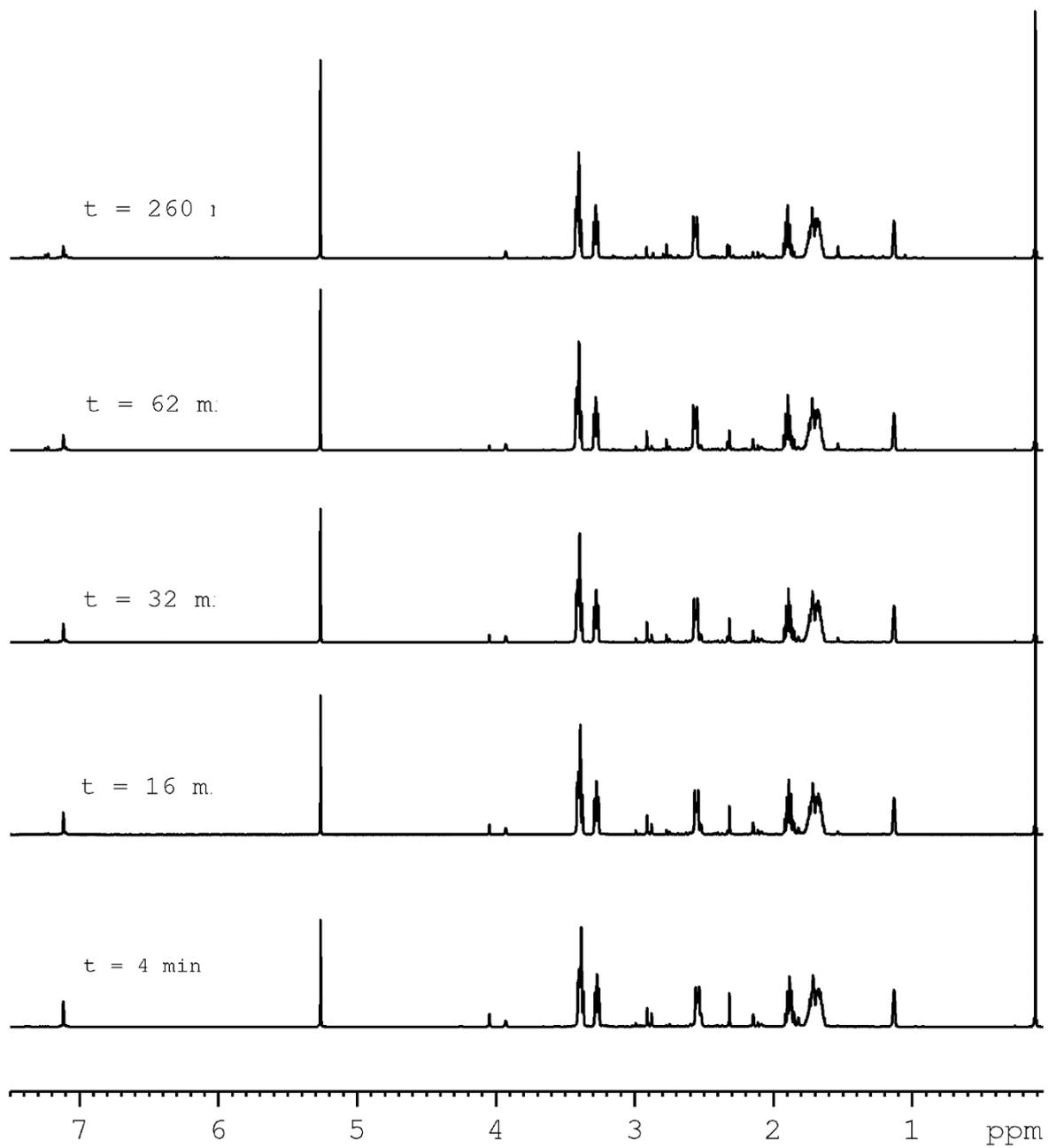


Abbildung A 86: Ausschnitt der ausgewählten  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 2 mit Cyclobutanon **32b** zu angegebenen Zeitpunkten.

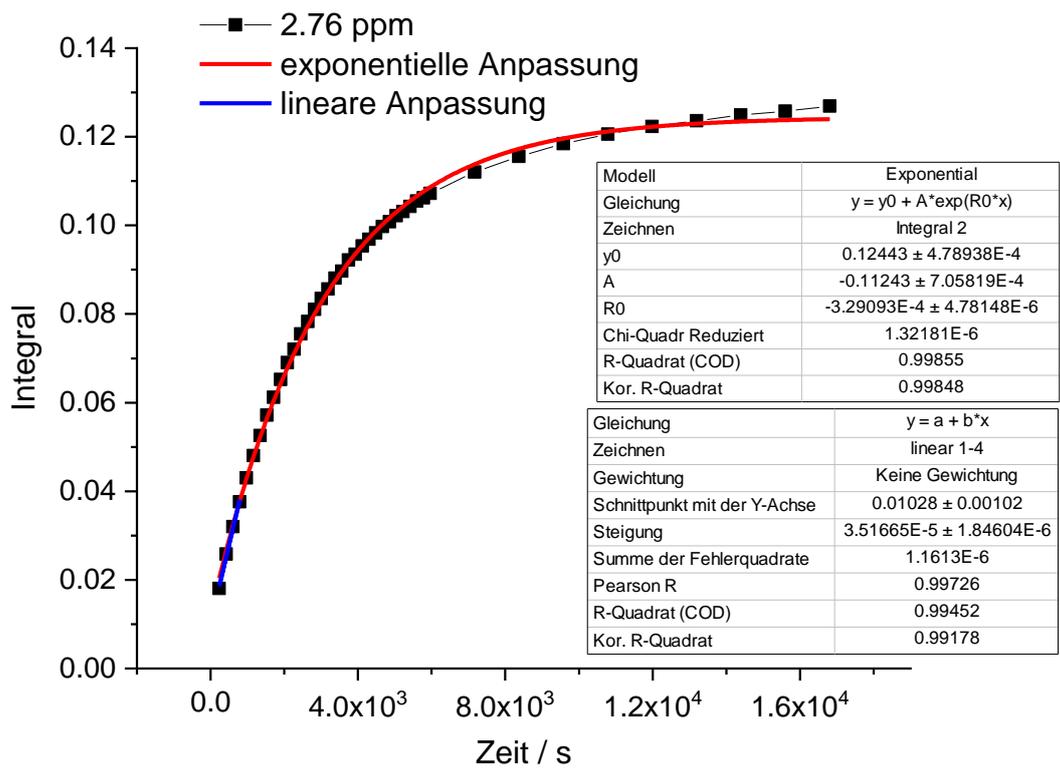
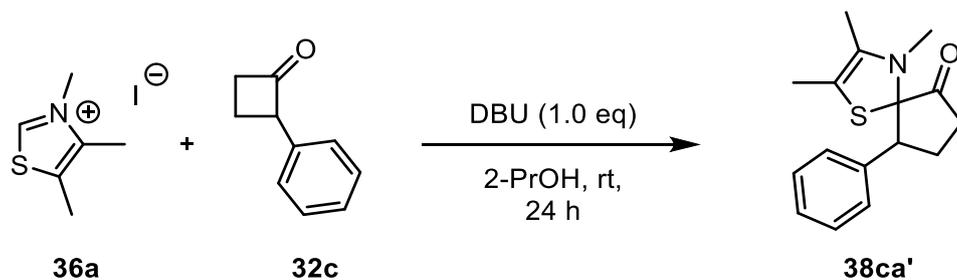


Abbildung A 87: Auftragung der zeitlichen Veränderung des Integrals des Singulett bei 2.76 ppm des Kinetikexperiments 2 mit Cyclobutanon **32b** mit linearer Anpassung des Anfangsbereichs (blaue Linie) und exponentieller Anpassung (rote Linie).



Schema A 3: Reaktionsschema der mittels zeitaufgelöster NMR-Spektroskopie untersuchten Reaktion von Thiazoliumsalz **36a**, Cyclobutanon **32c** und DBU.

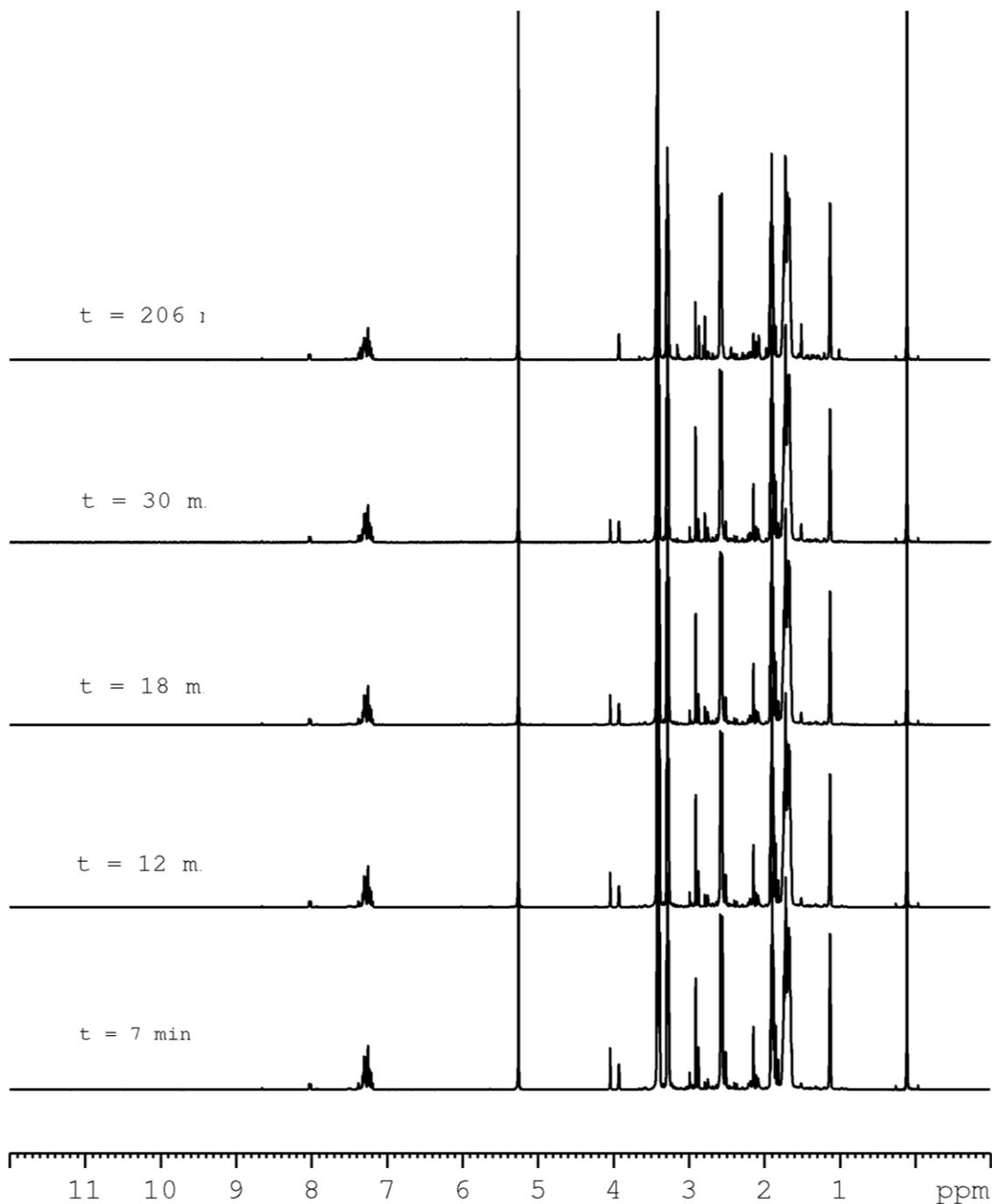


Abbildung A 88: Ausgewählte  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 1 mit Cyclobutanon **32c** zu angegebenen Zeitpunkten.

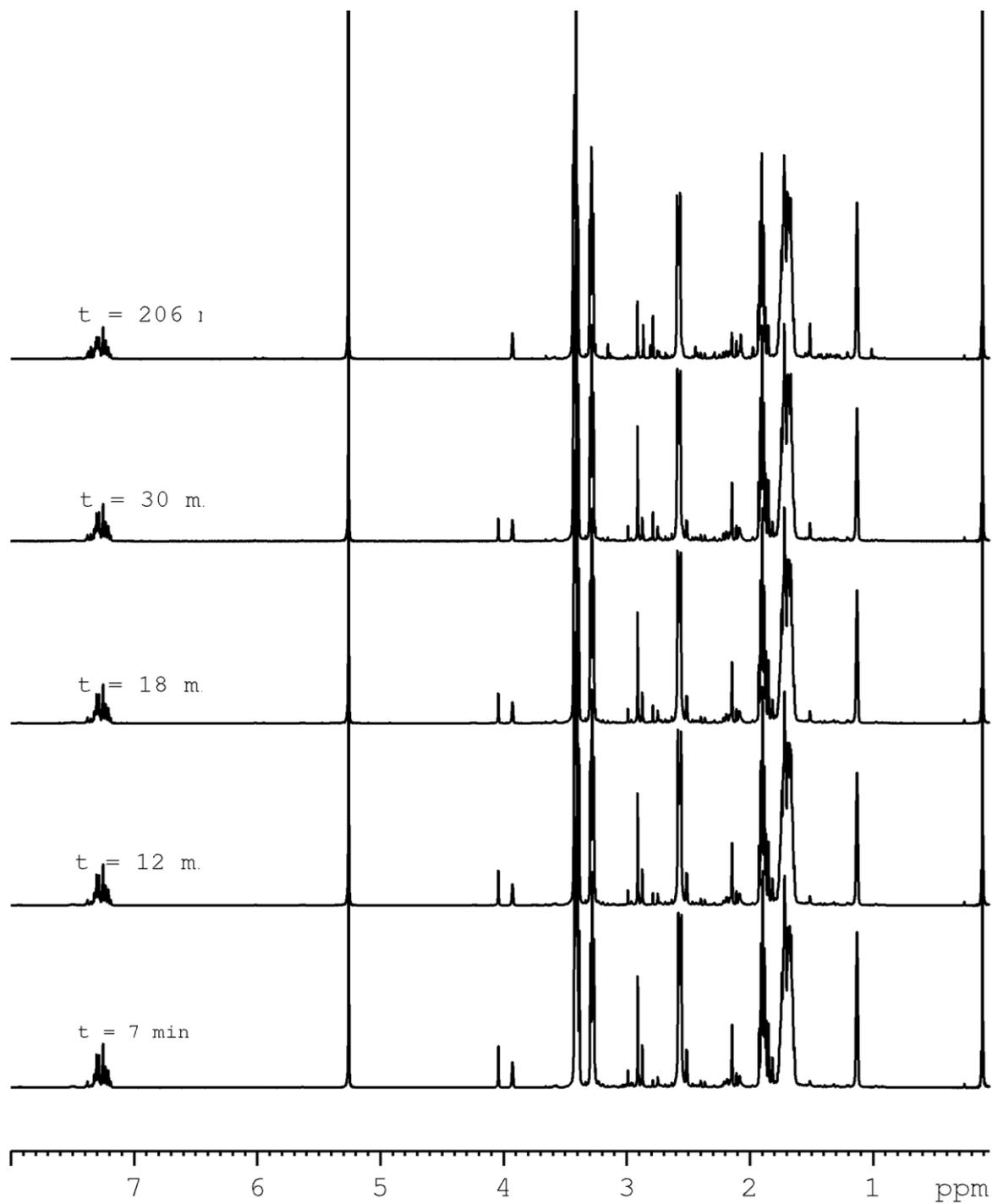


Abbildung A 89: Ausschnitt der ausgewählten  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 1 mit Cyclobutanon **32c** zu angegebenen Zeitpunkten.

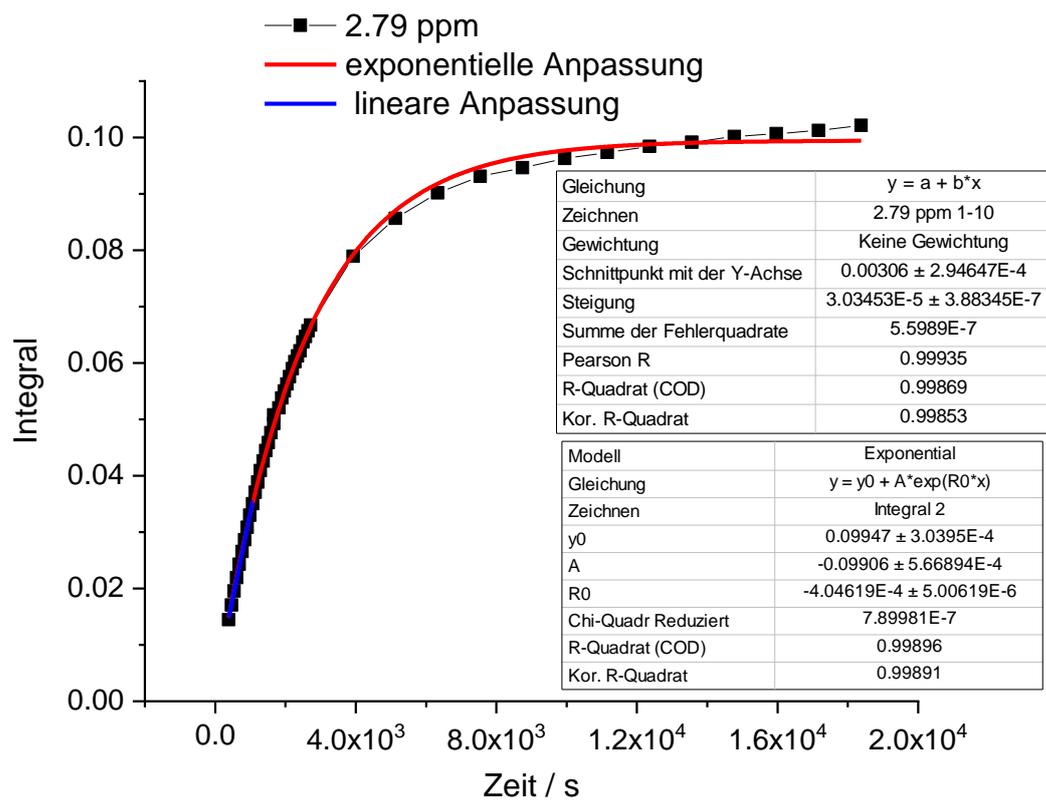


Abbildung A 90: Auftragung der zeitlichen Veränderung des Integrals des Singulett bei 2.79 ppm des Kinetikexperiments 1 mit Cyclobutanon **32c** mit linearer Anpassung des Anfangsbereichs (blaue Linie) und exponentieller Anpassung (rote Linie).

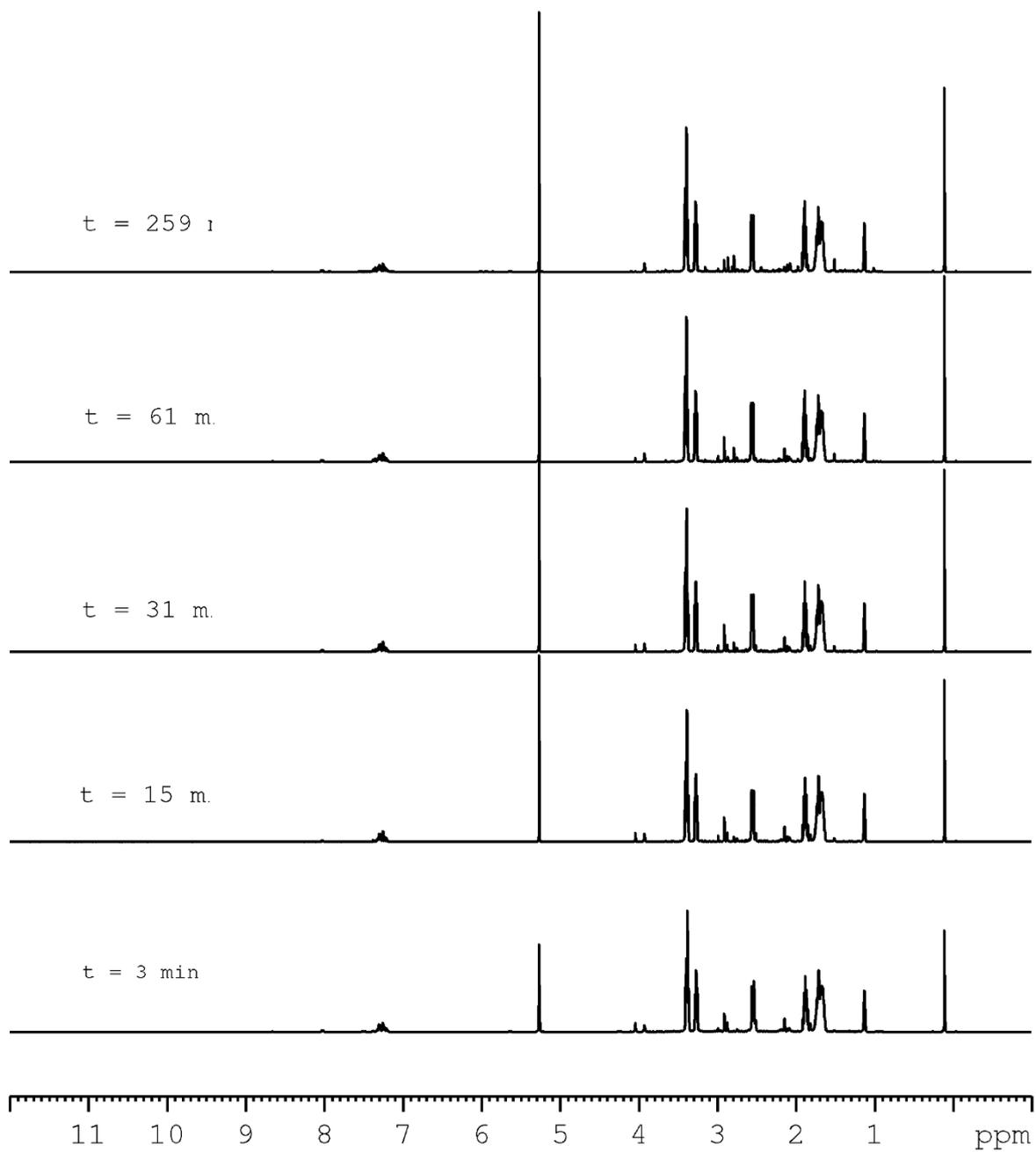


Abbildung A 91: Ausgewählte  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 2 mit Cyclobutanon **32c** zu angegebenen Zeitpunkten.

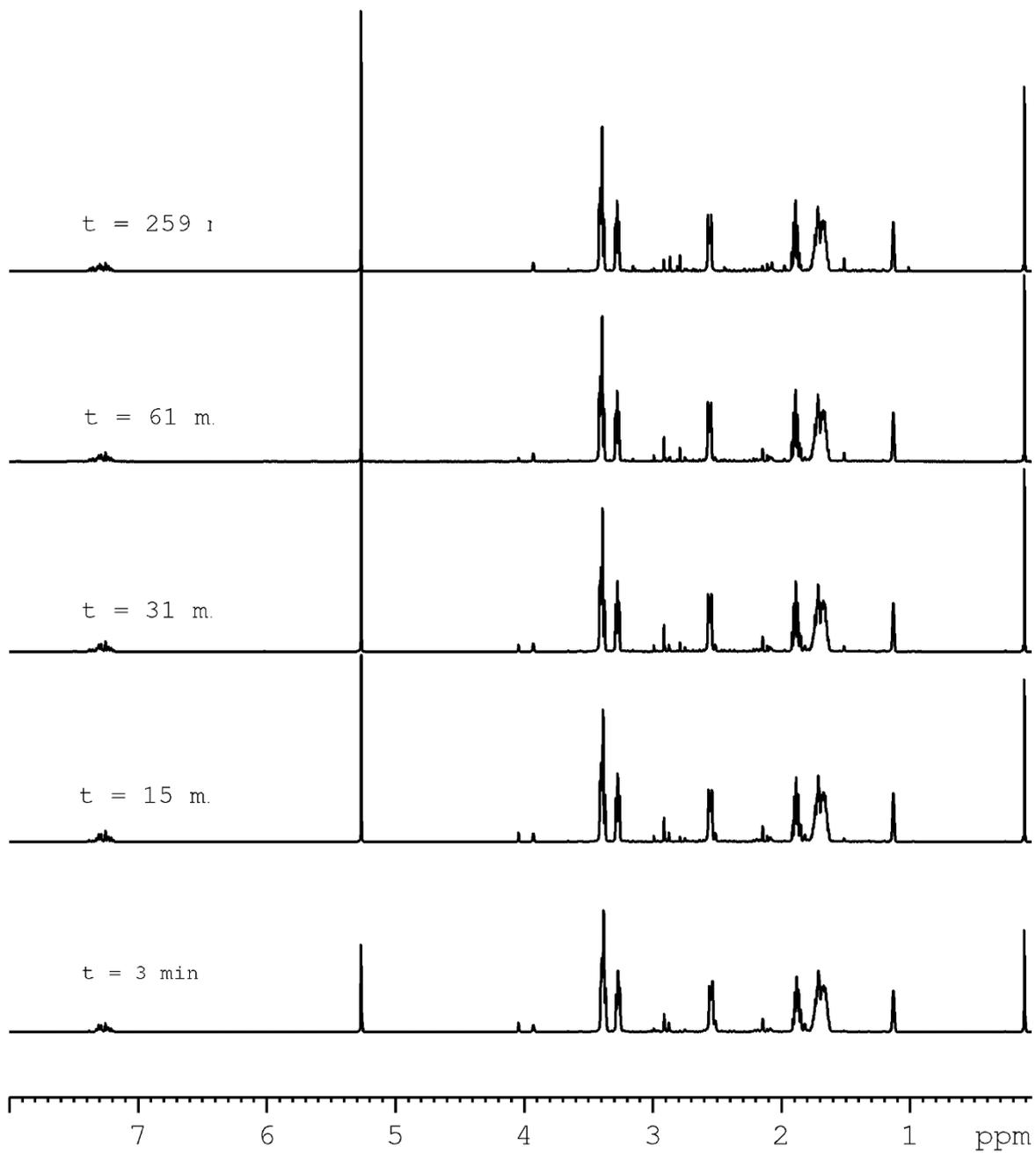


Abbildung A 92: Ausschnitt der ausgewählten  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 2 mit Cyclobutanon **32c** zu angegebenen Zeitpunkten.

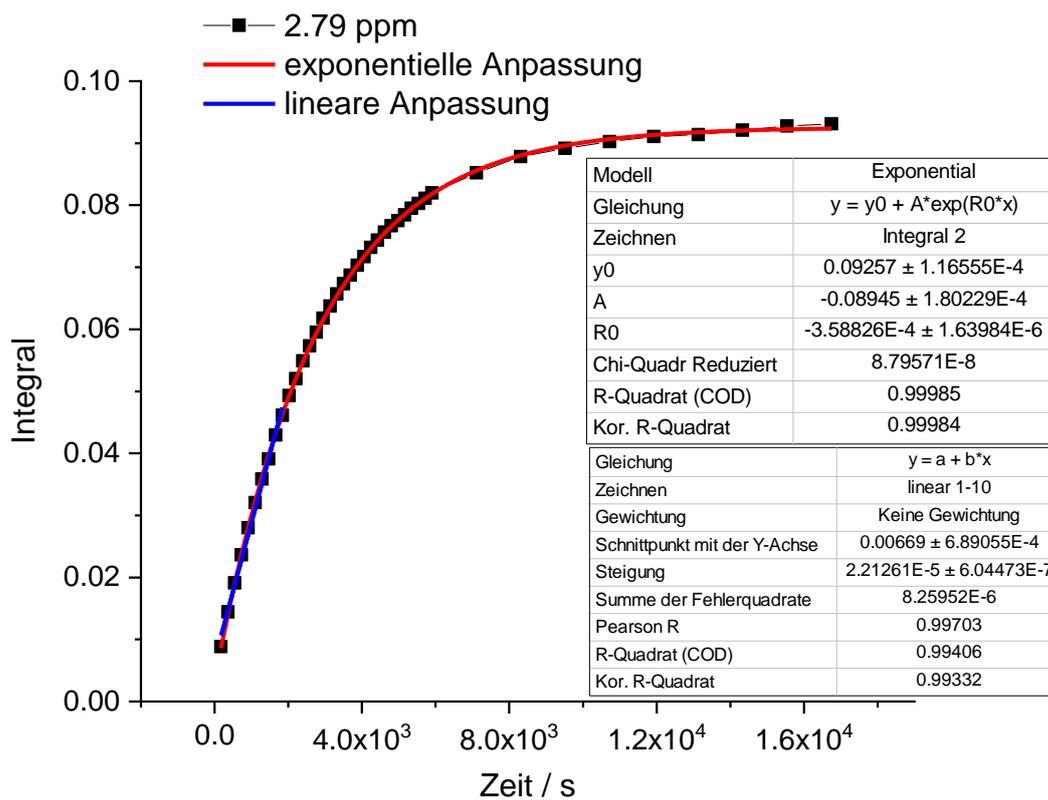
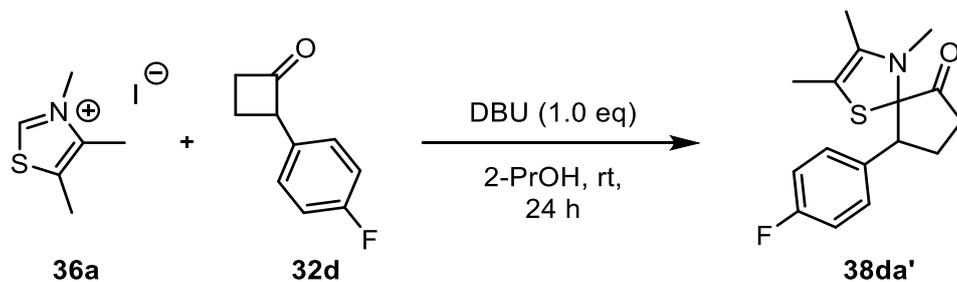


Abbildung A 93: Auftragung der zeitlichen Veränderung des Integrals des Singulett bei 2.79 ppm des Kinetikexperiments 2 mit Cyclobutanon **32c** mit linearer Anpassung des Anfangsbereichs (blaue Linie) und exponentieller Anpassung (rote Linie).



Schema A 4: Reaktionsschema der mittels zeitaufgelöster NMR-Spektroskopie untersuchten Reaktion von Thiazoliumsalz **36a**, Cyclobutanon **32d** und DBU.

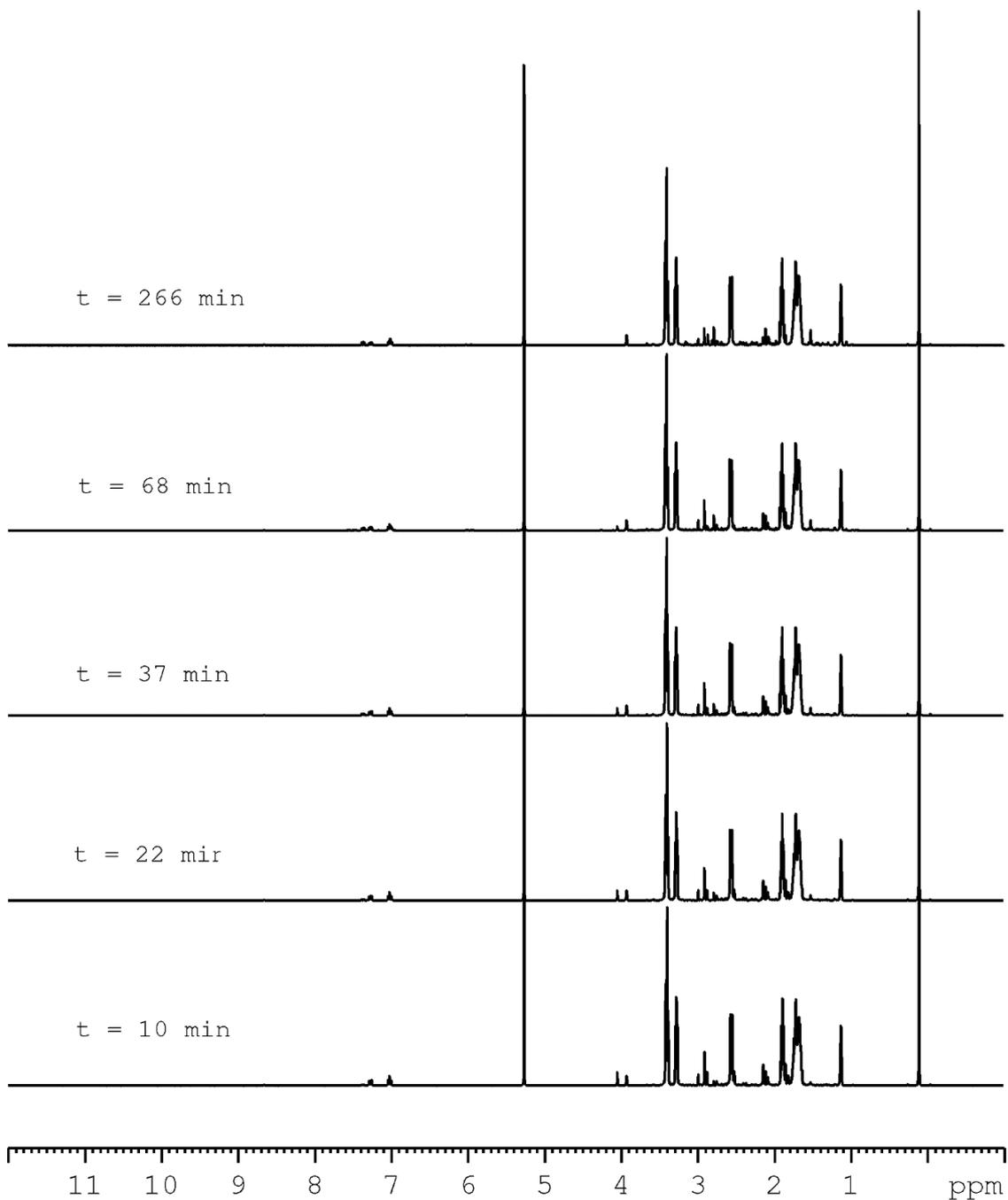


Abbildung A 94: Ausgewählte  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 1 mit Cyclobutanon **32d** zu angegebenen Zeitpunkten.

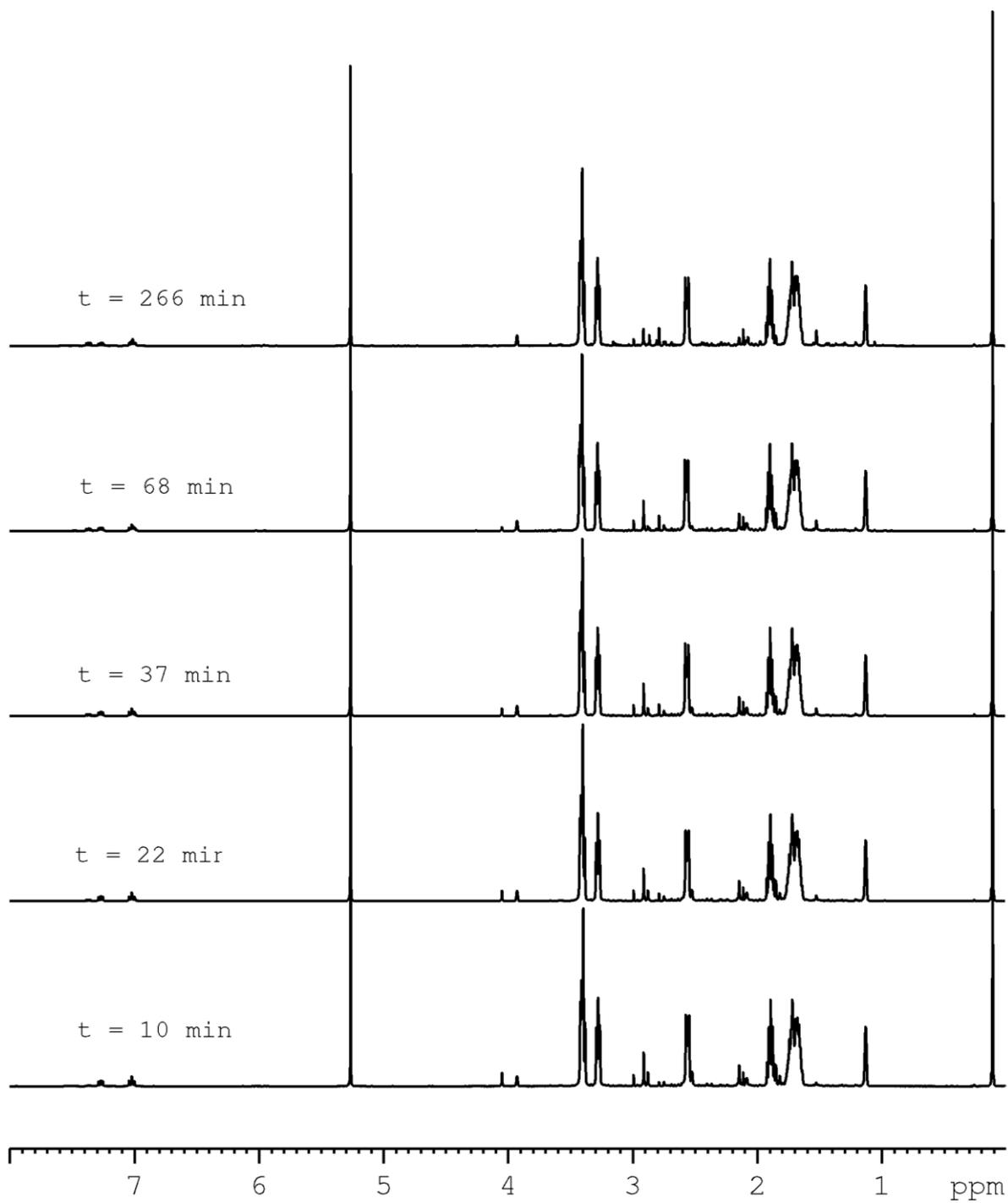


Abbildung A 95: Ausschnitt der ausgewählten  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 1 mit Cyclobutanon **32d** zu angegebenen Zeitpunkten.

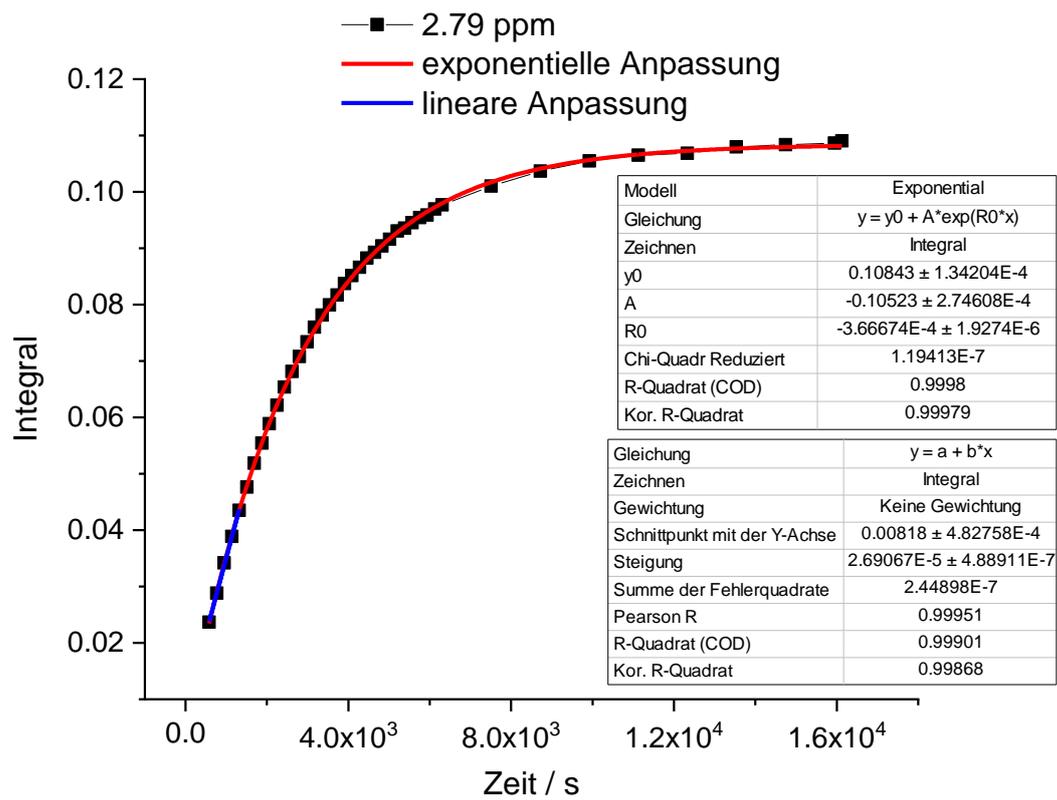


Abbildung A 96: Auftragung der zeitlichen Veränderung des Integrals des Singulett bei 2.79 ppm des Kinetikexperiments 1 mit Cyclobutanon **32d** mit linearer Anpassung des Anfangsbereichs (blaue Linie) und exponentieller Anpassung (rote Linie).

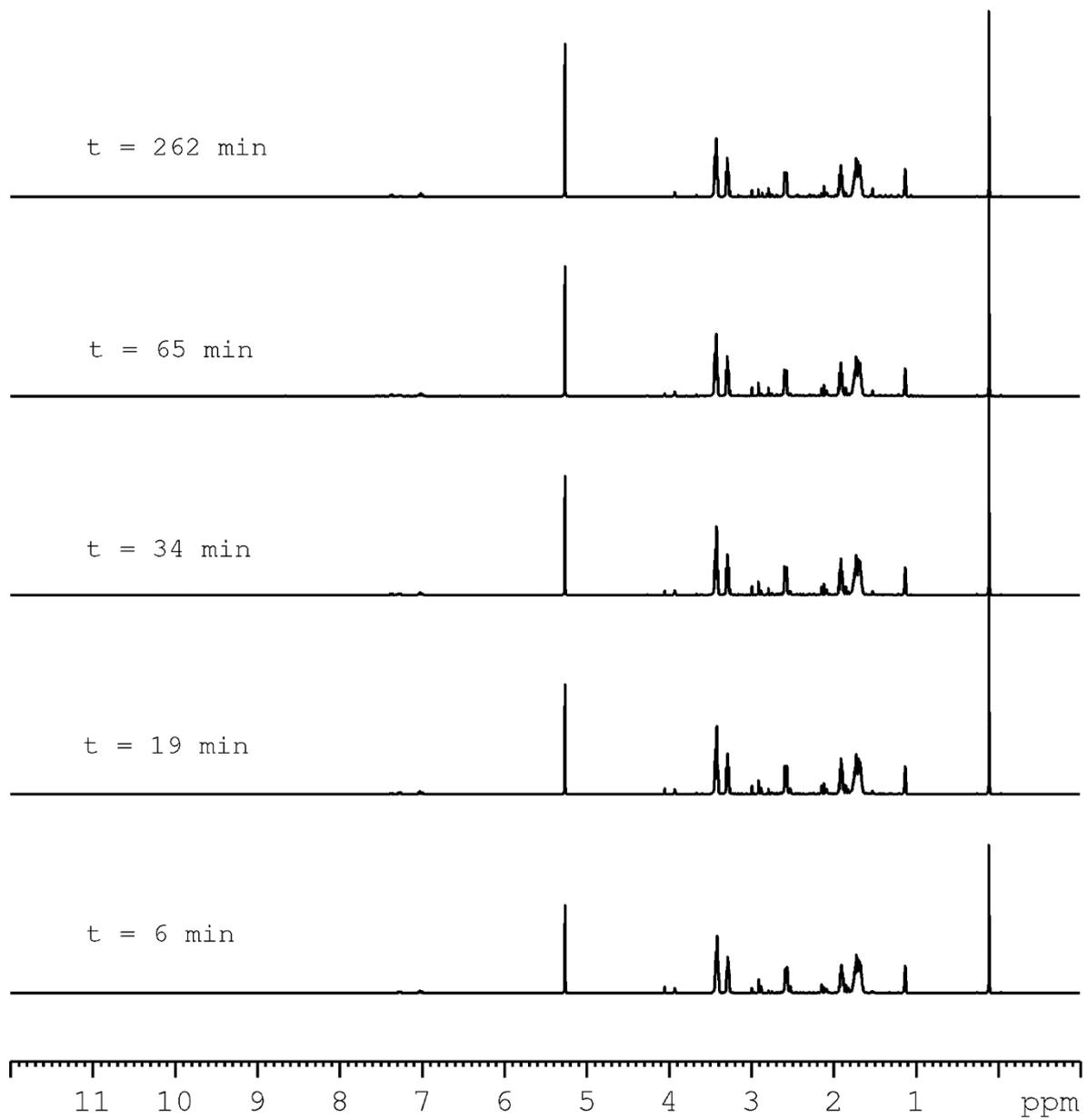


Abbildung A 97: Ausgewählte <sup>1</sup>H-NMR-Spektren des Kinetikexperiments 2 mit Cyclobutanon **32d** zu angegebenen Zeitpunkten.

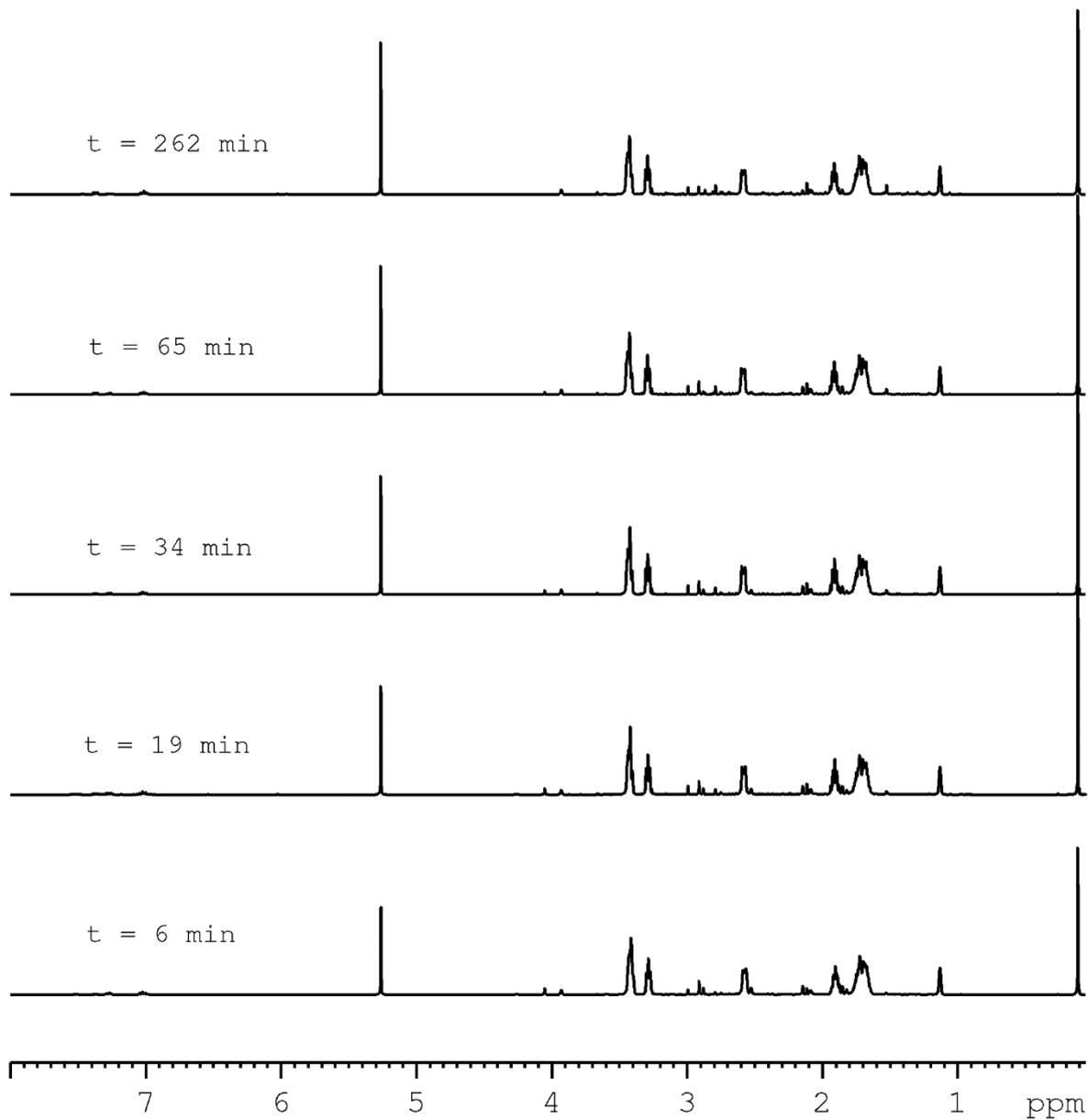


Abbildung A 98: Ausschnitt der ausgewählten  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 2 mit Cyclobutanon **32d** zu angegebenen Zeitpunkten.

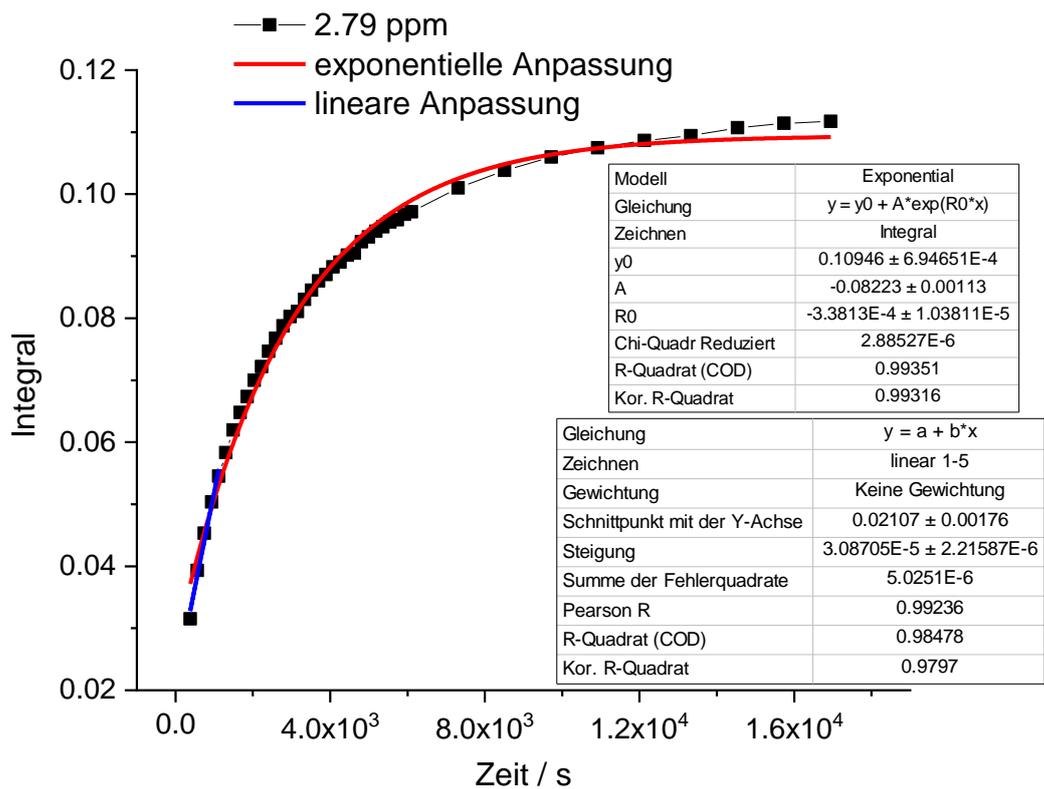
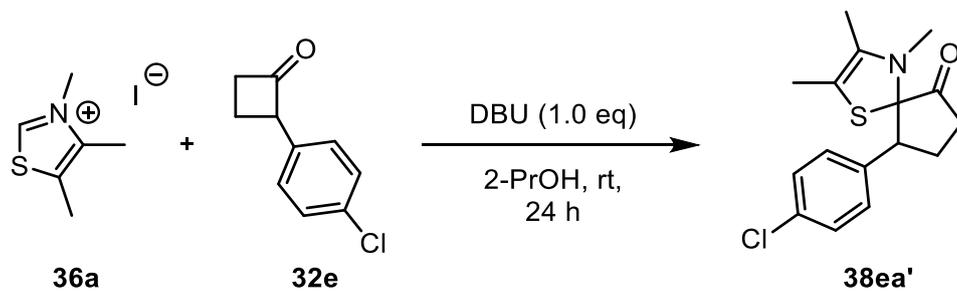


Abbildung A 99: Auftragung der zeitlichen Veränderung des Integrals des Singulett bei 2.79 ppm des Kinetikexperiments 2 mit Cyclobutanon **32d** mit linearer Anpassung des Anfangsbereichs (blaue Linie) und exponentieller Anpassung (rote Linie).



Schema A 5: Reaktionsschema der mittels zeitaufgelöster NMR-Spektroskopie untersuchten Reaktion von Thiazoliumsalz **36a**, Cyclobutanon **32e** und DBU.

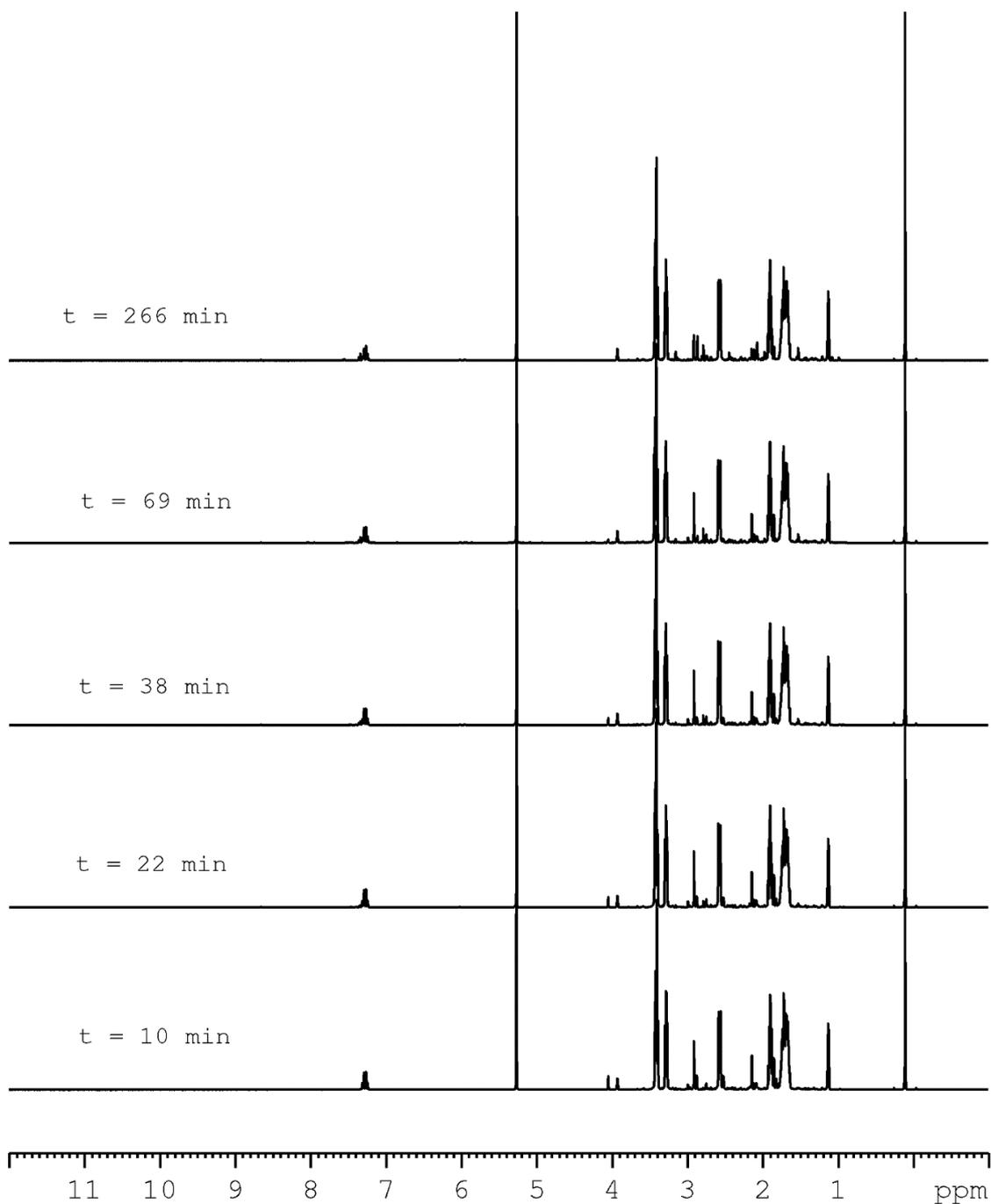


Abbildung A 100: Ausgewählte <sup>1</sup>H-NMR-Spektren des Kinetikexperiments 1 mit Cyclobutanon **32e** zu angegebenen Zeitpunkten.

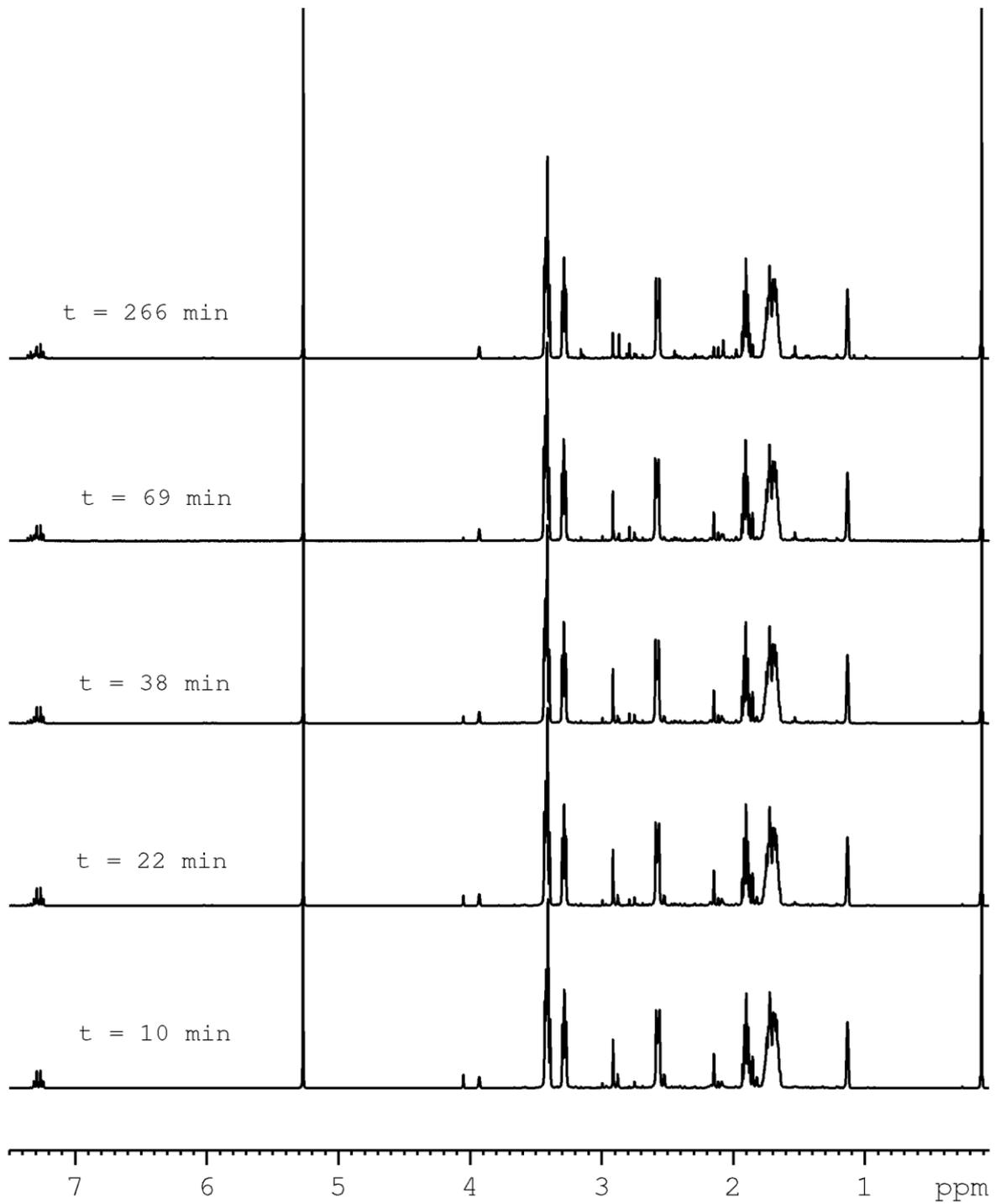


Abbildung A 101: Ausschnitt der ausgewählten <sup>1</sup>H-NMR-Spektren des Kinetikexperiments 1 mit Cyclobutanon **32e** zu angegebenen Zeitpunkten.

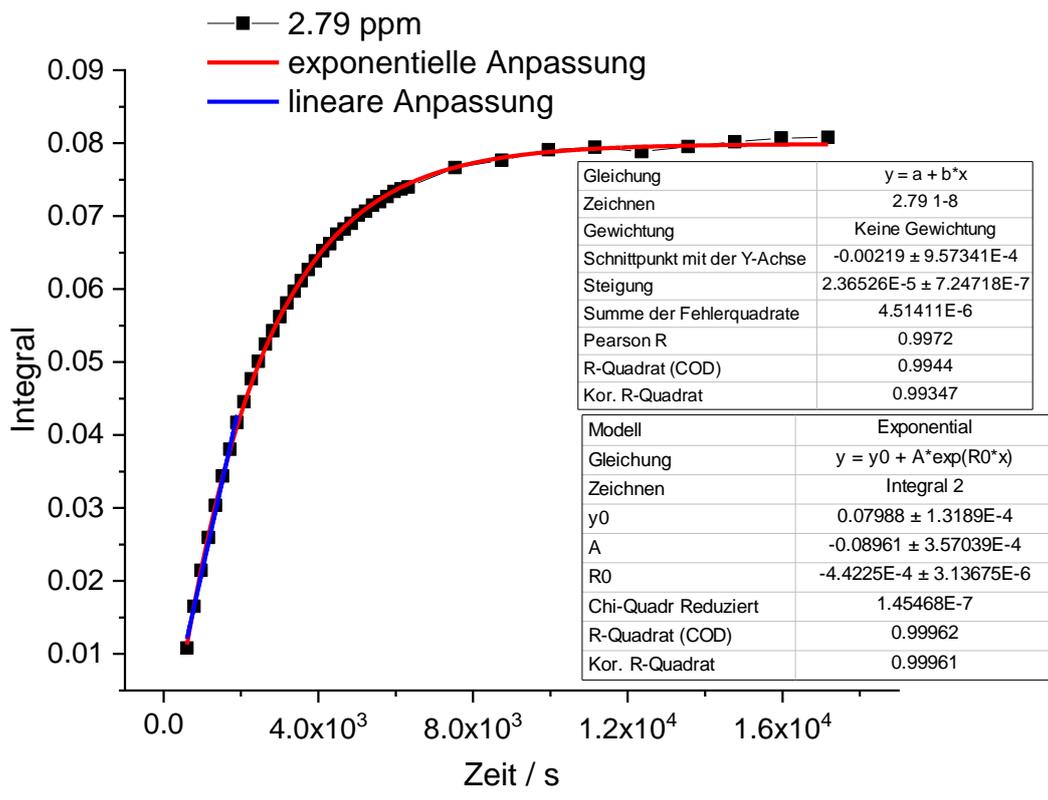


Abbildung A 102: Auftragung der zeitlichen Veränderung des Integrals des Singulett bei 2.79 ppm des Kinetikexperiments 1 mit Cyclobutanon **32e** mit linearer Anpassung des Anfangsbereichs (blaue Linie) und exponentieller Anpassung (rote Linie).

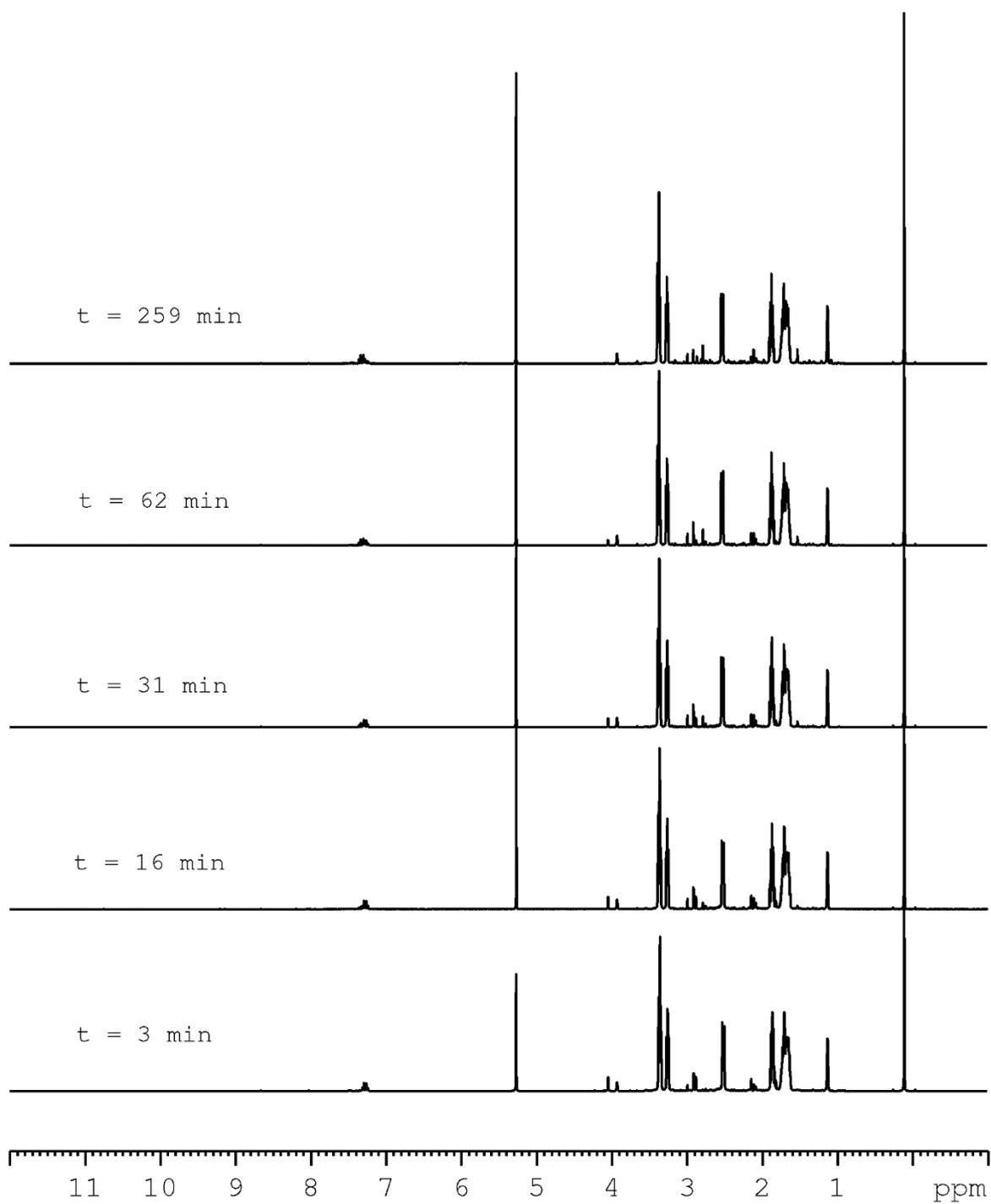


Abbildung A 103: Ausgewählte  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 2 mit Cyclobutanon **32e** zu angegebenen Zeitpunkten.

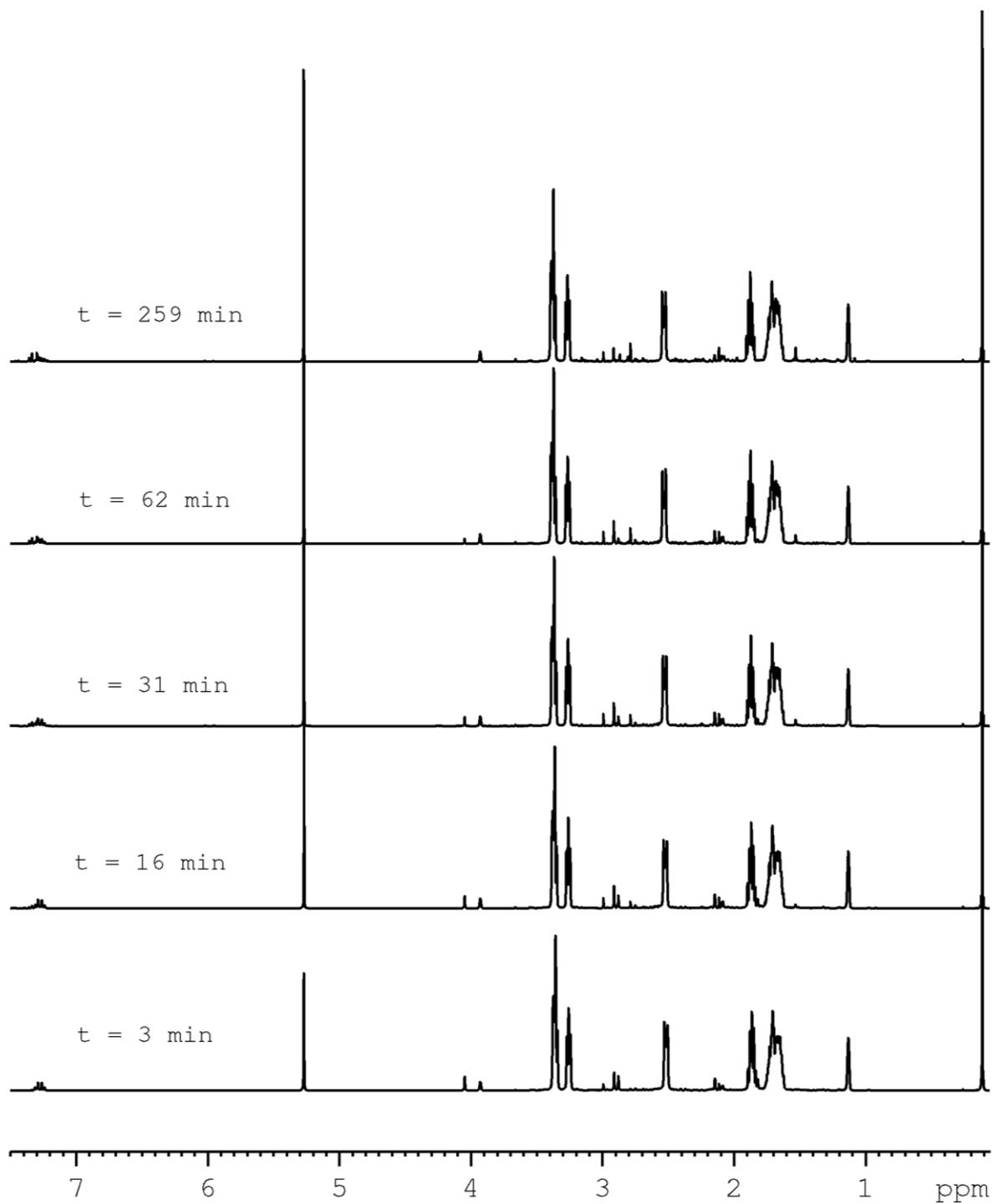


Abbildung A 104: Ausschnitt der ausgewählten  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 2 mit Cyclobutanon **32e** zu angegebenen Zeitpunkten.

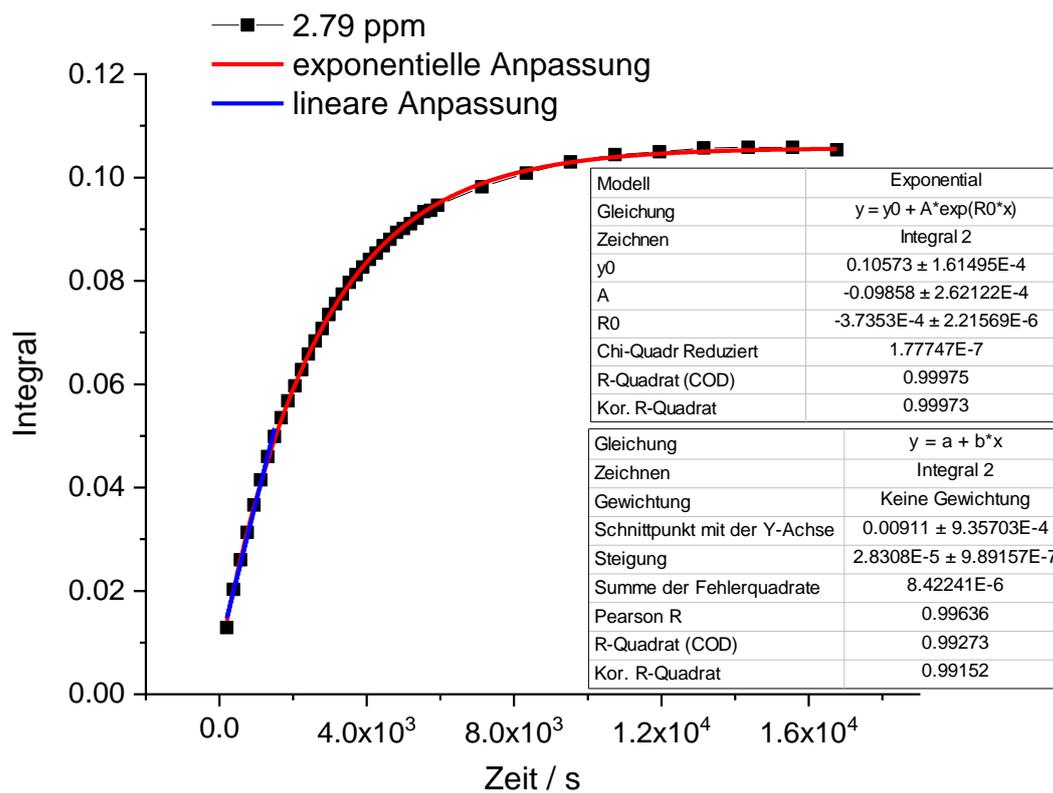


Abbildung A 105: Auftragung der zeitlichen Veränderung des Integrals des Singulett bei 2.79 ppm des Kinetikexperiments 2 mit Cyclobutanon **32e** mit linearer Anpassung des Anfangsbereichs (blaue Linie) und exponentieller Anpassung (rote Linie).

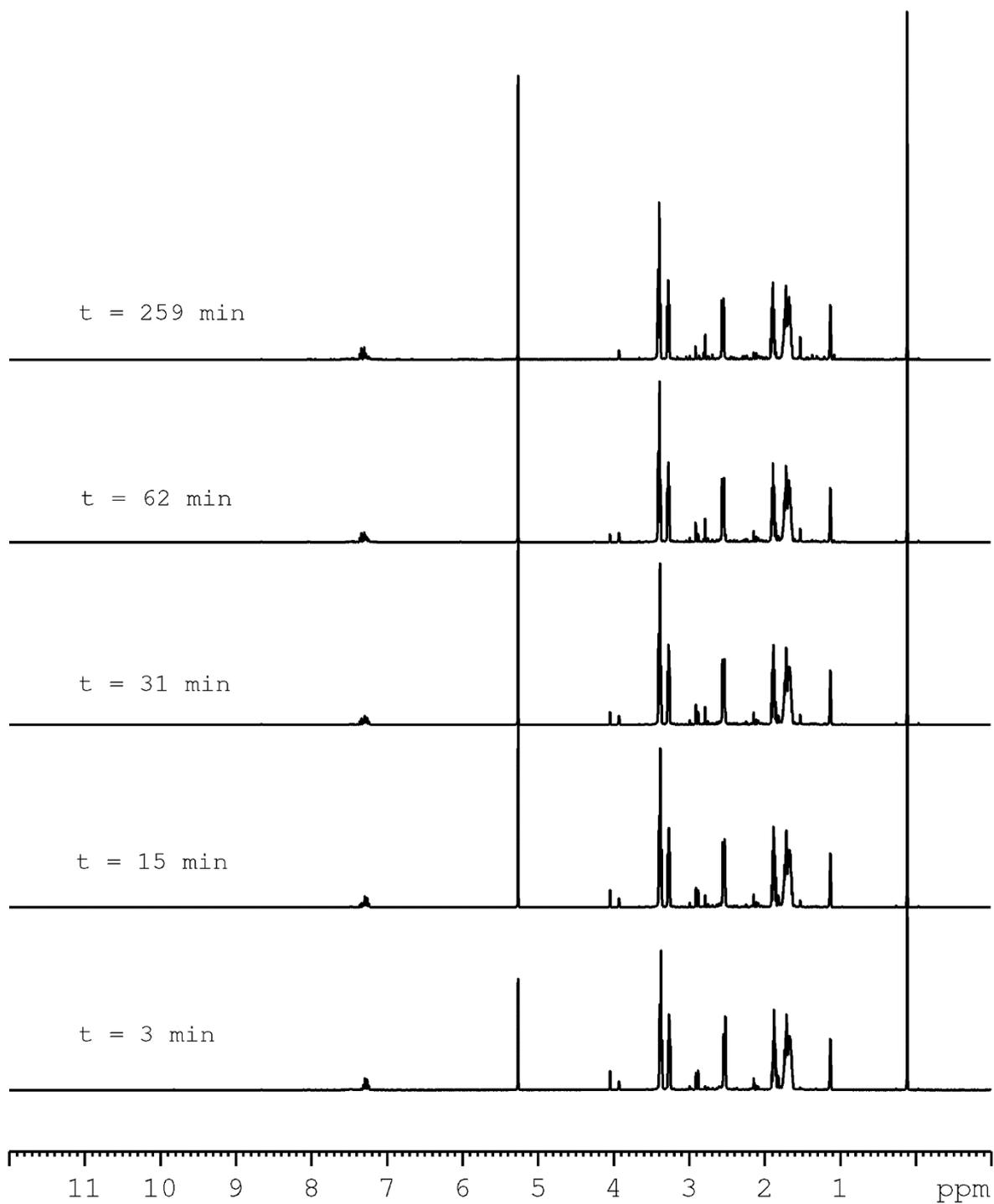


Abbildung A 106: Ausgewählte  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 3 mit Cyclobutanon **32e** zu angegebenen Zeitpunkten.

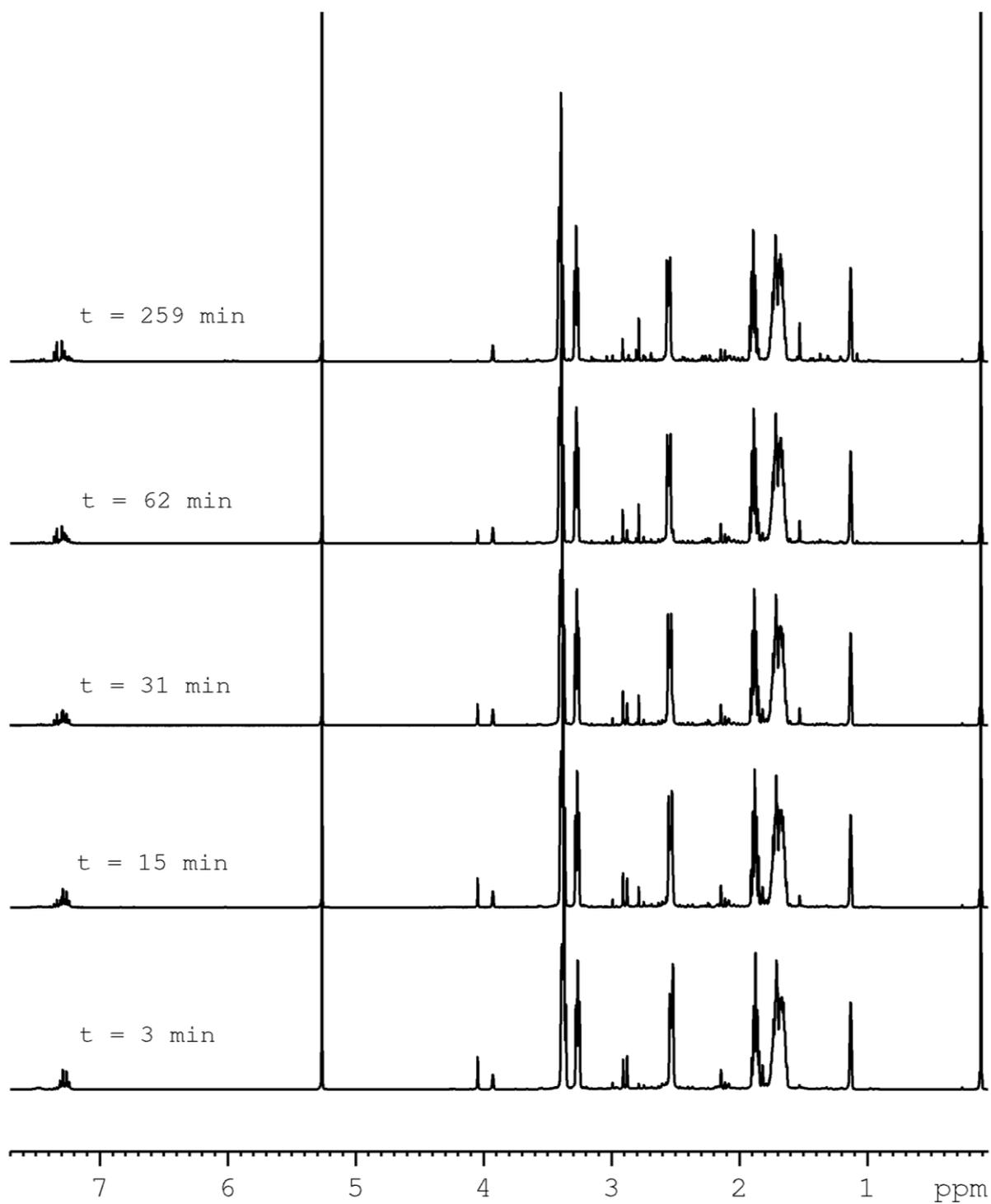


Abbildung A 107: Ausschnitt der ausgewählten  $^1\text{H-NMR}$ -Spektren des Kinetikexperiments 3 mit Cyclobutanon **32e** zu angegebenen Zeitpunkten.

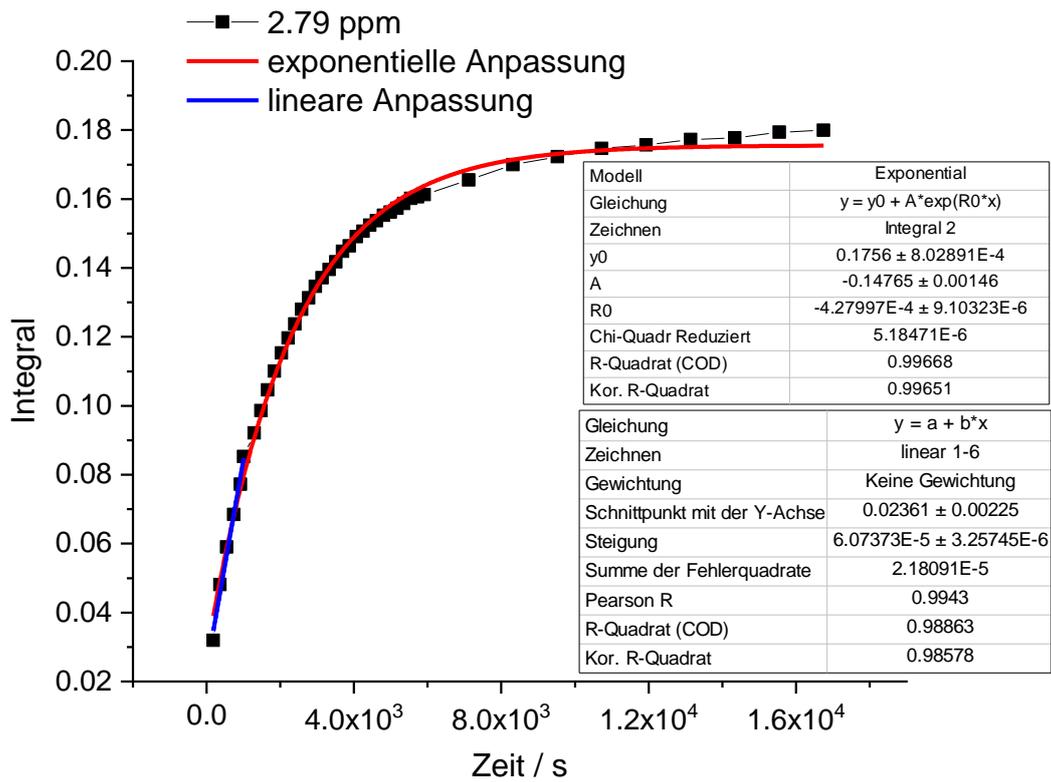


Abbildung A 108: Auftragung der zeitlichen Veränderung des Integrals des Singulett bei 2.79 ppm des Kinetikexperiments 3 mit Cyclobutanon **32e** mit linearer Anpassung des Anfangsbereichs (blaue Linie) und exponentieller Anpassung (rote Linie).

## Kristallstrukturanalyse:

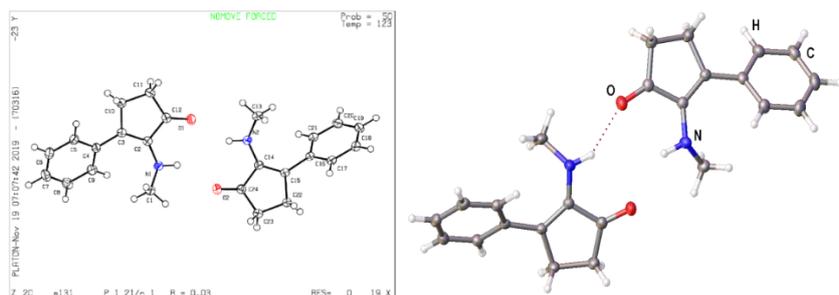


Abbildung A 109: Darstellungen aus der Kristallstrukturanalyse von 3-Phenyl-2-methylaminocyclopent-2-enon **37ca'**.

Compound	<b>37ca'</b>
Formula	C <sub>12</sub> H <sub>13</sub> NO
<i>D</i> <sub>calc.</sub> / g cm <sup>-3</sup>	1.270
$\mu$ /mm <sup>-1</sup>	0.639
Formula Weight	187.23
Colour	clear colourless
Shape	prism
Size/mm <sup>3</sup>	0.26×0.17×0.11
<i>T</i> /K	123.01(10)
Crystal System	monoclinic
Space Group	<i>P</i> 2 <sub>1</sub> / <i>n</i>
<i>a</i> /Å	11.2335(3)
<i>b</i> /Å	14.5084(3)
<i>c</i> /Å	12.8257(3)
$\alpha$ /°	90
$\beta$ /°	110.495(2)
$\gamma$ /°	90
<i>V</i> /Å <sup>3</sup>	1958.02(8)
<i>Z</i>	8
<i>Z</i> '	2
Wavelength/Å	1.54184
Radiation type	Cu K $\alpha$
$\theta$ <sub>min</sub> /°	4.514
$\theta$ <sub>max</sub> /°	76.191
Measured Refl's.	12304
Ind't Refl's	4013
Refl's with <i>I</i> > 2( <i>I</i> )	3699
<i>R</i> <sub>int</sub>	0.0161
Parameters	357
Restraints	0
Largest Peak	0.233
Deepest Hole	-0.195
GooF	1.040
<i>wR</i> <sub>2</sub> (all data)	0.0887
<i>wR</i> <sub>2</sub>	0.0865
<i>R</i> <sub>1</sub> (all data)	0.0367
<i>R</i> <sub>1</sub>	0.0340

## IR-Spektren:

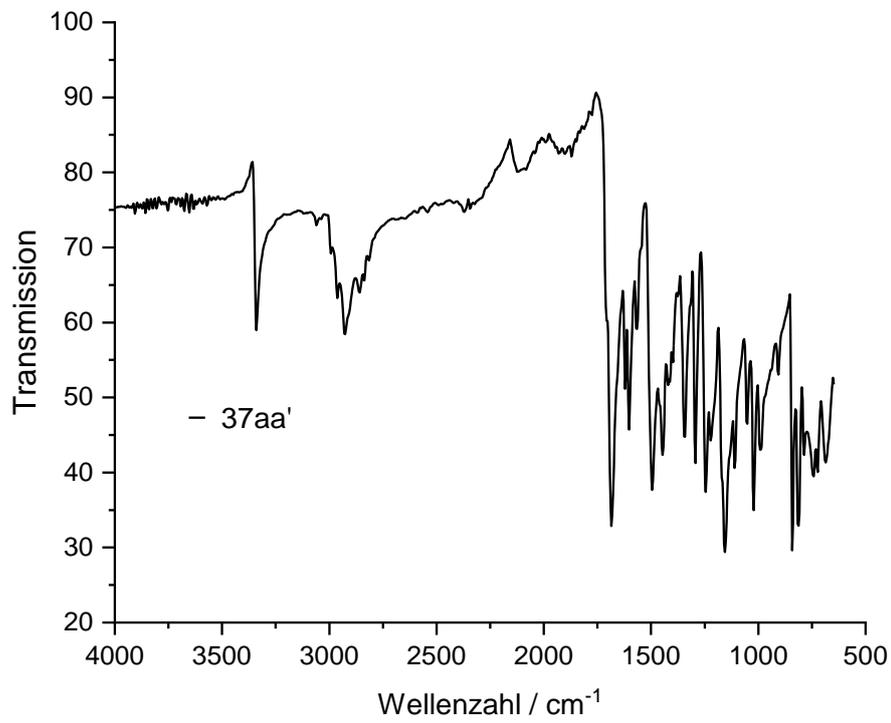


Abbildung A 110: IR-Spektrum von 3-(4-Methoxyphenyl)-2-methylaminocyclopent-2-enon **37aa'**.

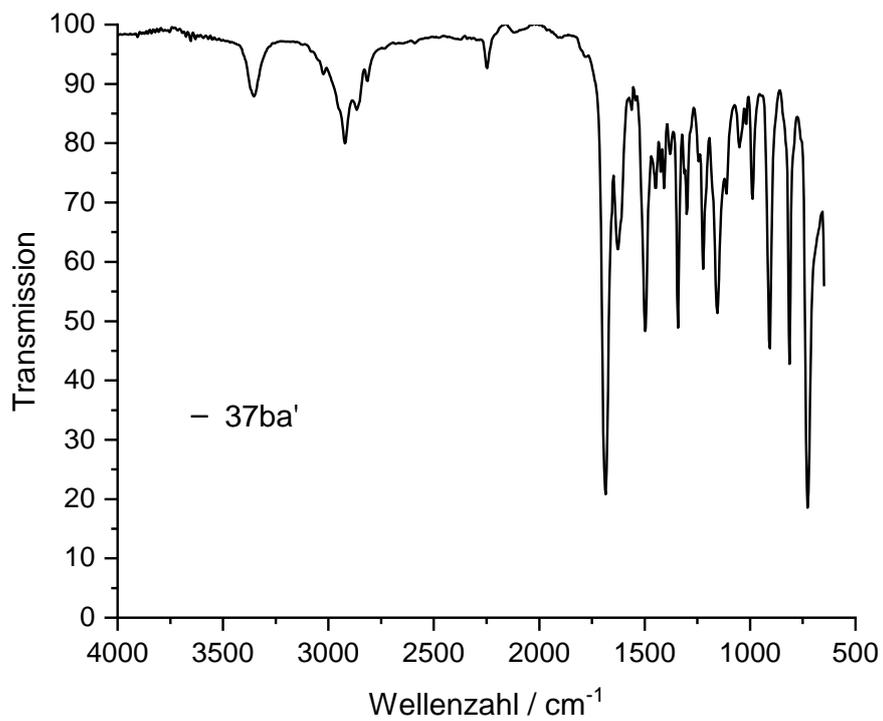


Abbildung A 111: IR-Spektrum von 3-(4-Methylphenyl)-2-methylaminocyclopent-2-enon **37ba'**.

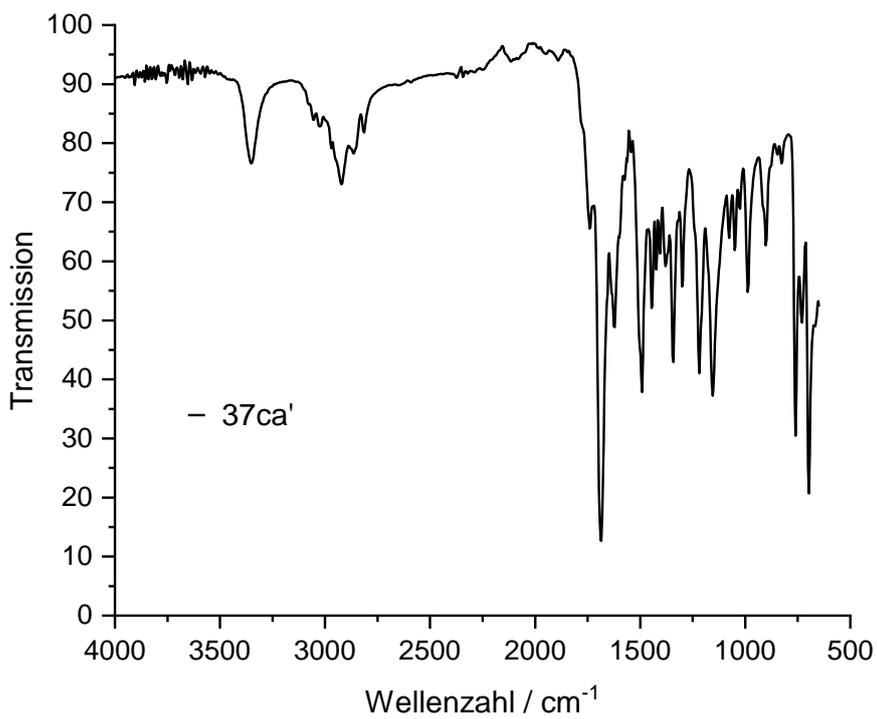


Abbildung A 112: IR-Spektrum von 3-Phenyl-2-methylaminocyclopent-2-enon **37ca'**.

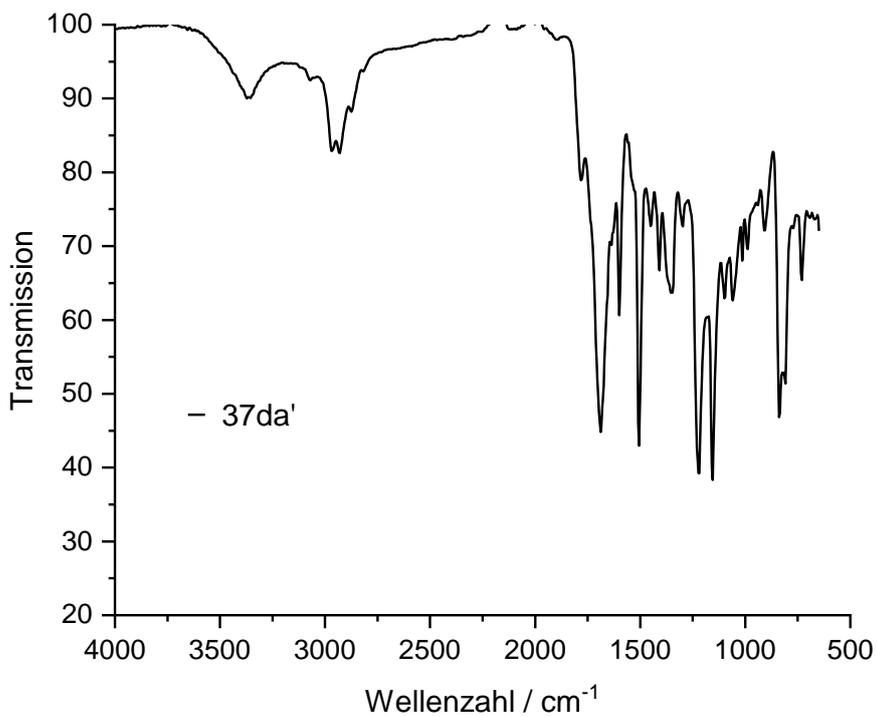


Abbildung A 113: IR-Spektrum von 3-(4-Fluorphenyl)-2-methylaminocyclopent-2-enon **37da'**.

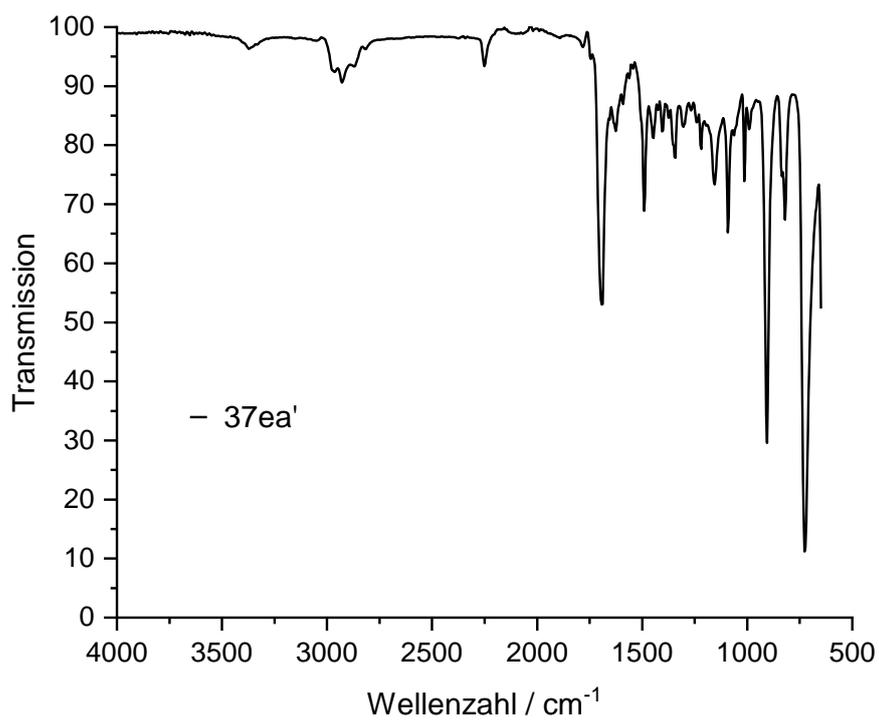


Abbildung A 114: IR-Spektrum von 3-(4-Chlorphenyl)-2-methylaminocyclopent-2-enon **37ea'**.

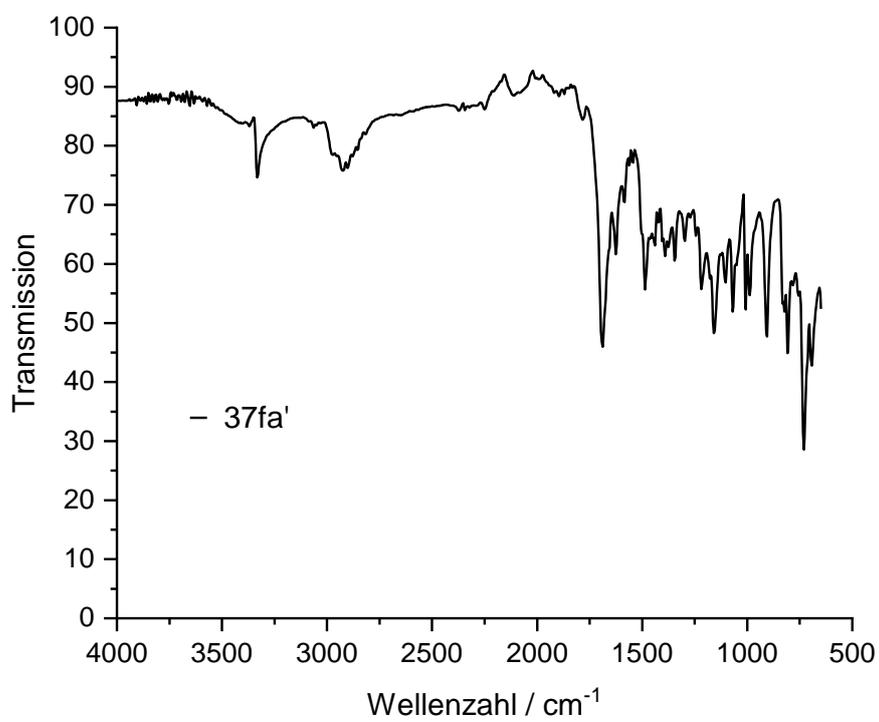


Abbildung A 115: IR-Spektrum von 3-(4-Bromphenyl)-2-methylaminocyclopent-2-enon **37fa'**.

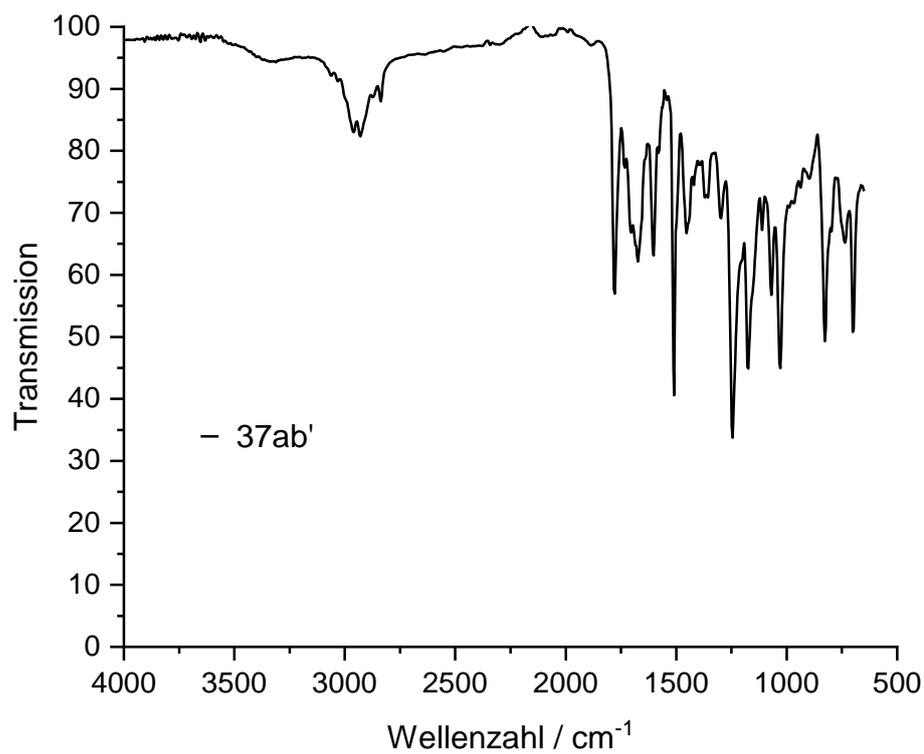


Abbildung A 116: IR-Spektrum von 3-(4-Methoxyphenyl)-2-benzylaminocyclopent-2-enon **37ab'**.

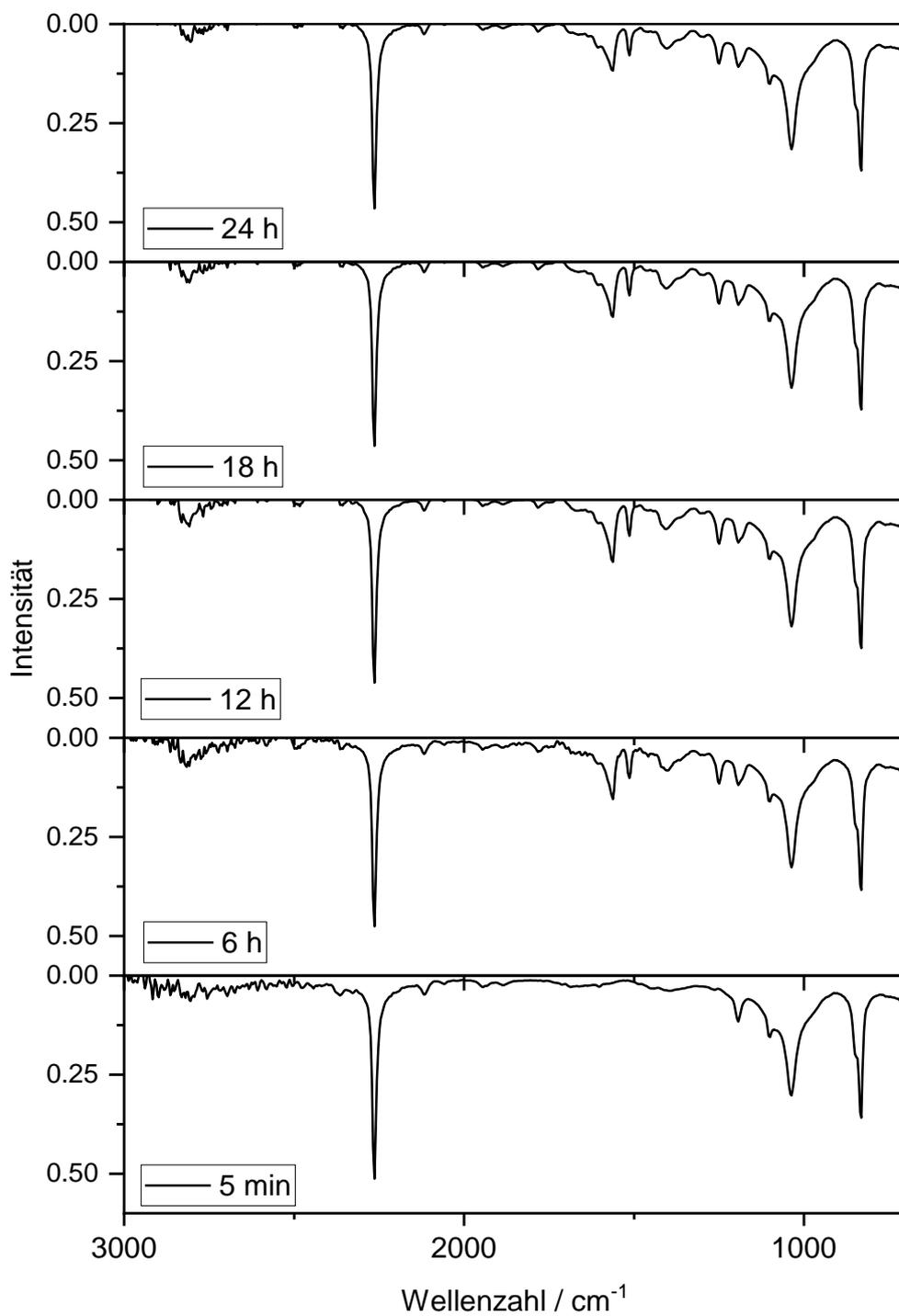


Abbildung A 117: Ausgewählte IR-Spektren des Kinetikexperiments mit Cyclobutanon **32a** in Acetonitril-D3 zu angegebenen Zeitpunkten.

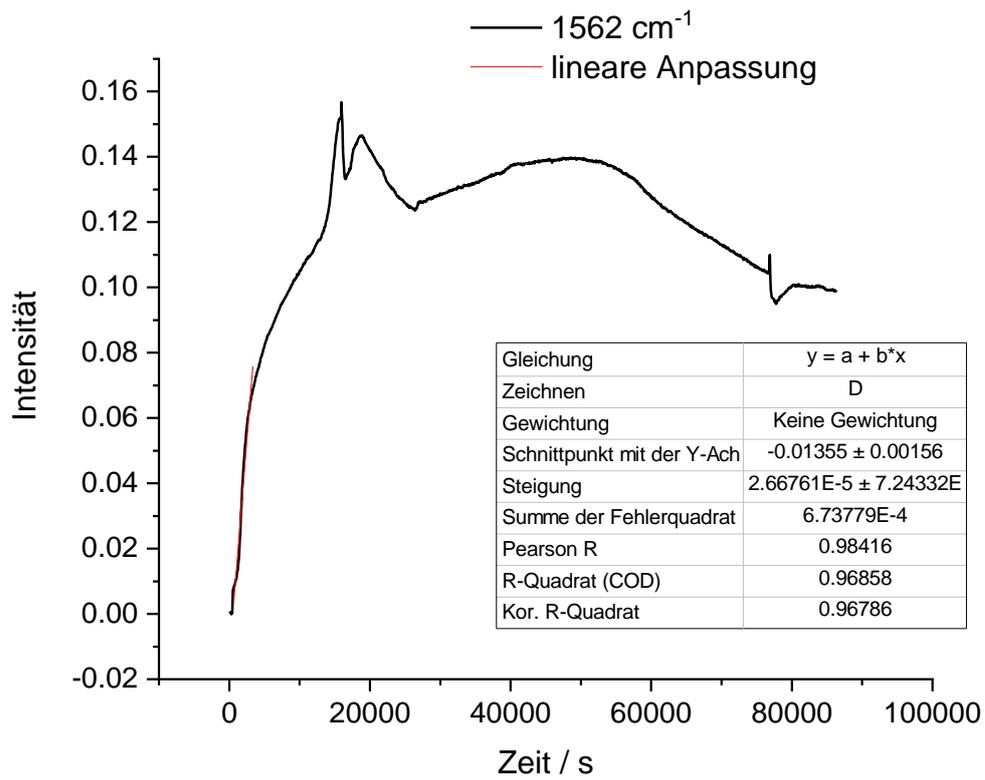


Abbildung A 118: Auftragung der zeitlichen Veränderung der Intensität der Schwingungsbande bei  $1562 \text{ cm}^{-1}$  des IR-spektroskopischen Kinetikexperiments 1 mit Cyclobutanon **32e** in Acetonitril-D<sub>3</sub> mit linearer Anpassung des Anfangsbereichs (rote Linie).

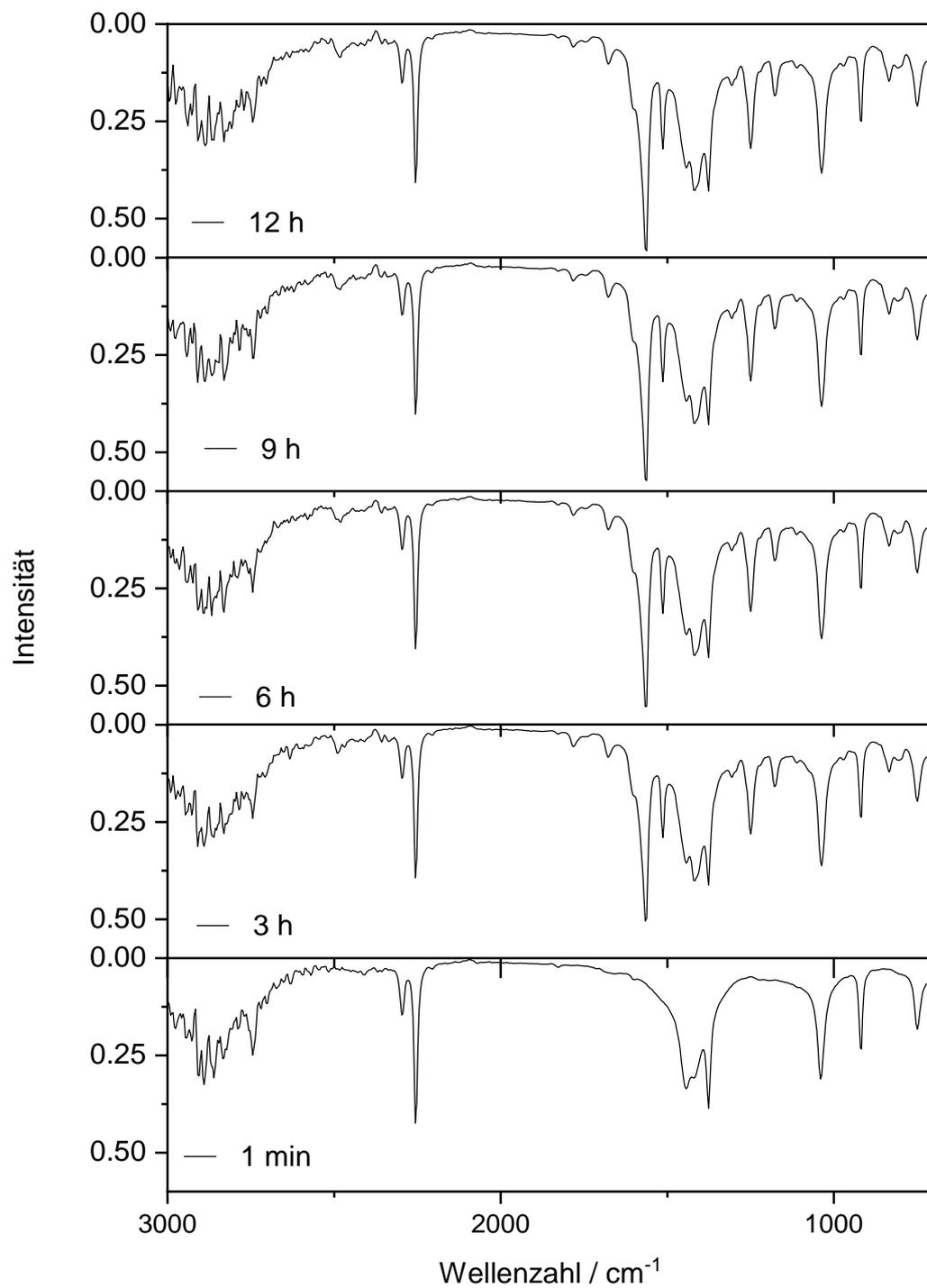


Abbildung A 119: Ausgewählte IR-Spektren des Kinetikexperiments mit Cyclobutanon **32a** in Acetonitril zu angegebenen Zeitpunkten.

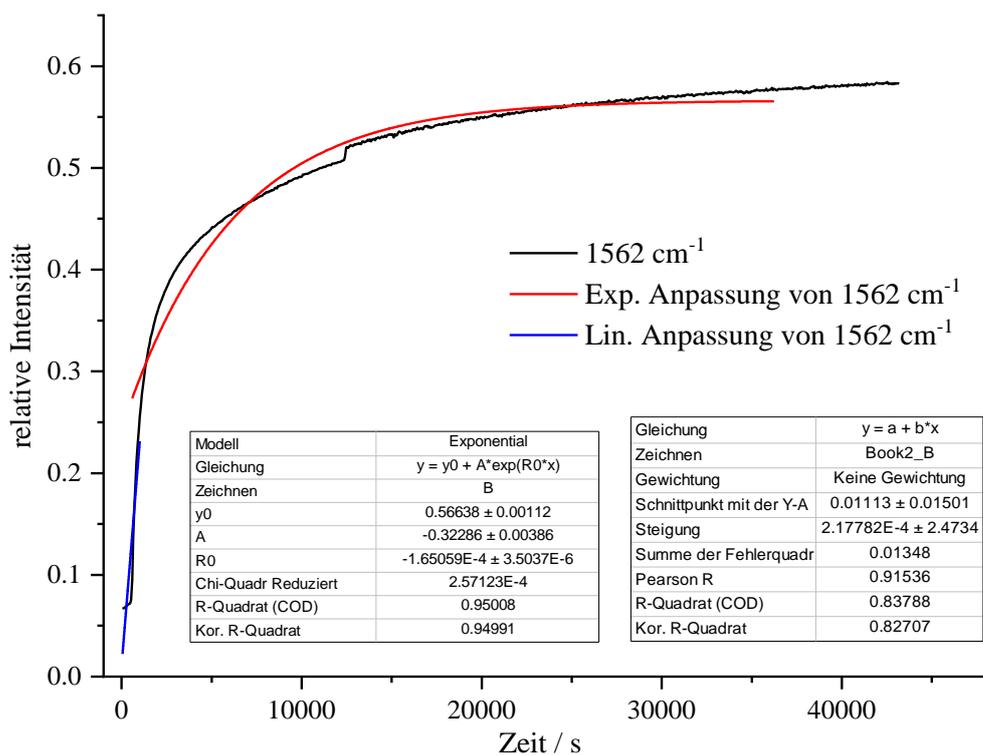


Abbildung A 120: Auftragung der zeitlichen Veränderung der Intensität der Schwingungsbande bei  $1562 \text{ cm}^{-1}$  des IR-spektroskopischen Kinetikexperiment 2 mit Cyclobutanon **32e** in Acetonitril mit linearer Anpassung des Anfangsbereichs (rote Linie).

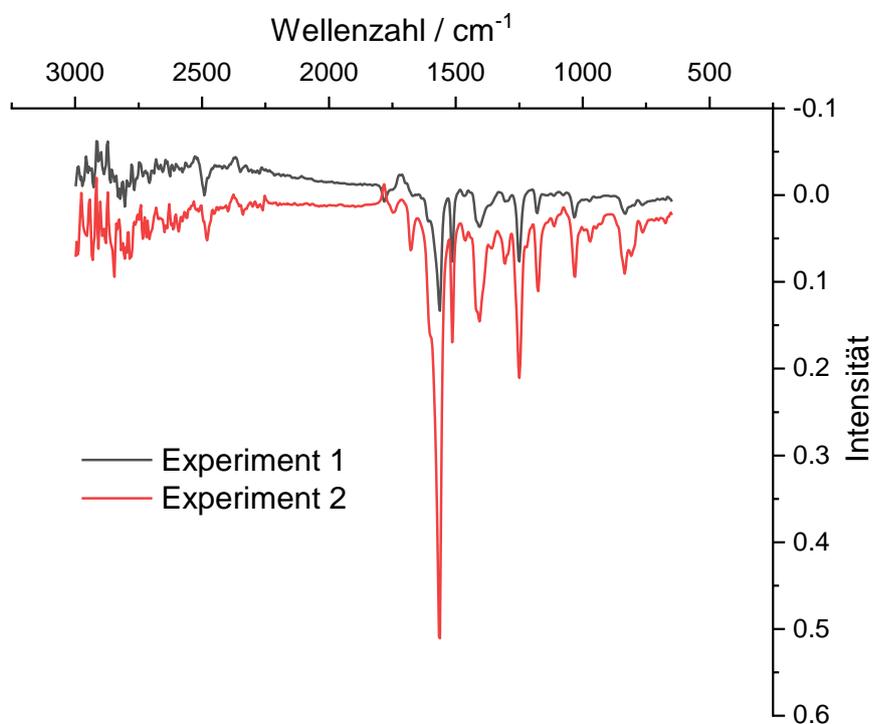


Abbildung A 121: Vergleich der Veränderungsspektren aus den kinetischen, IR-spektroskopischen Experimenten 1 (Acetonitril-D<sub>3</sub>) und 2 (Acetonitril) nach jeweils 10 h Reaktionszeit.

## EPR-Spektren:

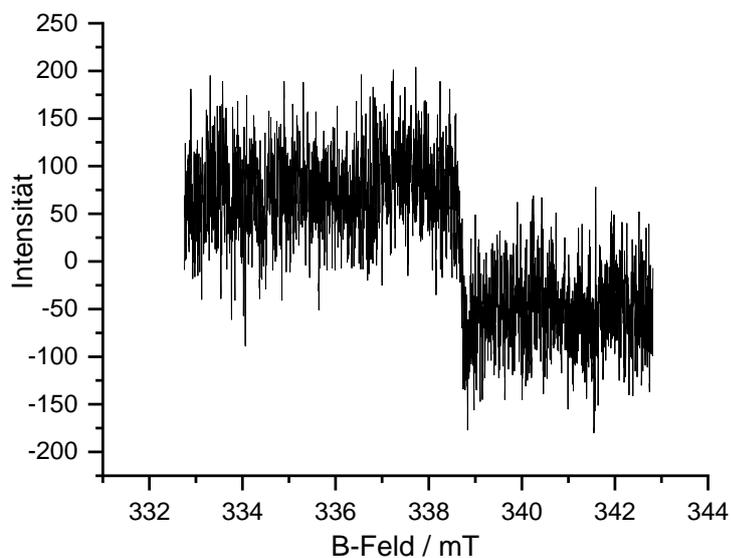


Abbildung A 122: EPR-Spektrum der Reaktionslösung 3,4,5-Trimethylthiazoliumiodid **36a**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in THF nach 10 min (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

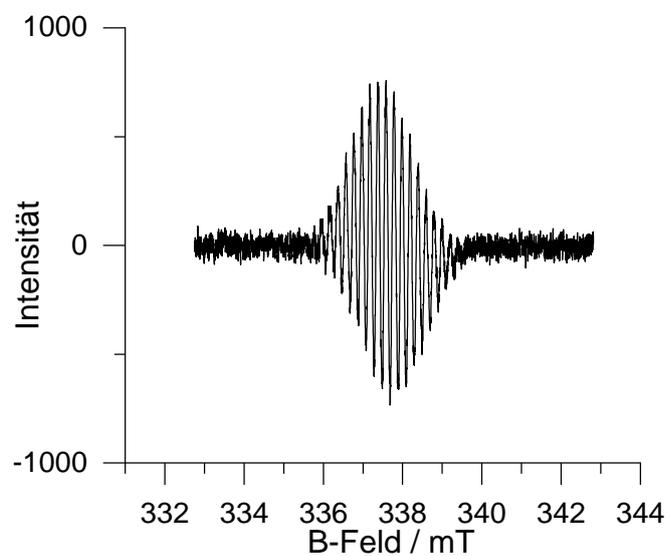


Abbildung A 123: EPR-Spektrum der Reaktionslösung 3,4,5-Trimethylthiazoliumiodid **36a**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in ACN nach 10 min (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

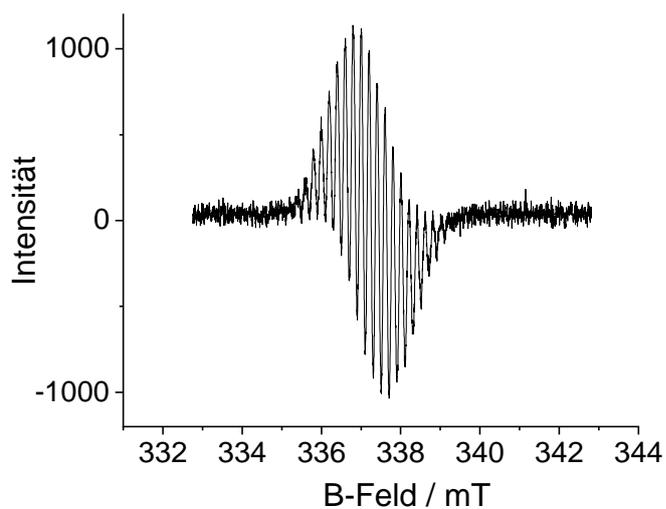


Abbildung A 124: EPR-Spektrum der Reaktionslösung 3,4,5-Trimethylthiazoliumiodid **36a**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in DCM nach 10 min (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

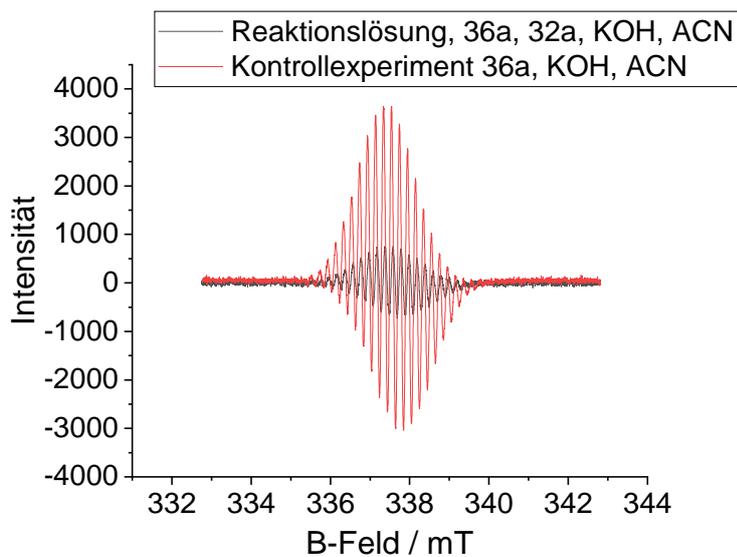


Abbildung A 125: Vergleich der EPR-Spektren der Reaktionslösung 3,4,5-Trimethylthiazoliumiodid **36a**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in ACN nach 10 min (schwarz) und des Kontrollexperimentes mit 3,4,5-Trimethylthiazoliumiodid und KOH in ACN (rot), Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT.

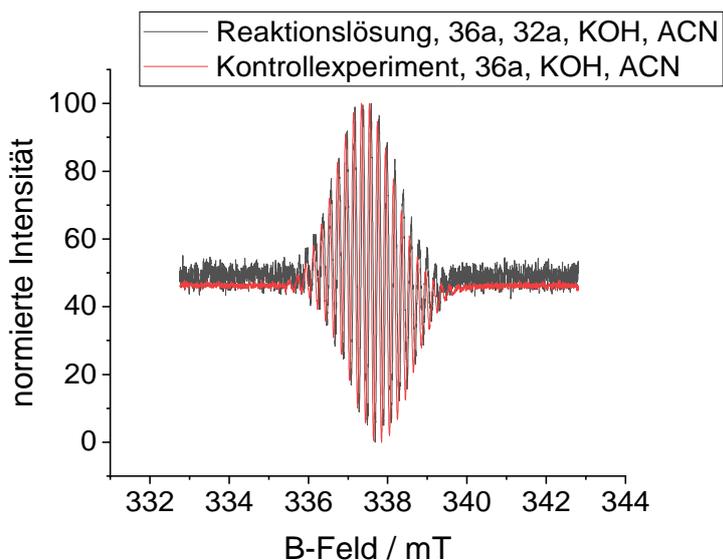


Abbildung A 126: Vergleich der EPR-Spektren der Reaktionslösung 3,4,5-Trimethylthiazoliumiodid **36a**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in ACN nach 10 min (schwarz) und des Kontrollexperiments mit 3,4,5-Trimethylthiazoliumiodid und KOH in ACN (rot) mit normierten Intensitäten (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

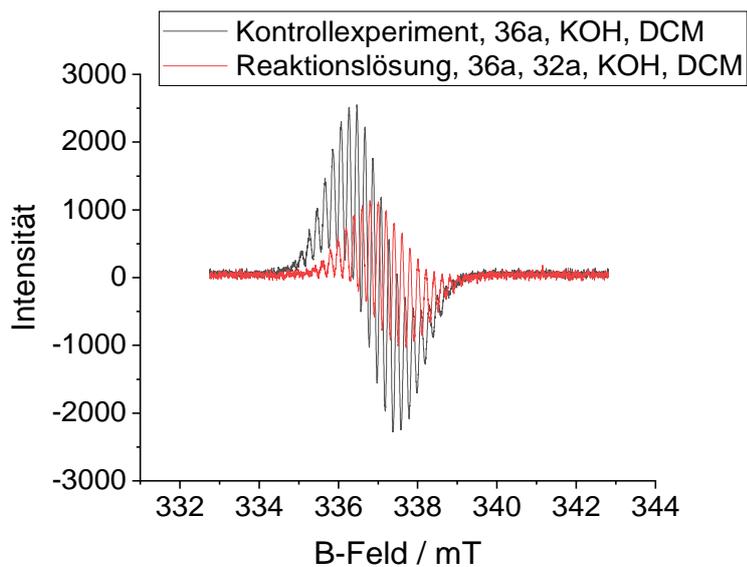


Abbildung A 127: Vergleich der EPR-Spektren der Reaktionslösung 3,4,5-Trimethylthiazoliumiodid **36a**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in DCM nach 10 min (rot) und des Kontrollexperiments mit 3,4,5-Trimethylthiazoliumiodid und KOH in DCM (schwarz), Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT.

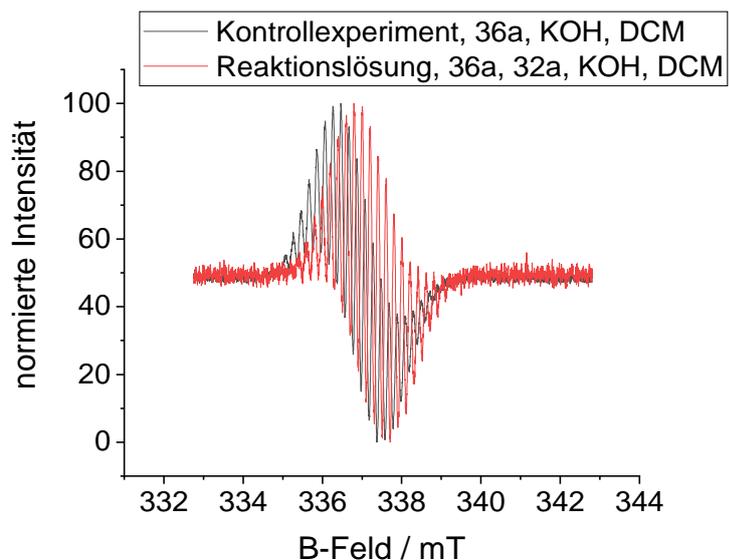


Abbildung A 128: Vergleich der EPR-Spektren der Reaktionslösung 3,4,5-Trimethylthiazoliumiodid **36a**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in DCM nach 10 min (rot) und des Kontrollexperiments mit 3,4,5-Trimethylthiazoliumiodid und KOH in DCM (schwarz) mit normierten Intensitäten (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

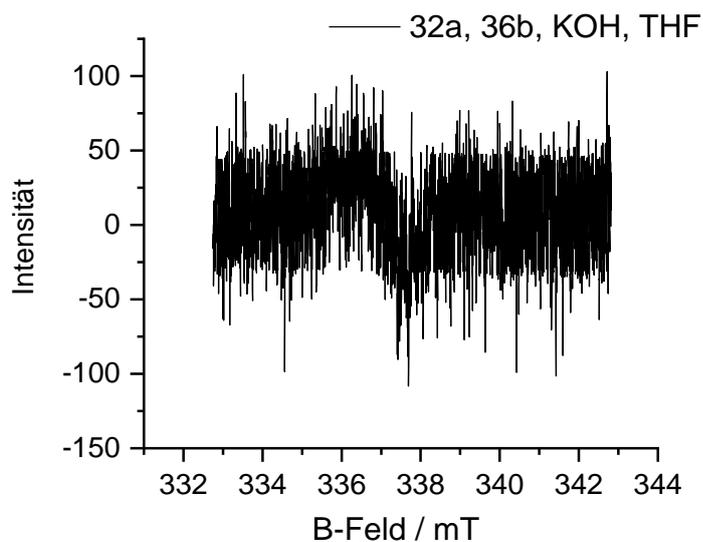


Abbildung A 129: EPR-Spektrum der Reaktionslösung 3-Benzyl-4,5-dimethylthiazoliumbromid **36b**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in THF nach 10 min (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

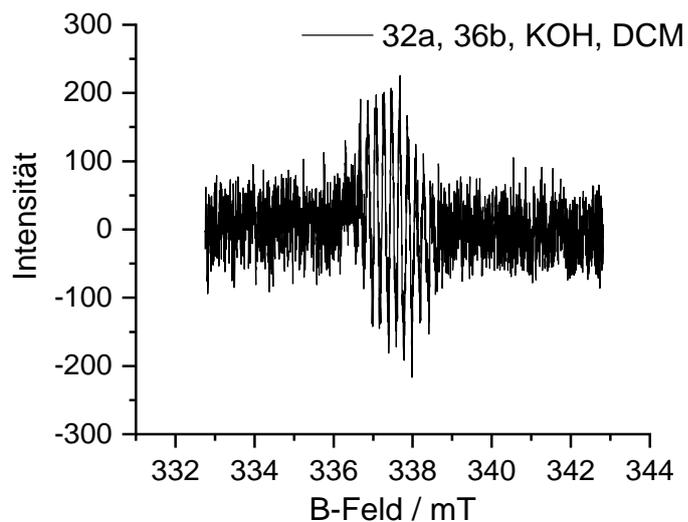


Abbildung A 130: EPR-Spektrum der Reaktionslösung 3-Benzyl-4,5-dimethylthiazoliumbromid **36b**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in DCM nach 10 min (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

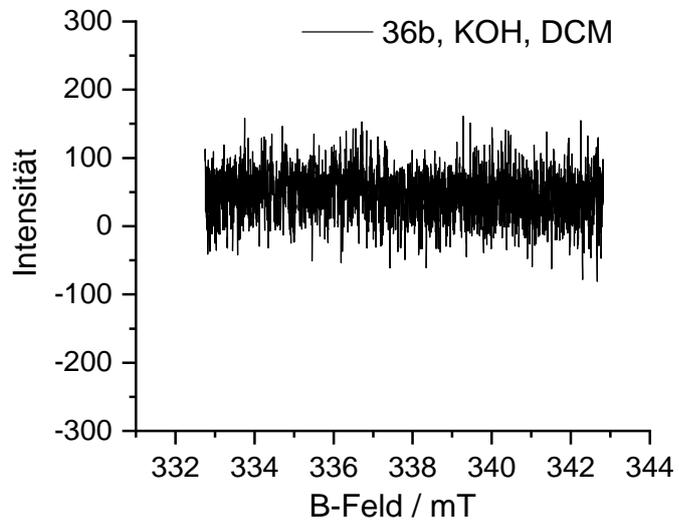


Abbildung A 131: EPR-Spektrum des Kontrollversuchs 3-Benzyl-4,5-dimethylthiazoliumbromid **36b** und KOH in THF (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

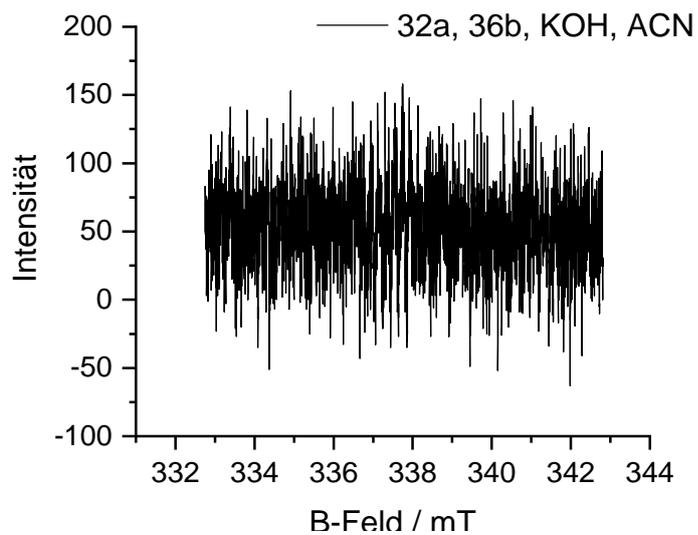


Abbildung A 132: EPR-Spektrum der Reaktionslösung 3-Benzyl-4,5-dimethylthiazoliumbromid **36b**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in ACN nach 10 min (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

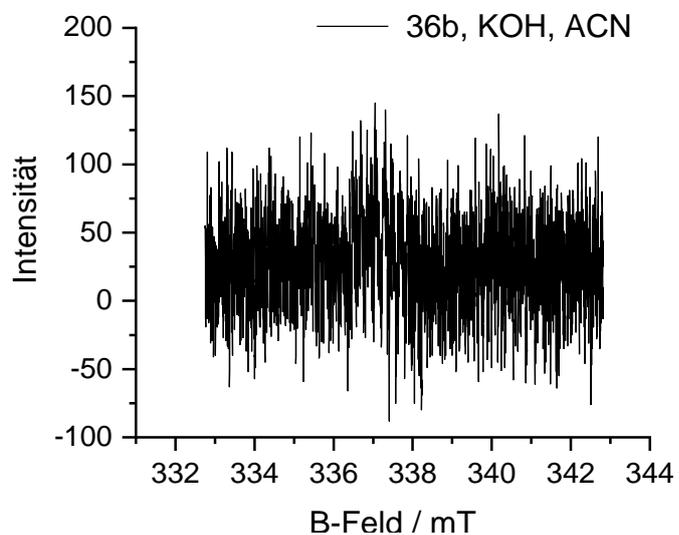


Abbildung A 133: EPR-Spektrum des Kontrollexperiments 3-Benzyl-4,5-dimethylthiazoliumbromid **36b** und KOH in ACN (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

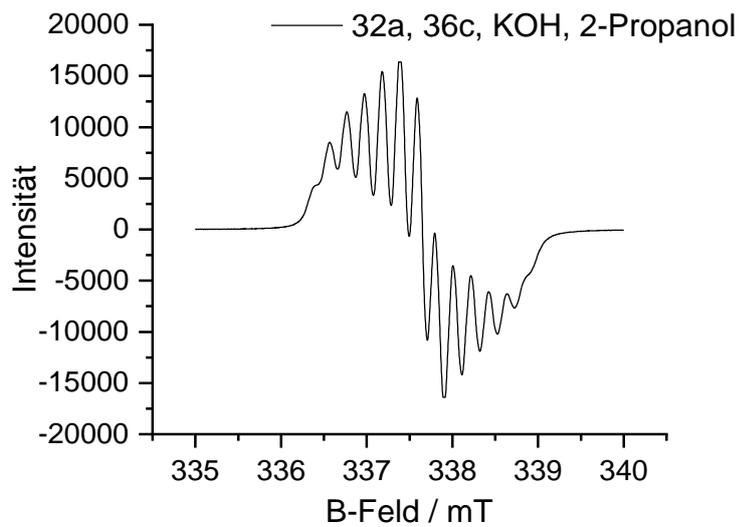


Abbildung A 134: EPR-Spektrum der Reaktionslösung 3-Mesityl-4,5-cycloheptanthiazoliumperchlorat **36c**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in 2-Propanol nach 10 min (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

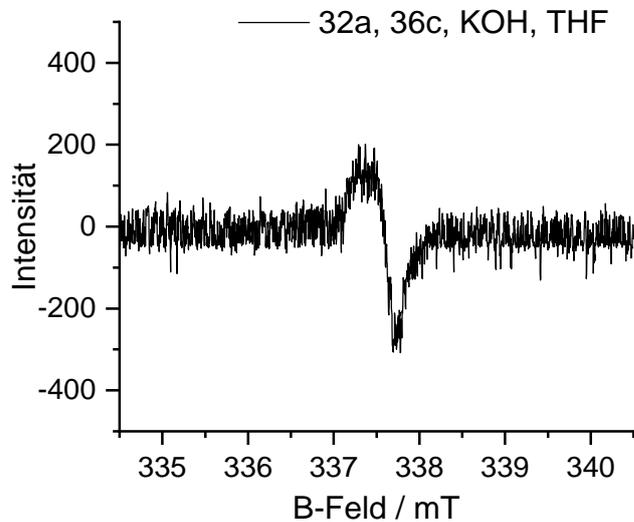


Abbildung A 135: EPR-Spektrum der Reaktionslösung 3-Mesityl-4,5-cycloheptanthiazoliumperchlorat **36c**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in THF nach 10 min (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

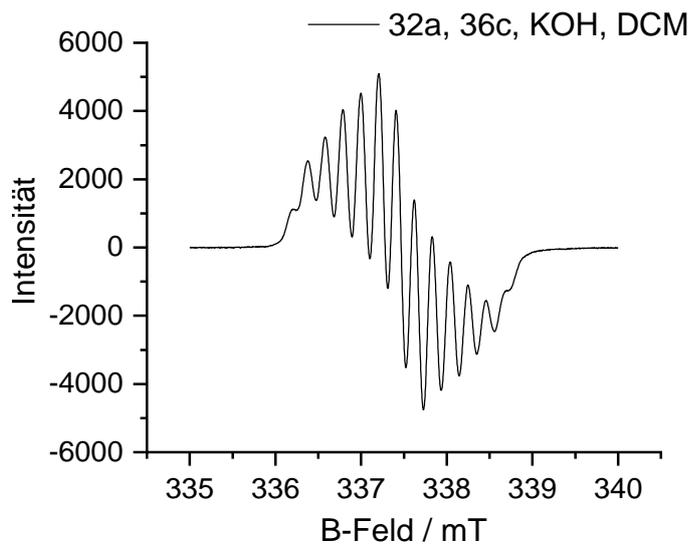


Abbildung A 136: EPR-Spektrum der Reaktionslösung 3-Mesityl-4,5-cycloheptanthiazoliumperchlorat **36c**, KOH und 2-(4-Methoxyphenyl)cyclobutanon **32a** in DCM nach 10 min (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

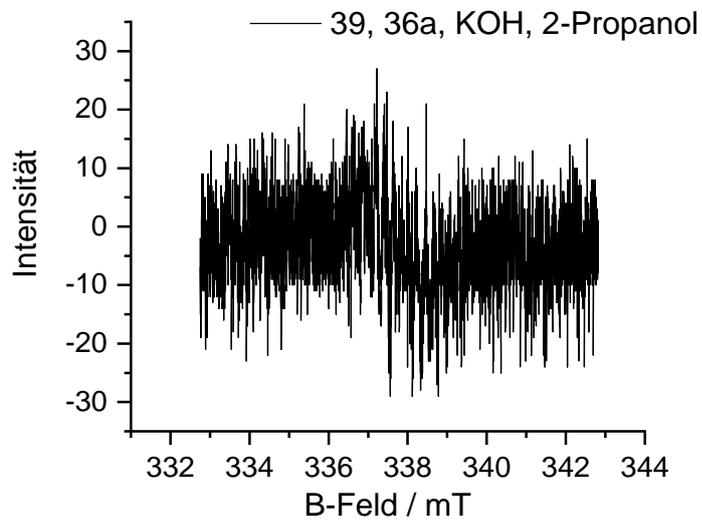


Abbildung A 137: EPR-Spektrum der Reaktionslösung 3,4,5-Trimethylthiazoliumiodid **36a**, KOH und 2-(4-Methoxyphenyl)cyclopentanon **32a** in 2-Propanol nach 10 min (Mikrowellenstärke: 10 mW, Messzeit= 30 s, Messbereich = 10.064 mT).

## Computerchemische Strukturen:

Zur Unterscheidung der computerchemisch als Minima bestimmten Isomere der Strukturen **40**, **41** und **42** sowie **46**, **22** und **23** wurden zwei Diederwinkel definiert (Abbildung A 138).

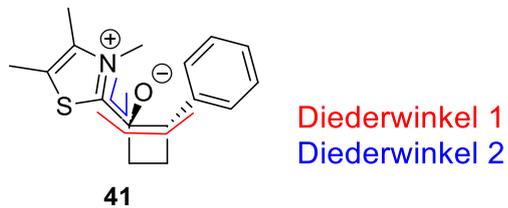
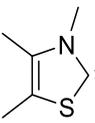
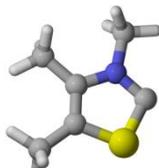


Abbildung A 138: Struktur **41** mit Diederwinkel 1 (rot) und Diederwinkel 2 (blau).

Die Strukturen wurden nach folgendem Schema benannt: **structure-dihedral 1-dihedral 2**. Ein Diederwinkel von annähernd  $0^\circ$  wurde mit *syn* bezeichnet, ein Diederwinkel von annähernd  $180^\circ$  mit *anti*.

## C-C-Info Phenyl

#M062X/6-311+G**	(20)
------------------	------

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

17

XYZ file generated by gabedit : coordinates in Angstrom

H	1.5009070000	2.2434890000	0.8605480000
H	2.8936980000	0.2635200000	0.9101580000
C	0.8502340000	2.0822590000	-0.0026180000
C	-2.2592180000	1.1949510000	0.0012100000
H	1.4406100000	2.2631010000	-0.9047440000
C	0.2681080000	0.7045740000	0.0014540000
C	-1.0319190000	0.3400390000	0.0023890000
H	0.0579610000	2.8279720000	0.0331680000
C	2.5718970000	-0.2510670000	0.0028480000
N	1.1197740000	-0.4197380000	-0.0016600000
S	-1.1137780000	-1.4062450000	-0.0003450000
C	0.5901160000	-1.6512960000	-0.0027990000
H	3.0084710000	-1.2450070000	-0.0290390000
H	2.8920290000	0.3211240000	-0.8697000000
H	-2.0032660000	2.2548160000	0.0143040000
H	-2.8794310000	0.9867920000	0.8757900000
H	-2.8642560000	1.0055240000	-0.8882500000

Zero-point correction=  
(Hartree/Particle)

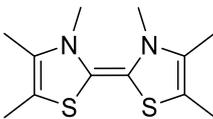
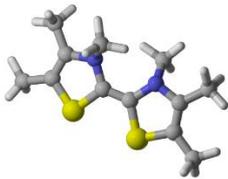
0.139288

Thermal correction to Energy=	0.148315
Thermal correction to Enthalpy=	0.149260
Thermal correction to Gibbs Free Energy=	0.104713
Sum of electronic and zero-point Energies=	-686.747420
Sum of electronic and thermal Energies=	-686.738392
Sum of electronic and thermal Enthalpies=	-686.737448
Sum of electronic and thermal Free Energies=	-686.781994

	E (Thermal) KCal/Mol	CV cal/Mol-Kelvin	S cal/Mol-kelvin
Total	93.069	31.772	93.756

#M062X/6-311+G\*\*

(Bis-20a)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

34

XYZ file generated by gabedit : coordinates in Angstrom

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H	3.5373890000	2.5263440000	0.6906570000
H	-5.2587790000	-0.7128160000	-0.2548420000
H	1.4069390000	1.4655220000	-2.1965490000
C	1.1696050000	1.9016520000	-1.2182190000
C	-4.4160020000	-1.4021170000	-0.2953660000
H	0.1042850000	2.1278180000	-1.1853710000
H	-4.8406150000	1.3856780000	-0.3372230000
C	3.8660870000	1.7396570000	0.0065100000
H	-3.5367260000	2.5269380000	-0.6900240000
H	4.8409550000	1.3853270000	0.3357810000
H	-4.5584660000	-2.1537600000	0.4858790000
H	3.9873020000	2.1849940000	-0.9849440000
C	-3.8660560000	1.7397640000	-0.0067550000
C	-3.1201070000	-0.6857580000	-0.0990730000
N	1.4992730000	0.9754510000	-0.1295860000
C	2.8680770000	0.6241040000	-0.0077970000
C	-2.8680410000	0.6241930000	0.0075890000
S	-1.6366060000	-1.6620420000	-0.0232350000
H	-3.9881810000	2.1843480000	0.9849220000
H	-1.7293760000	2.8273070000	1.0898800000
N	-1.4991810000	0.9755720000	0.1294310000
C	0.6707580000	-0.1716270000	-0.0391670000
C	-0.6707600000	-0.1716050000	0.0387660000
H	5.2588430000	-0.7129840000	0.2544940000
C	3.1201590000	-0.6858390000	0.0989560000
C	-1.1696540000	1.9007290000	1.2190490000
H	4.4390770000	-1.9186770000	1.2586670000
C	4.4160260000	-1.4022190000	0.2953130000
H	-1.4058620000	1.4630720000	2.1969780000
H	-0.1045540000	2.1279560000	1.1858200000
S	1.6365320000	-1.6620450000	0.0232240000
H	4.5583700000	-2.1541380000	-0.4856810000

Zero-point correction= 0.282748

(Hartree/Particle)

Thermal correction to Energy= 0.301316

Thermal correction to Enthalpy= 0.302260

Thermal correction to Gibbs Free Energy= 0.236848

Sum of electronic and zero-point Energies= -1373.549538

Sum of electronic and thermal Energies= -1373.530970

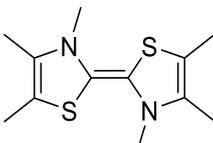
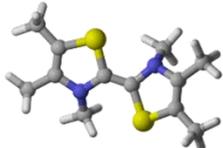
Sum of electronic and thermal Enthalpies= -1373.530026

Sum of electronic and thermal Free Energies= -1373.595438

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-kelvin
Total	189.079	67.971	137.671

#M062X/6-311+G\*\*

(Bis-20b)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

34

XYZ file generated by gabedit : coordinates in Angstrom

H	-2.3100460000	-2.7428110000	-1.0721400000
H	4.1037910000	-1.8095120000	1.8057710000
H	-3.7542940000	-2.4135670000	0.8473520000
H	5.1008760000	-0.6144250000	0.9595800000
H	-0.9939250000	-1.8733480000	-1.8939660000
C	-1.3792610000	-2.2008110000	-0.9215820000
C	4.2742020000	-1.3151480000	0.8458070000
H	-0.6615870000	-2.8877300000	-0.4730350000
H	4.6412770000	1.4932260000	0.9580820000
C	-4.0492430000	-1.5622900000	0.2290390000
H	3.2818060000	2.6262810000	0.9266100000
H	-4.9305270000	-1.1079100000	0.6772770000
H	4.5799690000	-2.0822390000	0.1287050000
H	-4.3352630000	-1.9411860000	-0.7558470000
C	3.7721440000	1.8133510000	0.3858850000
C	3.0408800000	-0.6202150000	0.3690950000
N	-1.6202350000	-1.0457640000	-0.0629850000
C	-2.9320550000	-0.5683700000	0.1472140000
C	2.8081470000	0.6847890000	0.1868660000
S	1.6259770000	-1.6250770000	-0.0375760000
H	4.1275720000	2.2106540000	-0.5692410000
H	1.9922190000	2.6899450000	-1.4371170000
N	1.4994010000	1.0193440000	-0.2613890000
C	-0.6688690000	-0.0163670000	-0.0512490000
C	0.6615750000	-0.1290830000	-0.1909500000
H	-5.1400260000	1.0111420000	0.6037320000
C	-3.0324490000	0.7589630000	0.3025320000
C	1.4763220000	1.7349970000	-1.5454170000
H	-4.1320620000	2.0918470000	1.5772460000
C	-4.2264040000	1.6048580000	0.6026460000
H	1.9558250000	1.1496620000	-2.3410810000
H	0.4426880000	1.9404220000	-1.8215630000
S	-1.4542410000	1.5592160000	0.1713750000
H	-4.3401560000	2.3902160000	-0.1498540000

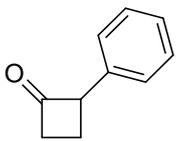
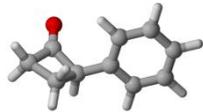
Zero-point correction= 0.282878  
(Hartree/Particle)

Thermal correction to Energy=	0.301587
Thermal correction to Enthalpy=	0.302531
Thermal correction to Gibbs Free Energy=	0.236431
Sum of electronic and zero-point Energies=	-1373.547228
Sum of electronic and thermal Energies=	-1373.528519
Sum of electronic and thermal Enthalpies=	-1373.527575
Sum of electronic and thermal Free Energies=	-1373.593676

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.249	68.021	139.120

#M062X/6-311+G\*\*

(32)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

21

XYZ file generated by gabedit : coordinates in Angstrom

```

O      -2.0110050000      1.4437400000      -1.1332590000
H       1.1518120000      -2.0967320000      -1.0685070000
H      -1.1506300000      -1.4749560000      -0.9692000000
H       3.5390430000      -1.5194330000      -0.8099570000
C       1.4333730000      -1.1681050000      -0.5828900000
C      -2.0518540000       0.4191820000      -0.5250090000
C       2.7782850000      -0.8432410000      -0.4379370000
C      -1.0103900000      -0.6754790000      -0.2338960000
C       0.4383010000      -0.3122450000      -0.1118080000
H      -3.7658740000      -0.8370800000      -0.0835840000
C       3.1435500000       0.3481930000       0.1781380000
H       4.1901690000       0.6053790000       0.2887860000
C       0.8156930000       0.8853100000       0.5001870000
C      -3.0576030000      -0.1948190000       0.4451030000
C       2.1577330000       1.2130100000       0.6451000000
H       0.0539810000       1.5742680000       0.8507410000
H       2.4354990000       2.1482180000       1.1166960000
C      -1.8627370000      -0.9902000000       1.0376020000
H      -3.6011260000       0.4999450000       1.0844120000
H      -2.0289150000      -2.0431690000       1.2551980000
H      -1.4420230000      -0.4959930000       1.9139460000

```

Zero-point correction=  
(Hartree/Particle)

0.173354

Thermal correction to Energy=

0.182544

Thermal correction to Enthalpy=

0.183488

Thermal correction to Gibbs Free Energy=

0.137762

Sum of electronic and zero-point Energies=

-462.028157

Sum of electronic and thermal Energies=

-462.018967

Sum of electronic and thermal Enthalpies=

-462.018022

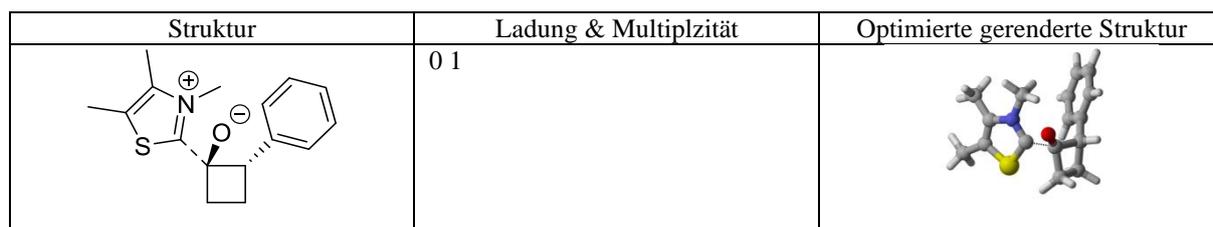
Sum of electronic and thermal Free Energies=

-462.063749

Total	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
	114.548	35.362	96.239

#M062X/6-311+G\*\*

(40-syn-syn)



38

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.5280280000	-3.4730670000	-0.1327600000
H	0.5590650000	-1.9647730000	-1.8507080000
H	-0.5395040000	1.5337260000	2.5512910000
H	1.0831750000	-3.9975980000	0.4008040000
C	0.5067880000	-3.1586720000	0.0022550000
C	1.2465040000	-2.4623460000	-1.1670800000
H	2.8252510000	-1.9520380000	0.2217990000
C	-0.0125740000	1.0807410000	1.7126850000
H	1.9290080000	-3.0806850000	-1.7485050000
H	0.5269480000	1.8450210000	1.1476330000
N	-0.9864490000	0.4222450000	0.8297860000
C	1.9105520000	-1.4896110000	-0.1662150000
C	0.8151650000	-1.9236490000	0.8889850000
C	-0.7107660000	-0.7379490000	0.2475900000
H	-4.6406170000	1.5545680000	-0.6734330000
H	0.6727420000	0.3212490000	2.0814960000
C	-2.5587680000	2.3575740000	1.1154500000
C	-2.2103630000	1.0369140000	0.5091700000
S	-2.0437760000	-1.1537440000	-0.7439700000
C	-2.9371050000	0.2942670000	-0.3561380000
H	0.7261090000	0.1696870000	-2.0275500000
C	-4.2918960000	0.5555430000	-0.9339070000
H	-4.2736680000	0.4786280000	-2.0227440000
O	0.8621290000	-1.8218700000	2.1102280000
C	2.1698090000	-0.0449140000	-0.4449260000
C	1.4491570000	0.6783780000	-1.3999670000
H	3.6684200000	0.0975600000	1.0837290000
H	-5.0219060000	-0.1648760000	-0.5581210000
C	3.1015630000	0.6454520000	0.3379700000
C	1.6409240000	2.0479070000	-1.5553490000
H	1.0742870000	2.5873020000	-2.3061370000
C	3.2959050000	2.0140380000	0.1869800000
C	2.5619970000	2.7238460000	-0.7594420000
H	4.0221450000	2.5267880000	0.8071990000
H	2.7149750000	3.7894330000	-0.8842490000
H	-1.7592340000	3.0838110000	0.9530060000
H	-2.7213790000	2.2692500000	2.1926160000
H	-3.4706170000	2.7500370000	0.6694890000

Zero-point correction=  
(Hartree/Particle)

0.315879

Thermal correction to Energy=

0.333624

Thermal correction to Enthalpy=

0.334569

Thermal correction to Gibbs Free Energy=

0.270362

Sum of electronic and zero-point Energies=

-1148.780095

Sum of electronic and thermal Energies=

-1148.762350

Sum of electronic and thermal Enthalpies=

-1148.761406

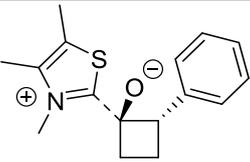
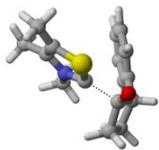
Sum of electronic and thermal Free Energies=

-1148.825612

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	209.352	69.420	135.134

#M062X/6-311+G\*\*

(40-syn-anti)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.2557020000	-2.7350580000	1.9260870000
H	-2.2240080000	-1.2095260000	1.9941290000
H	-0.4626840000	1.7812320000	1.3598280000
H	-1.1660390000	-3.8746820000	0.9074300000
C	-0.9711070000	-2.8197690000	1.1079790000
C	-2.2594320000	-1.9653620000	1.2079860000
H	-2.6172730000	-1.9367780000	-0.9524830000
C	-0.0082100000	0.9062660000	1.8302120000
H	-3.1852500000	-2.5263520000	1.3332560000
H	0.4795970000	1.1879570000	2.7630860000
N	0.9715150000	0.3100200000	0.9228120000
C	-2.0205980000	-1.3915170000	-0.2133030000
C	-0.6200030000	-2.1159090000	-0.2402630000
C	0.7011700000	-0.7856920000	0.2159860000
H	4.3321270000	0.5074740000	-1.8255220000
H	-0.7781730000	0.1689370000	2.0270880000
C	2.5657580000	2.1807850000	1.4293530000
C	2.2110890000	0.9279060000	0.6948810000
S	2.0387650000	-1.1309020000	-0.7935960000
C	2.9361640000	0.2433020000	-0.2207010000
H	-3.6629300000	0.4062840000	1.0301210000
C	4.3125040000	0.5306200000	-0.7345230000
H	4.6564500000	1.5133230000	-0.4126650000
O	-0.1250390000	-2.6661930000	-1.2376420000
C	-2.1475580000	0.0826380000	-0.4573820000
C	-3.0295270000	0.8724420000	0.2819960000
H	-0.6899550000	0.0842790000	-2.0299410000
H	5.0260010000	-0.2128410000	-0.3717900000
C	-1.3573860000	0.6992300000	-1.4334010000
C	-3.1014160000	2.2485240000	0.0780510000
H	-3.7938660000	2.8449610000	0.6614190000
C	-1.4164210000	2.0740130000	-1.6298110000
C	-2.2851370000	2.8566990000	-0.8693700000
H	-0.7898280000	2.5366810000	-2.3841000000
H	-2.3340810000	3.9277940000	-1.0267040000
H	2.6862410000	1.9977460000	2.5004900000
H	1.7950970000	2.9444950000	1.3005040000
H	3.5043900000	2.5828430000	1.0526090000

Zero-point correction=  
(Hartree/Particle)

0.315506

Thermal correction to Energy=

0.333492

Thermal correction to Enthalpy=

0.334436

Thermal correction to Gibbs Free Energy=

0.269097

Sum of electronic and zero-point Energies=

-1148.771364

Sum of electronic and thermal Energies=

-1148.753378

Sum of electronic and thermal Enthalpies=

-1148.752434

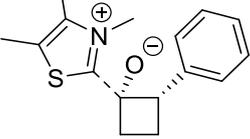
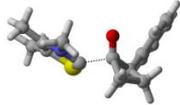
Sum of electronic and thermal Free Energies=

-1148.817773

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	209.269	69.507	137.518

#M062X/6-311+G\*\*

(40-anti-syn)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	0.098660000	2.879345000	-1.797957000
H	-2.348778000	2.527419000	-2.225866000
H	3.601714000	2.236167000	0.925947000
H	-0.440023000	3.802017000	-0.351717000
C	-0.533283000	2.869357000	-0.909227000
C	-1.962971000	2.355234000	-1.221187000
H	-1.098258000	0.465023000	-1.816453000
C	2.541241000	1.987202000	0.938192000
H	-2.685299000	2.710807000	-0.485117000
H	2.171888000	1.881691000	1.958559000
N	2.323567000	0.734508000	0.209747000
C	-1.514722000	0.900721000	-0.904232000
C	-0.374611000	1.583018000	-0.063673000
C	1.258291000	0.590375000	-0.572370000
H	2.558283000	-3.576990000	0.030212000
H	1.968045000	2.767200000	0.445802000
C	4.337923000	-0.284104000	1.301212000
C	3.144336000	-0.387142000	0.407709000
S	1.248823000	-1.020709000	-1.146679000
C	2.700747000	-1.461848000	-0.283845000
H	-2.207872000	-1.575302000	-1.744104000
C	3.265968000	-2.844438000	-0.363612000
H	3.490987000	-3.115429000	-1.397263000
O	-0.321336000	1.579516000	1.173308000
C	-2.431019000	-0.067776000	-0.232906000
C	-2.682767000	-1.317631000	-0.802252000
H	-2.824025000	1.197330000	1.456256000
H	4.188725000	-2.921915000	0.210859000
C	-3.042076000	0.246251000	0.985119000
C	-3.534357000	-2.229235000	-0.186201000
H	-3.721473000	-3.191946000	-0.648248000
C	-3.893627000	-0.662102000	1.602015000
C	-4.145710000	-1.901423000	1.018399000
H	-4.359023000	-0.405356000	2.546792000
H	-4.812009000	-2.606583000	1.501581000
H	4.052817000	0.078010000	2.291521000
H	5.083455000	0.402343000	0.891447000
H	4.806539000	-1.258925000	1.421065000

Zero-point correction=  
(Hartree/Particle)

0.315071

Thermal correction to Energy=

0.333442

Thermal correction to Enthalpy=

0.334386

Thermal correction to Gibbs Free Energy=

0.267209

Sum of electronic and zero-point Energies=

-1148.769927

Sum of electronic and thermal Energies=

-1148.751556

Sum of electronic and thermal Enthalpies=

-1148.750612

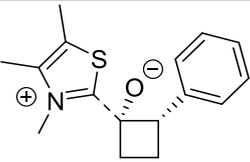
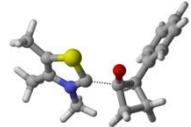
Sum of electronic and thermal Free Energies=

-1148.817789

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	209.238	69.916	141.386

#M062X/6-311+G\*\*

(40-anti-anti)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.2299410000	3.2036010000	-0.1240870000
H	2.0606960000	3.2184570000	0.9137850000
H	-1.8146090000	0.9492950000	2.7369220000
H	0.6250440000	3.3247580000	-1.6883820000
C	0.5675900000	2.7878090000	-0.7420620000
C	1.8821060000	2.5733640000	0.0527180000
H	0.8786600000	1.0953750000	1.2892130000
C	-1.9898740000	1.5022780000	1.8127000000
H	2.7536300000	2.5960820000	-0.6029580000
H	-2.8936400000	2.1039810000	1.9144400000
N	-2.1264870000	0.5766810000	0.6889310000
C	1.4668940000	1.1082980000	0.3677190000
C	0.5223380000	1.2472160000	-0.8892820000
C	-1.2359090000	0.5523150000	-0.3025540000
H	-3.4872830000	-3.1129700000	-1.1202760000
H	-1.1423860000	2.1521440000	1.6135590000
C	-4.2300500000	-0.3521730000	1.6956410000
C	-3.1939790000	-0.3346470000	0.6180230000
S	-1.6916530000	-0.6593490000	-1.4130050000
C	-3.1070080000	-1.0974890000	-0.4967910000
H	2.0419130000	-0.5590370000	2.4213020000
C	-4.0290960000	-2.1770780000	-0.9709310000
H	-4.8253950000	-2.3596150000	-0.2498300000
O	0.7098320000	0.6631580000	-1.9637520000
C	2.4810240000	0.0118990000	0.3993350000
C	2.6528590000	-0.7640260000	1.5472450000
H	3.1219120000	0.3005450000	-1.6288940000
H	-4.4908050000	-1.9028840000	-1.9218460000
C	3.2735060000	-0.2678940000	-0.7193820000
C	3.5968810000	-1.7851680000	1.5915600000
H	3.7179100000	-2.3711390000	2.4955400000
C	4.2150200000	-1.2892810000	-0.6781590000
C	4.3830800000	-2.0498230000	0.4760360000
H	4.8163140000	-1.4994930000	-1.5553980000
H	5.1186740000	-2.8453320000	0.5037020000
H	-4.7863520000	0.5882970000	1.7298260000
H	-3.7797020000	-0.5135000000	2.6781970000
H	-4.9437420000	-1.1546150000	1.5198590000

Zero-point correction=  
(Hartree/Particle)

0.313883

Thermal correction to Energy=

0.332657

Thermal correction to Enthalpy=

0.333601

Thermal correction to Gibbs Free Energy=

0.262965

Sum of electronic and zero-point Energies=

-1148.764961

Sum of electronic and thermal Energies=

-1148.746187

Sum of electronic and thermal Enthalpies=

-1148.745243

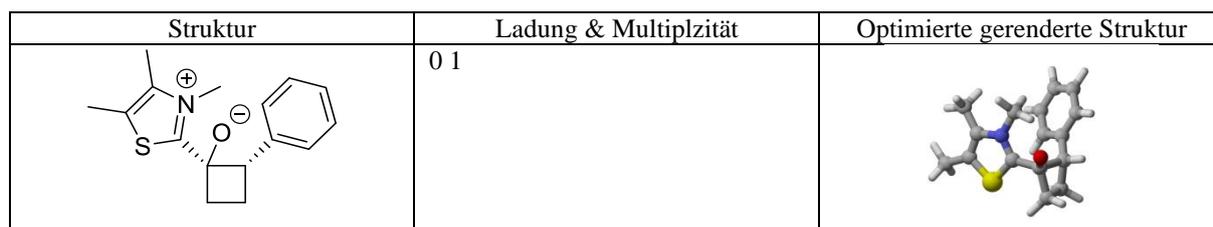
Sum of electronic and thermal Free Energies=

-1148.815879

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	208.745	70.230	148.665

#M062X/6-311+G\*\*

(41-syn-syn)



38

XYZ file generated by gabedit : coordinates in Angstrom

H	0.9718300000	3.4598980000	-0.4219980000
H	-0.2965450000	1.9282810000	-2.0128280000
H	0.3001550000	-1.3071840000	2.7783580000
H	-0.5759930000	3.9846150000	0.2721870000
C	-0.0531010000	3.1505320000	-0.1962390000
C	-0.9040150000	2.4965890000	-1.3045090000
H	-2.3575030000	2.1524990000	0.2587550000
C	-0.2110930000	-0.8388680000	1.9378770000
H	-1.5716010000	3.1443230000	-1.8724760000
H	-0.8599310000	-1.5585650000	1.4349140000
N	0.8062610000	-0.3724250000	0.9796480000
C	-1.5630910000	1.5976160000	-0.2461780000
C	-0.2886510000	1.9156770000	0.7481930000
C	0.7706260000	0.8274110000	0.4196390000
H	4.0541690000	-2.1733510000	-0.7668230000
H	-0.7566330000	0.0436490000	2.2753900000
C	1.9280430000	-2.6005180000	1.0933240000
C	1.8437660000	-1.2099510000	0.5550050000
S	2.0869900000	1.0056270000	-0.6558780000
C	2.6532980000	-0.6099750000	-0.3490400000
H	-0.4380640000	-0.2972000000	-1.9055490000
C	3.8732880000	-1.1341710000	-1.0381400000
H	3.7618530000	-1.0831770000	-2.1230970000
O	-0.4601950000	2.0350610000	2.0247690000
C	-1.9959200000	0.1952440000	-0.4974790000
C	-1.2790860000	-0.6740570000	-1.3311160000
H	-3.6561810000	0.3277610000	0.8547350000
H	4.7571180000	-0.5554010000	-0.7617240000
C	-3.0857220000	-0.3306670000	0.2080850000
C	-1.6142600000	-2.0205130000	-1.4252510000
H	-1.0406810000	-2.6723920000	-2.0753150000
C	-3.4295730000	-1.6742590000	0.1109440000
C	-2.6883260000	-2.5306630000	-0.6986620000
H	-4.2762400000	-2.0546610000	0.6711280000
H	-2.9528910000	-3.5786680000	-0.7753700000
H	0.9838390000	-3.1275520000	0.9373390000
H	2.1450490000	-2.5996580000	2.1639760000
H	2.7170440000	-3.1533330000	0.5880320000

Zero-point correction=  
(Hartree/Particle)

0.316806

Thermal correction to Energy=

0.334726

Thermal correction to Enthalpy=

0.335670

Thermal correction to Gibbs Free Energy=

0.271653

Sum of electronic and zero-point Energies=

-1148.787794

Sum of electronic and thermal Energies=

-1148.769874

Sum of electronic and thermal Enthalpies=

-1148.768930

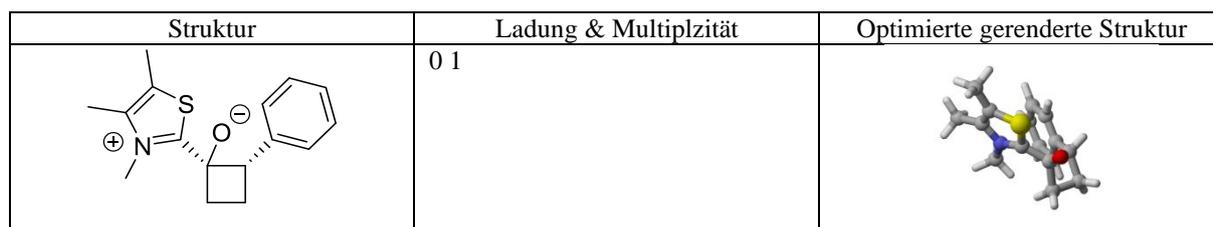
Sum of electronic and thermal Free Energies=

-1148.832947

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-kelvin
Total	210.044	70.529	134.736

#M062X/6-311+G\*\*

(41-syn-anti)



38

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.5460430000	1.5676510000	-2.0273100000
H	-3.4454150000	2.0807860000	-0.4771850000
H	-0.5712860000	-1.8226620000	-1.2703690000
H	-1.0654560000	3.2673600000	-1.7605200000
C	-1.3377100000	2.3315090000	-1.2740770000
C	-2.4363940000	2.3775940000	-0.1907130000
H	-1.4742440000	1.7420690000	1.7348000000
C	-0.1334730000	-0.9551930000	-1.7668750000
H	-2.4738940000	3.3627810000	0.2693470000
H	0.3480660000	-1.2544130000	-2.6979010000
N	0.8657760000	-0.3398020000	-0.8922870000
C	-1.6255530000	1.4170180000	0.7047570000
C	-0.3247170000	1.9417060000	-0.1464230000
C	0.7501610000	0.8582370000	-0.3278100000
H	4.5120320000	-1.6330930000	0.4642390000
H	-0.9138850000	-0.2358260000	-1.9747730000
C	2.2757760000	-2.3902590000	-1.1413390000
C	2.0557220000	-1.0189840000	-0.5881980000
S	2.1278230000	1.2560140000	0.5903130000
C	2.8602380000	-0.2808930000	0.2131840000
H	-3.6007930000	0.0571110000	-0.7261420000
C	4.2145650000	-0.6248200000	0.7500530000
H	4.9674960000	0.0693080000	0.3701850000
O	0.2739950000	2.9606120000	0.4265560000
C	-1.9534470000	-0.0435380000	0.6571020000
C	-2.9696420000	-0.5920430000	-0.1307970000
H	-0.3862310000	-0.5215500000	2.0471110000
H	4.2265950000	-0.5643610000	1.8401640000
C	-1.1712940000	-0.9294150000	1.4158230000
C	-3.1900460000	-1.9674580000	-0.1710020000
H	-3.9903770000	-2.3637200000	-0.7857440000
C	-1.3806520000	-2.3011640000	1.3735550000
C	-2.3939600000	-2.8305590000	0.5733060000
H	-0.7632480000	-2.9589790000	1.9755820000
H	-2.5684480000	-3.8996250000	0.5456180000
H	2.3644530000	-2.3782770000	-2.2306920000
H	1.4517300000	-3.0564950000	-0.8742480000
H	3.1939430000	-2.8109900000	-0.7369040000

Zero-point correction=  
(Hartree/Particle)

0.316653

Thermal correction to Energy=

0.334708

Thermal correction to Enthalpy=

0.335652

Thermal correction to Gibbs Free Energy=

0.270769

Sum of electronic and zero-point Energies=

-1148.775393

Sum of electronic and thermal Energies=

-1148.757338

Sum of electronic and thermal Enthalpies=

-1148.756394

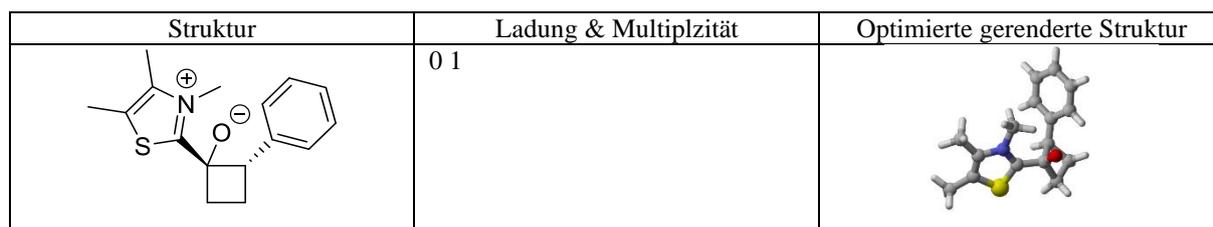
Sum of electronic and thermal Free Energies=

-1148.821276

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	210.032	70.686	136.557

#M062X/6-311+G\*\*

(41-anti-syn)



38

XYZ file generated by gabedit : coordinates in Angstrom

H	0.6765900000	3.1620950000	-0.6164120000
H	-1.7029050000	3.3622080000	-1.3849930000
H	0.4938250000	-2.1663330000	1.8917170000
H	0.0252380000	3.6158290000	0.9947710000
C	-0.0778310000	2.9399660000	0.1466390000
C	-1.4725730000	2.7764250000	-0.4941860000
H	-0.6270930000	1.1439230000	-1.6345430000
C	0.0788940000	-1.4830980000	1.1529160000
H	-2.2522090000	2.9215210000	0.2530650000
H	-0.4289740000	-2.0368890000	0.3619360000
N	1.1885020000	-0.7036400000	0.5658290000
C	-1.1905780000	1.2763060000	-0.7042760000
C	-0.1561420000	1.4367390000	0.5637700000
C	1.0865980000	0.5893640000	0.2897250000
H	5.4001510000	-0.1573410000	-0.0589210000
H	-0.5933600000	-0.7588890000	1.6218850000
C	2.6311230000	-2.7468540000	0.4953130000
C	2.4163800000	-1.2918160000	0.2337430000
S	2.5383800000	1.1647540000	-0.3993940000
C	3.2840130000	-0.4058420000	-0.3073750000
H	-1.6343950000	-0.8286900000	-2.3524300000
C	4.6953430000	-0.6076580000	-0.7615860000
H	4.9280780000	-1.6689150000	-0.8401130000
O	-0.6440850000	1.2070120000	1.7576670000
C	-2.2284140000	0.2224150000	-0.5738290000
C	-2.2954130000	-0.8335460000	-1.4901690000
H	-3.0247530000	0.9993570000	1.2601270000
H	4.8592270000	-0.1555050000	-1.7413160000
C	-3.0947120000	0.2066040000	0.5264770000
C	-3.1951860000	-1.8800770000	-1.3174140000
H	-3.2394340000	-2.6828270000	-2.0450940000
C	-3.9907940000	-0.8427170000	0.7019630000
C	-4.0451900000	-1.8893600000	-0.2144240000
H	-4.6487540000	-0.8454950000	1.5636880000
H	-4.7500150000	-2.7009910000	-0.0758920000
H	1.8272940000	-3.3435590000	0.0594600000
H	2.6637500000	-2.9551980000	1.5673120000
H	3.5737180000	-3.0721000000	0.0601810000

Zero-point correction=  
(Hartree/Particle)

0.316508

Thermal correction to Energy=

0.334704

Thermal correction to Enthalpy=

0.335648

Thermal correction to Gibbs Free Energy=

0.269801

Sum of electronic and zero-point Energies=

-1148.783196

Sum of electronic and thermal Energies=

-1148.765000

Sum of electronic and thermal Enthalpies=

-1148.764056

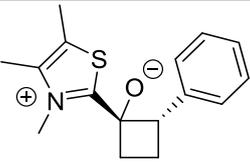
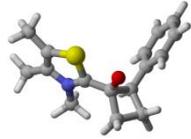
Sum of electronic and thermal Free Energies=

-1148.829903

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	210.030	70.651	138.586

#M062X/6-311+G\*\*

(41-anti-anti)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.3243450000	3.3306070000	0.0607580000
H	2.1051750000	3.3245110000	0.7448110000
H	-1.4951020000	0.9393750000	2.6934110000
H	0.2976700000	3.3143450000	-1.6125660000
C	0.3626460000	2.8396140000	-0.6344740000
C	1.7687340000	2.6312630000	-0.0276170000
H	0.8832680000	1.2934420000	1.4256240000
C	-1.7957100000	1.4990610000	1.8063340000
H	2.5195930000	2.5701100000	-0.8147180000
H	-2.7621340000	1.9707100000	1.9808940000
N	-1.9012840000	0.5916400000	0.6643490000
C	1.3558920000	1.2183190000	0.4403400000
C	0.2488210000	1.2780090000	-0.7408350000
C	-1.0493140000	0.5660090000	-0.3595060000
H	-4.6297470000	-1.8498480000	-1.4157190000
H	-1.0561030000	2.2617880000	1.5935350000
C	-3.9559250000	-0.4423950000	1.6722850000
C	-2.9198110000	-0.3684590000	0.5976930000
S	-1.4403960000	-0.6520400000	-1.4749850000
C	-2.8146850000	-1.1300890000	-0.5171880000
H	1.8157310000	-0.5361210000	2.4408330000
C	-3.7215210000	-2.2417790000	-0.9516840000
H	-3.2238050000	-2.8812680000	-1.6812210000
O	0.6159020000	0.7844610000	-1.9042450000
C	2.2980010000	0.0639680000	0.4352860000
C	2.4032300000	-0.7645460000	1.5557280000
H	2.9464480000	0.3649300000	-1.5850440000
H	-4.0102610000	-2.8671440000	-0.1054090000
C	3.0616690000	-0.2432580000	-0.6970280000
C	3.2557200000	-1.8639440000	1.5627200000
H	3.3275290000	-2.4883930000	2.4461320000
C	3.9120760000	-1.3433180000	-0.6913140000
C	4.0156690000	-2.1553470000	0.4350590000
H	4.4935270000	-1.5739780000	-1.5769220000
H	4.6823100000	-3.0100550000	0.4328500000
H	-4.5840600000	0.4524900000	1.6887950000
H	-3.5060610000	-0.5605000000	2.6610970000
H	-4.6044890000	-1.2981690000	1.4913370000

Zero-point correction=  
(Hartree/Particle)

0.316303

Thermal correction to Energy=

0.334703

Thermal correction to Enthalpy=

0.335647

Thermal correction to Gibbs Free Energy=

0.268721

Sum of electronic and zero-point Energies=

-1148.772953

Sum of electronic and thermal Energies=

-1148.754554

Sum of electronic and thermal Enthalpies=

-1148.753609

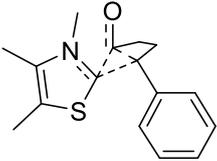
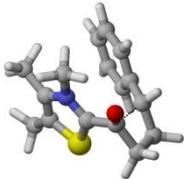
Sum of electronic and thermal Free Energies=

-1148.820536

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	210.029	70.814	140.858

#M062X/6-311+G\*\*

(42-syn-syn)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	3.2252320000	-1.5066170000	-1.0636630000
H	1.9406320000	0.2381970000	-2.2748440000
H	-0.2961050000	-1.2085230000	3.2760130000
H	4.1737740000	-0.2550120000	-0.2411910000
C	3.1841550000	-0.5059700000	-0.6211970000
C	2.5869750000	0.6217590000	-1.4847020000
H	2.4237160000	1.8572550000	0.3137470000
C	-0.0670220000	-0.3759800000	2.6081670000
H	3.3132390000	1.2883920000	-1.9529050000
H	-0.7850710000	0.4290190000	2.7565800000
N	-0.1669690000	-0.8501320000	1.2170890000
C	1.8035700000	1.2344670000	-0.3298220000
C	2.2189820000	-0.3270050000	0.5854600000
C	0.8686260000	-0.9497880000	0.3796330000
H	-3.2784320000	-2.4696280000	-0.9439980000
H	0.9565140000	-0.0406900000	2.7673250000
C	-2.6379350000	-1.0788600000	1.5015380000
C	-1.3972860000	-1.2761100000	0.6950400000
S	0.3718830000	-1.7117490000	-1.0749470000
C	-1.2894540000	-1.7848570000	-0.5495710000
H	0.0308130000	1.0889480000	-2.4579090000
C	-2.3510230000	-2.2734460000	-1.4809110000
H	-2.5531460000	-1.5277400000	-2.2546960000
O	2.6613070000	-0.2128760000	1.7687210000
C	0.4203980000	1.7164850000	-0.4305550000
C	-0.3971580000	1.5009330000	-1.5519670000
H	0.4485150000	2.5084480000	1.5668830000
H	-2.0472470000	-3.1996000000	-1.9726980000
C	-0.1738890000	2.3078070000	0.6995430000
C	-1.7526020000	1.8140210000	-1.5242640000
H	-2.3588440000	1.6408770000	-2.4070190000
C	-1.5263120000	2.6165280000	0.7281670000
C	-2.3311720000	2.3582600000	-0.3819850000
H	-1.9556890000	3.0714930000	1.6146770000
H	-3.3862770000	2.6051980000	-0.3651030000
H	-2.8221740000	-0.0109660000	1.6486610000
H	-2.5594330000	-1.5537350000	2.4818410000
H	-3.4949320000	-1.5028520000	0.9826040000

Zero-point correction=  
(Hartree/Particle)

0.315750

Thermal correction to Energy=

0.333311

Thermal correction to Enthalpy=

0.334255

Thermal correction to Gibbs Free Energy=

0.271701

Sum of electronic and zero-point Energies=

-1148.785891

Sum of electronic and thermal Energies=

-1148.768330

Sum of electronic and thermal Enthalpies=

-1148.767386

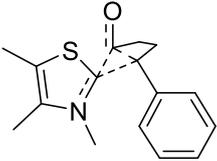
Sum of electronic and thermal Free Energies=

-1148.829940

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	209.156	69.572	131.657

#M062X/6-311+G\*\*

(42-syn-anti)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	1.9813280000	1.4843490000	1.6947450000
H	3.4963900000	1.8967470000	-0.2467990000
H	0.6380530000	-1.6243140000	1.6270920000
H	1.7538820000	3.2489650000	1.5725960000
C	1.6950920000	2.3019140000	1.0339180000
C	2.4510270000	2.2088940000	-0.2998650000
H	1.0066930000	1.5195450000	-1.8851090000
C	0.1914010000	-0.7021080000	2.0016120000
H	2.3992730000	3.1673620000	-0.8125150000
H	-0.3501350000	-0.8954510000	2.9293940000
N	-0.7351370000	-0.1662900000	1.0066330000
C	1.4851660000	1.2220240000	-0.9553210000
C	0.3218850000	2.1534670000	0.3485990000
C	-0.6686310000	1.0513200000	0.4532760000
H	-4.2996030000	-1.6377760000	-0.4227470000
H	0.9736420000	0.0199260000	2.1908820000
C	-1.9875240000	-2.3275910000	1.1227950000
C	-1.8579870000	-0.9250180000	0.6242490000
S	-2.0609630000	1.3567030000	-0.5179570000
C	-2.6795340000	-0.2475330000	-0.2026310000
H	3.5044630000	-0.0807220000	0.3987900000
C	-3.9570990000	-0.6919330000	-0.8411060000
H	-4.7446910000	0.0480470000	-0.6835640000
O	-0.1670720000	3.2020330000	-0.1492350000
C	1.7176220000	-0.2092040000	-0.8094970000
C	2.7754410000	-0.7455270000	-0.0495340000
H	-0.0103340000	-0.7451380000	-1.9779270000
H	-3.8320740000	-0.8201340000	-1.9191550000
C	0.8131970000	-1.1286710000	-1.3810070000
C	2.9138630000	-2.1154730000	0.1351540000
H	3.7471400000	-2.4939200000	0.7169120000
C	0.9451980000	-2.4952200000	-1.1876270000
C	1.9951110000	-3.0032290000	-0.4203240000
H	0.2311170000	-3.1726510000	-1.6444640000
H	2.1060330000	-4.0714600000	-0.2772620000
H	-2.0684690000	-2.3663760000	2.2119370000
H	-1.1214500000	-2.9233660000	0.8224090000
H	-2.8786830000	-2.7897660000	0.7033860000

Zero-point correction=  
(Hartree/Particle)

0.315984

Thermal correction to Energy=

0.333556

Thermal correction to Enthalpy=

0.334501

Thermal correction to Gibbs Free Energy=

0.271868

Sum of electronic and zero-point Energies=

-1148.771671

Sum of electronic and thermal Energies=

-1148.754098

Sum of electronic and thermal Enthalpies=

-1148.753154

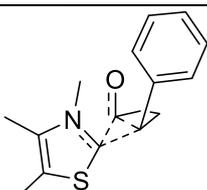
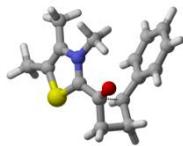
Sum of electronic and thermal Free Energies=

-1148.815787

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	209.310	69.706	131.821

#M062X/6-311+G\*\*

(42-anti-syn)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

```

H      -1.5840810000      3.3175090000     -1.7077730000
C      -1.4614610000      2.7735030000     -0.7690870000
H      -0.2760950000      1.2002210000     -1.6813640000
H      -2.3704010000      2.8641790000     -0.1753760000
H      -0.6622060000     -1.0291270000     -2.1395820000
C      -1.4964860000     -1.0590280000     -1.4441210000
H      -1.8563770000     -3.1547310000     -1.7371410000
C      -1.0358460000      1.3116330000     -0.9061160000
H      0.3993270000       -1.6594600000     2.5304910000
C      -1.8809280000      0.1269570000     -0.7927980000
C      -2.1610990000     -2.2550740000     -1.2135740000
C      -3.2242730000     -2.2970550000     -0.3111710000
C      -2.9625010000      0.0729780000      0.0997830000
H      0.6374270000      3.3338890000     -0.5238070000
H      -3.7458060000     -3.2286570000     -0.1250830000
C      -3.6208850000     -1.1294030000      0.3353370000
H      -3.2529160000      0.9664460000      0.6366890000
C      -0.2368910000      3.1189570000      0.0985680000
H      -4.4474120000     -1.1568430000      1.0363340000
H      -0.6204030000     -1.8935740000      1.0759030000
C      -0.0913140000     -1.1645770000      1.6916870000
H      -0.3563770000      3.8926460000      0.8568960000
H      -0.7758850000     -0.3913900000      2.0372500000
C      -0.2498530000      1.6982300000      0.7115930000
N       0.9452520000     -0.4975010000      0.8768860000
C       0.9149500000      0.7914000000      0.5226730000
C       2.1409370000     -2.6811250000      0.6739690000
O      -1.0036900000      1.5231300000      1.7261350000
C       2.0522070000     -1.2160870000      0.3960670000
H       5.0261070000     -0.2029630000     -0.5915180000
C       2.9166410000     -0.4490620000     -0.3005340000
S       2.3360880000      1.1984090000     -0.3609070000
C       4.2033750000     -0.8139750000     -0.9691650000
H       4.1411100000     -0.6640160000     -2.0493590000
H       4.4520070000     -1.8582270000     -0.7849280000
H       2.2510080000     -2.8779360000      1.7428260000
H       2.9971790000     -3.1120630000      0.1599080000
H       1.2396970000     -3.1926050000      0.3281850000

```

Zero-point correction=  
(Hartree/Particle)

0.315652

Thermal correction to Energy=

0.333478

Thermal correction to Enthalpy=

0.334422

Thermal correction to Gibbs Free Energy=

0.269866

Sum of electronic and zero-point Energies=

-1148.782739

Sum of electronic and thermal Energies=

-1148.764914

Sum of electronic and thermal Enthalpies=

-1148.763969

Sum of electronic and thermal Free Energies=

-1148.828526

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	209.260	69.540	135.870

#M062X/6-311+G\*\*

(42-anti-anti)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

```

H      -1.7223860000      3.2900260000     -1.5529290000
C      -1.5584400000      2.7296380000     -0.6297200000
H      -0.3268860000      1.2315330000     -1.6241600000
H      -2.4681760000      2.7491690000     -0.0314390000
H      -0.6751060000     -1.0078810000     -2.1268240000
C      -1.5080290000     -1.0637310000     -1.4308200000
H      -1.9067330000     -3.1299860000     -1.8516850000
C      -1.0554170000      1.2957160000     -0.8113960000
H      1.8198160000       2.1452260000     -1.7526090000
C      -1.8740650000      0.0879500000     -0.7154510000
C      -2.1959690000     -2.2587000000     -1.2744240000
C      -3.2617170000     -2.3343740000     -0.3798030000
C      -2.9339620000     -0.0090750000      0.1972230000
H      0.4808670000      3.4636880000     -0.3904600000
H      -3.8041140000     -3.2643180000     -0.2554060000
C      -3.6196990000     -1.2091580000      0.3556720000
H      -3.1950090000      0.8489930000      0.8022410000
C      -0.3488910000      3.1297650000      0.2333350000
H      -4.4361060000     -1.2670160000      1.0664370000
H      3.4767510000       1.7006410000     -1.2975440000
C      2.4783150000       1.8973590000     -0.9180710000
H      -0.5210690000      3.8432680000      1.0392680000
H      2.5230900000       2.7381120000     -0.2288650000
C      -0.2319140000      1.6829560000      0.7735070000
N      1.9911870000       0.7165500000     -0.2106580000
C      0.9127170000       0.7512570000     0.5870940000
C      3.8132340000     -0.7327380000     -1.1604040000
O      -0.9346910000      1.3964420000      1.8008750000
C      2.6222530000     -0.5399580000     -0.2766140000
H      3.2680770000     -3.1715120000      0.2017530000
C      2.0280280000     -1.4476150000      0.5289160000
S      0.6705830000     -0.7447850000      1.3771550000
C      2.3708530000     -2.8869220000      0.7498280000
H      1.5518690000     -3.5319110000      0.4228710000
H      2.5483130000     -3.0843700000      1.8093290000
H      3.5899320000     -0.4659730000     -2.1963950000
H      4.1164870000     -1.7773540000     -1.1455360000
H      4.6664930000     -0.1353780000     -0.8281520000

```

Zero-point correction=  
(Hartree/Particle)

0.315585

Thermal correction to Energy=

0.333620

Thermal correction to Enthalpy=

0.334564

Thermal correction to Gibbs Free Energy=

0.269604

Sum of electronic and zero-point Energies=

-1148.771542

Sum of electronic and thermal Energies=

-1148.753508

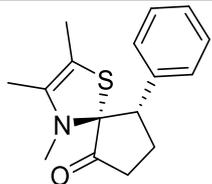
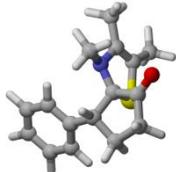
Sum of electronic and thermal Enthalpies=

-1148.752563

Sum of electronic and thermal Free Energies=

-1148.817524

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-kelvin
Total	209.350	69.794	136.720

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	4.9673490000	-2.1214010000	-0.1607440000
H	3.3657370000	-2.4246640000	1.7106190000
C	4.1356890000	-1.4378110000	-0.0384220000
C	3.2366990000	-1.6074810000	1.0106980000
H	4.6559530000	-0.2412120000	-1.7440390000
C	3.9597960000	-0.3838990000	-0.9258460000
C	2.1734910000	-0.7284560000	1.1640590000
H	1.4704820000	-0.8700680000	1.9773390000
C	2.8901820000	0.4947190000	-0.7709570000
C	1.9826370000	0.3320740000	0.2741030000
H	2.7724140000	1.3081050000	-1.4766310000
H	-2.0438300000	-2.9971030000	1.6024120000
H	-0.4958590000	0.3431480000	2.8104380000
H	-1.3905490000	-1.1597310000	2.9270160000
H	0.7782430000	1.5166210000	1.5486160000
C	0.7986070000	1.2423530000	0.4847170000
N	-1.0099240000	-0.5126380000	0.9757950000
C	-1.3184450000	-0.2243490000	2.3720020000
C	-2.6964480000	-2.3496340000	1.0091010000
C	-1.8866220000	-1.3527010000	0.2448370000
H	-3.2735100000	-2.9772110000	0.3338870000
H	1.5113030000	3.2610370000	0.0142160000
C	-0.5797680000	0.6166430000	0.1794120000
S	-0.6568060000	0.0293980000	-1.5700370000
C	-1.8395440000	-1.2179420000	-1.0840250000
C	0.7468090000	2.5571230000	-0.3160520000
H	0.9149480000	2.3551830000	-1.3765950000
H	-3.3918960000	-1.8542690000	1.6915160000
C	-2.5212240000	-1.9830270000	-2.1688800000
H	-2.2450350000	0.3457980000	2.4983250000
C	-1.5119240000	1.8440740000	0.2247350000
C	-0.6838320000	3.0783150000	-0.1081710000
H	-0.7544540000	3.7486410000	0.7537000000
O	-2.6731890000	1.8184050000	0.5262780000
H	-1.1021750000	3.6043830000	-0.9665720000
H	-1.7901780000	-2.4545010000	-2.8331700000
H	-3.1450990000	-1.3236890000	-2.7784440000
H	-3.1566070000	-2.7681990000	-1.7599540000

Zero-point correction=  
(Hartree/Particle)

0.318299

Thermal correction to Energy=

0.336473

Thermal correction to Enthalpy=

0.337418

Thermal correction to Gibbs Free Energy=

0.271953

Sum of electronic and zero-point Energies=

-1148.844195

Sum of electronic and thermal Energies=

-1148.826020

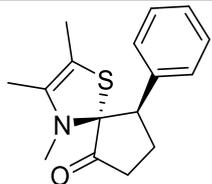
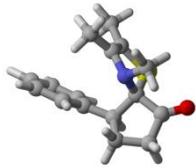
Sum of electronic and thermal Enthalpies=

-1148.825076

Sum of electronic and thermal Free Energies=

-1148.890540

	E (Thermal) KCal/Mol	CV Cal/Mol-kelvin	S Cal/Mol-kelvin
Total	211.140	70.227	137.781

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-4.8721960000	-0.7348340000	0.2074590000
H	-3.4375200000	-1.3779270000	2.1230890000
C	-3.8088240000	-0.8870410000	0.0643020000
C	-3.0023850000	-1.2482250000	1.1383900000
H	-3.8633310000	-0.4727930000	-2.0459020000
C	-3.2421810000	-0.7394960000	-1.1983730000
C	-1.6360770000	-1.4403410000	0.9582520000
H	-1.0184630000	-1.6998300000	1.8096830000
C	-1.8787690000	-0.9394160000	-1.3771390000
C	-1.0539640000	-1.2736880000	-0.2995030000
H	-1.4388770000	-0.8177430000	-2.3613960000
H	-1.2449340000	0.8716470000	2.6090230000
H	2.7451750000	0.2578350000	2.0533060000
H	1.6369980000	1.4376660000	2.7435780000
H	0.5966690000	-1.6368560000	-1.5769980000
C	0.4304620000	-1.3875960000	-0.5214560000
N	0.9020380000	0.4738490000	1.0456740000
C	2.0256290000	1.0404950000	1.8063010000
C	-0.9629680000	1.7842550000	2.0790510000
C	-0.1547720000	1.4328130000	0.8692060000
H	-1.8741950000	2.3124800000	1.8022020000
H	0.9908600000	-2.2413210000	1.3893510000
C	1.2338510000	-0.0792820000	-0.2691320000
S	0.8879590000	1.2296900000	-1.5096870000
C	-0.2994490000	1.9118740000	-0.3701130000
C	1.2002750000	-2.4096210000	0.3316630000
H	0.9230110000	-3.4348770000	0.0854850000
H	-0.4032310000	2.4202770000	2.7711810000
C	-1.3169000000	2.8615360000	-0.9103170000
H	2.5402240000	1.8392620000	1.2586430000
C	2.6858990000	-0.6062990000	-0.3187730000
C	2.6690500000	-2.0885020000	0.0324290000
H	3.3627420000	-2.2850070000	0.8516180000
O	3.6493340000	0.0368230000	-0.6194790000
H	3.0379140000	-2.6323760000	-0.8428630000
H	-1.9872070000	2.3441960000	-1.6031130000
H	-0.8301950000	3.6720840000	-1.4596990000
H	-1.9129940000	3.3027630000	-0.1122730000

Zero-point correction=  
(Hartree/Particle)

0.318052

Thermal correction to Energy=

0.336222

Thermal correction to Enthalpy=

0.337166

Thermal correction to Gibbs Free Energy=

0.272266

Sum of electronic and zero-point Energies=

-1148.844921

Sum of electronic and thermal Energies=

-1148.826752

Sum of electronic and thermal Enthalpies=

-1148.825808

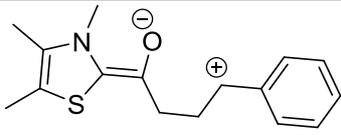
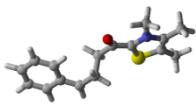
Sum of electronic and thermal Free Energies=

-1148.890708

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	210.982	70.133	136.594

#M062X/6-311+G\*\*

(44ion)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.4433900000	0.5020800000	-0.9454650000
H	-0.4032300000	-0.9439500000	-0.8732710000
H	-2.5014450000	-2.1614430000	1.1034500000
C	-0.6582300000	-0.0052570000	-0.3837990000
C	-2.5316350000	-1.0897370000	0.9337600000
C	0.4651850000	0.9131230000	-0.1409780000
O	0.2529000000	2.0949970000	0.1960310000
H	4.5768100000	-2.8595140000	-1.2250210000
S	2.0759360000	-1.3804950000	-0.2604430000
C	-1.3122660000	-0.3264910000	1.0829180000
C	1.7870510000	0.3238340000	-0.1173500000
H	-1.4469130000	0.6764680000	1.5037140000
H	2.1181510000	2.8616380000	0.2351340000
H	3.5440850000	2.8070140000	-0.8393920000
C	3.8055170000	-1.1518340000	-0.1841860000
N	2.9748440000	0.9781020000	0.0239620000
H	-0.5606720000	-0.8614760000	1.6659390000
C	4.7094450000	-2.3382920000	-0.2739600000
C	3.1065640000	2.4373370000	0.0911810000
C	4.1001460000	0.1602960000	-0.0356580000
H	5.6035820000	1.5497990000	-0.6798960000
H	5.7538170000	-2.0399730000	-0.1953570000
H	4.5017850000	-3.0492780000	0.5294900000
C	5.4572000000	0.7771670000	0.0777650000
H	6.2279400000	0.0218300000	-0.0561380000
H	3.7541720000	2.7010680000	0.9272470000
H	5.5984750000	1.2372350000	1.0589120000
C	-3.7271610000	-0.5475210000	0.4049460000
C	-3.8702630000	0.8325750000	0.0974050000
C	-5.0583980000	1.3277810000	-0.4169200000
C	-6.1450260000	0.4863920000	-0.6468140000
C	-6.0273710000	-0.8762910000	-0.3510150000
C	-4.8498380000	-1.3833260000	0.1584060000
H	-3.0482860000	1.5159770000	0.2790850000
H	-5.1398130000	2.3857400000	-0.6399460000
H	-7.0699000000	0.8818610000	-1.0487110000
H	-6.8662680000	-1.5406110000	-0.5257310000
H	-4.7665200000	-2.4417780000	0.3828670000

Zero-point correction=  
(Hartree/Particle)

0.314814

Thermal correction to Energy=

0.334050

Thermal correction to Enthalpy=

0.334994

Thermal correction to Gibbs Free Energy=

0.265008

Sum of electronic and zero-point Energies=

-1148.749887

Sum of electronic and thermal Energies=

-1148.730650

Sum of electronic and thermal Enthalpies=

-1148.729706

Sum of electronic and thermal Free Energies=

-1148.799692

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	209.620	72.592	147.298

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.4433900000	0.5020800000	-0.9454650000
H	-0.4032300000	-0.9439500000	-0.8732710000
H	-2.5014450000	-2.1614430000	1.1034500000
C	-0.6582300000	-0.0052570000	-0.3837990000
C	-2.5316350000	-1.0897370000	0.9337600000
C	0.4651850000	0.9131230000	-0.1409780000
O	0.2529000000	2.0949970000	0.1960310000
H	4.5768100000	-2.8595140000	-1.2250210000
S	2.0759360000	-1.3804950000	-0.2604430000
C	-1.3122660000	-0.3264910000	1.0829180000
C	1.7870510000	0.3238340000	-0.1173500000
H	-1.4469130000	0.6764680000	1.5037140000
H	2.1181510000	2.8616380000	0.2351340000
H	3.5440850000	2.8070140000	-0.8393920000
C	3.8055170000	-1.1518340000	-0.1841860000
N	2.9748440000	0.9781020000	0.0239620000
H	-0.5606720000	-0.8614760000	1.6659390000
C	4.7094450000	-2.3382920000	-0.2739600000
C	3.1065640000	2.4373370000	0.0911810000
C	4.1001460000	0.1602960000	-0.0356580000
H	5.6035820000	1.5497990000	-0.6798960000
H	5.7538170000	-2.0399730000	-0.1953570000
H	4.5017850000	-3.0492780000	0.5294900000
C	5.4572000000	0.7771670000	0.0777650000
H	6.2279400000	0.0218300000	-0.0561380000
H	3.7541720000	2.7010680000	0.9272470000
H	5.5984750000	1.2372350000	1.0589120000
C	-3.7271610000	-0.5475210000	0.4049460000
C	-3.8702630000	0.8325750000	0.0974050000
C	-5.0583980000	1.3277810000	-0.4169200000
C	-6.1450260000	0.4863920000	-0.6468140000
C	-6.0273710000	-0.8762910000	-0.3510150000
C	-4.8498380000	-1.3833260000	0.1584060000
H	-3.0482860000	1.5159770000	0.2790850000
H	-5.1398130000	2.3857400000	-0.6399460000
H	-7.0699000000	0.8818610000	-1.0487110000
H	-6.8662680000	-1.5406110000	-0.5257310000
H	-4.7665200000	-2.4417780000	0.3828670000

Zero-point correction=  
(Hartree/Particle)

0.314813

Thermal correction to Energy=

0.334050

Thermal correction to Enthalpy=

0.334994

Thermal correction to Gibbs Free Energy=

0.265006

Sum of electronic and zero-point Energies=

-1148.749887

Sum of electronic and thermal Energies=

-1148.730651

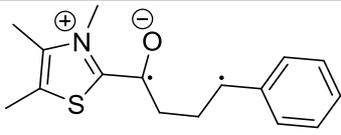
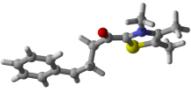
Sum of electronic and thermal Enthalpies=

-1148.729706

Sum of electronic and thermal Free Energies=

-1148.799695

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	209.619	72.592	147.303

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.3681350000	0.5301900000	-1.1155640000
H	-0.3521410000	-0.9115220000	-1.1015900000
H	-2.5196640000	-2.2902060000	0.6605860000
C	-0.6355370000	-0.0255690000	-0.5265690000
C	-2.5480170000	-1.2065010000	0.6179760000
C	0.5268480000	0.9164630000	-0.2674320000
O	0.2856390000	2.1171360000	-0.0529240000
H	4.6760860000	-2.8833210000	-1.0148330000
S	2.1347780000	-1.3660650000	-0.3654380000
C	-1.2764380000	-0.4514760000	0.8162460000
C	1.8353120000	0.3514020000	-0.2122210000
H	-1.4506910000	0.4565940000	1.4022820000
H	2.1881760000	2.9070830000	0.1451990000
H	3.5784250000	2.7698150000	-0.9575360000
C	3.8509050000	-1.1370090000	-0.0864840000
N	3.0228210000	1.0056170000	0.0492330000
H	-0.5608680000	-1.0611370000	1.3747520000
C	4.7503490000	-2.3303410000	-0.0751620000
C	3.1671950000	2.4603900000	0.0082400000
C	4.1350490000	0.1698830000	0.1014480000
H	5.7143200000	1.5451870000	-0.3685440000
H	5.7902980000	-2.0361840000	0.0600530000
H	4.4857650000	-3.0134300000	0.7360800000
C	5.4794070000	0.7702450000	0.3645790000
H	6.2535050000	0.0083280000	0.3109380000
H	3.8380230000	2.7799950000	0.8050080000
H	5.5178520000	1.2250080000	1.3577650000
C	-3.7884330000	-0.5937560000	0.3064140000
C	-3.9348040000	0.8122110000	0.1951620000
C	-5.1631080000	1.3743070000	-0.1081350000
C	-6.2848230000	0.5704370000	-0.3120090000
C	-6.1626150000	-0.8172870000	-0.2099570000
C	-4.9417310000	-1.3895470000	0.0915910000
H	-3.0767810000	1.4582700000	0.3442830000
H	-5.2504280000	2.4518330000	-0.1886280000
H	-7.2421670000	1.0187470000	-0.5480070000
H	-7.0286330000	-1.4496190000	-0.3682950000
H	-4.8516010000	-2.4681180000	0.1696840000

Zero-point correction=  
(Hartree/Particle)

0.313785

Thermal correction to Energy=

0.333549

Thermal correction to Enthalpy=

0.334494

Thermal correction to Gibbs Free Energy=

0.260632

Sum of electronic and zero-point Energies=

-1148.785580

Sum of electronic and thermal Energies=

-1148.765816

Sum of electronic and thermal Enthalpies=

-1148.764871

Sum of electronic and thermal Free Energies=

-1148.838733

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	209.305	73.074	155.455



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XYZ file generated by gabedit : coordinates in Angstrom

H	-0.8019080000	-2.7139840000	-1.4850430000
H	-1.2424210000	-3.8160290000	-0.1723780000
C	-0.9626970000	-2.7896130000	-0.4048610000
H	1.1943630000	-2.9193770000	-0.1627690000
C	-2.0969140000	-1.8683010000	0.0217650000
O	-2.9816910000	-2.2541900000	0.7914200000
C	0.3591590000	-2.4260000000	0.3380810000
C	-1.9573350000	-0.5405860000	-0.4613750000
S	-0.3545770000	-0.1076890000	-0.9955030000
H	-4.4875150000	0.8562390000	-0.6008070000
H	0.3041040000	-2.8340370000	1.3498710000
H	0.1241350000	-0.4946630000	1.3222480000
C	0.6407850000	-0.9239680000	0.4613250000
N	-2.5436600000	0.5913450000	0.1809260000
C	-0.6040500000	1.5793220000	-0.5986840000
C	-3.9932510000	0.6043450000	0.3450330000
H	0.8284000000	2.4061300000	-1.9568560000
H	0.0473360000	3.5937390000	-0.9217130000
C	-1.8147220000	1.7233300000	0.0304100000
H	2.5118910000	-1.5265990000	-1.4240410000
H	-4.2699090000	1.3297140000	1.1092510000
C	0.4542260000	2.5820860000	-0.9443750000
H	-4.3002230000	-0.3884250000	0.6660360000
C	2.0576730000	-0.4729050000	0.3997950000
H	-3.2871840000	3.2750410000	-0.0822590000
C	2.8863270000	-0.8478790000	-0.6642200000
C	-2.3847280000	3.0314290000	0.4840180000
H	1.3125020000	2.5441490000	-0.2677590000
H	1.9216160000	0.7199490000	2.1808430000
H	-1.6642680000	3.8347440000	0.3511330000
C	2.5577450000	0.4169760000	1.3554790000
H	-2.6542060000	2.9836220000	1.5411640000
C	4.1801270000	-0.3511100000	-0.7639900000
H	4.8075590000	-0.6488100000	-1.5959120000
C	3.8544200000	0.9082430000	1.2601020000
C	4.6697050000	0.5271930000	0.1985240000
H	4.2294770000	1.5892890000	2.0152040000
H	5.6798120000	0.9110710000	0.1218210000

Zero-point correction=  
(Hartree/Particle)

0.317305

Thermal correction to Energy=

0.335738

Thermal correction to Enthalpy=

0.336682

Thermal correction to Gibbs Free Energy=

0.270832

Sum of electronic and zero-point Energies=

-1148.778700

Sum of electronic and thermal Energies=

-1148.760268

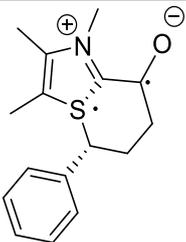
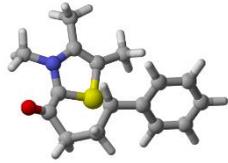
Sum of electronic and thermal Enthalpies=

-1148.759323

Sum of electronic and thermal Free Energies=

-1148.825173

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	210.679	70.881	138.593

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.8019080000	-2.7139840000	-1.4850430000
H	-1.2424210000	-3.8160290000	-0.1723780000
C	-0.9626970000	-2.7896130000	-0.4048610000
H	1.1943630000	-2.9193770000	-0.1627690000
C	-2.0969140000	-1.8683010000	0.0217650000
O	-2.9816910000	-2.2541900000	0.7914200000
C	0.3591590000	-2.4260000000	0.3380810000
C	-1.9573350000	-0.5405860000	-0.4613750000
S	-0.3545770000	-0.1076890000	-0.9955030000
H	-4.4875150000	0.8562390000	-0.6008070000
H	0.3041040000	-2.8340370000	1.3498710000
H	0.1241350000	-0.4946630000	1.3222480000
C	0.6407850000	-0.9239680000	0.4613250000
N	-2.5436600000	0.5913450000	0.1809260000
C	-0.6040500000	1.5793220000	-0.5986840000
C	-3.9932510000	0.6043450000	0.3450330000
H	0.8284000000	2.4061300000	-1.9568560000
H	0.0473360000	3.5937390000	-0.9217130000
C	-1.8147220000	1.7233300000	0.0304100000
H	2.5118910000	-1.5265990000	-1.4240410000
H	-4.2699090000	1.3297140000	1.1092510000
C	0.4542260000	2.5820860000	-0.9443750000
H	-4.3002230000	-0.3884250000	0.6660360000
C	2.0576730000	-0.4729050000	0.3997950000
H	-3.2871840000	3.2750410000	-0.0822590000
C	2.8863270000	-0.8478790000	-0.6642200000
C	-2.3847280000	3.0314290000	0.4840180000
H	1.3125020000	2.5441490000	-0.2677590000
H	1.9216160000	0.7199490000	2.1808430000
H	-1.6642680000	3.8347440000	0.3511330000
C	2.5577450000	0.4169760000	1.3554790000
H	-2.6542060000	2.9836220000	1.5411640000
C	4.1801270000	-0.3511100000	-0.7639900000
H	4.8075590000	-0.6488100000	-1.5959120000
C	3.8544200000	0.9082430000	1.2601020000
C	4.6697050000	0.5271930000	0.1985240000
H	4.2294770000	1.5892890000	2.0152040000
H	5.6798120000	0.9110710000	0.1218210000

Zero-point correction= 0.317309  
(Hartree/Particle)

Thermal correction to Energy= 0.335738

Thermal correction to Enthalpy= 0.336682

Thermal correction to Gibbs Free Energy= 0.270859

Sum of electronic and zero-point Energies= -1148.778697

Sum of electronic and thermal Energies= -1148.760267

Sum of electronic and thermal Enthalpies= -1148.759323

Sum of electronic and thermal Free Energies= -1148.825146

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	210.679	70.880	138.537



38

XYZ file generated by gabedit : coordinates in Angstrom

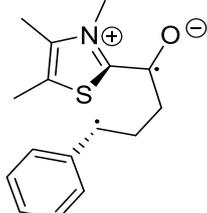
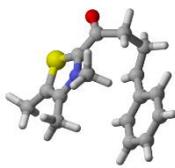
H	-4.3840260000	-0.8181320000	-1.8781210000
H	-3.1012250000	1.1932020000	-1.3112310000
C	-3.8841850000	-0.7559130000	-0.9181360000
O	1.6291140000	2.9514010000	0.1701170000
H	-1.0050270000	3.5950540000	0.6318120000
C	-3.1599740000	0.3799500000	-0.5970900000
H	-4.5446910000	-2.7039540000	-0.2770900000
C	-3.9767960000	-1.8183080000	-0.0191640000
S	0.4255030000	-0.6603530000	-0.9202000000
C	-1.4046750000	2.7509070000	0.0666430000
C	0.9729740000	2.0380720000	-0.3628820000
C	-2.4920350000	0.4900430000	0.6470970000
H	-2.3174730000	3.0932130000	-0.4324530000
H	-0.1881950000	3.2396750000	-1.6568900000
C	1.3950770000	-3.2660650000	-0.6313020000
C	-1.7001440000	1.6155560000	0.9917440000
C	1.3953600000	0.6788540000	-0.3550110000
C	-3.3364090000	-1.7260760000	1.2195530000
C	-0.3599050000	2.3743140000	-1.0113170000
C	1.6505340000	-1.8083730000	-0.4203540000
C	-2.6112710000	-0.5968490000	1.5484790000
H	-3.4089550000	-2.5438750000	1.9274360000
H	-1.2102280000	1.6035310000	1.9594690000
N	2.5836870000	0.2072990000	0.1671880000
H	-0.7380930000	1.5598520000	-1.6345910000
C	2.7119840000	-1.1777680000	0.1309280000
H	-2.1087460000	-0.5327380000	2.5079810000
H	4.8302660000	-1.5543110000	0.1045670000
C	3.9424610000	-1.8283870000	0.6800150000
H	3.8341400000	1.8655760000	-0.1107240000
H	3.8410820000	-2.9104180000	0.6436190000
C	3.6316790000	1.1081110000	0.6439040000
H	3.3130540000	1.6192380000	1.5513260000
H	4.1092120000	-1.5404360000	1.7206250000
H	4.5309780000	0.5292340000	0.8360670000
H	1.2171660000	-3.4803600000	-1.6881860000
H	0.5129910000	-3.5913270000	-0.0732970000
H	2.2429530000	-3.8680760000	-0.3070240000

Zero-point correction=  
(Hartree/Particle)

0.314277

Thermal correction to Energy=	0.333805
Thermal correction to Enthalpy=	0.334749
Thermal correction to Gibbs Free Energy=	0.263142
Sum of electronic and zero-point Energies=	-1148.787380
Sum of electronic and thermal Energies=	-1148.767852
Sum of electronic and thermal Enthalpies=	-1148.766908
Sum of electronic and thermal Free Energies=	-1148.838514

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	209.466	72.961	150.708

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3	

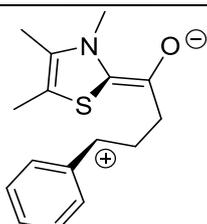
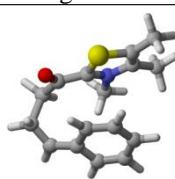
38

XYZ file generated by gabedit : coordinates in Angstrom

H	0.8049110000	2.0918600000	1.3541440000
H	0.1054420000	3.6979540000	1.0787690000
C	0.2052780000	2.6907170000	0.6698330000
H	1.9117610000	3.2240180000	-0.5635290000
C	-1.1976300000	2.1550010000	0.4289600000
O	-2.0629910000	2.9347620000	0.0001910000
C	0.9321610000	2.7565660000	-0.7024690000
C	-1.4860310000	0.7570800000	0.4552170000
S	-2.8465200000	0.1976870000	-0.4834170000
H	-0.1069630000	0.6641090000	2.6730180000
H	0.3483880000	3.4024540000	-1.3606300000
H	0.2917250000	1.0731580000	-1.9989100000
C	1.0577000000	1.3937170000	-1.2999990000
N	-0.7785830000	-0.3126120000	0.9615420000
C	-2.3466200000	-1.4690670000	-0.2552480000
C	0.1680860000	-0.1960710000	2.0634570000
H	-4.1878740000	-2.5098160000	-0.5801410000
H	-3.1157160000	-2.4912990000	-1.9809620000
C	-1.2482270000	-1.5533310000	0.5262540000
H	3.2052580000	1.7246270000	0.3606880000
H	1.1932440000	-0.0848350000	1.7019820000
C	-3.1412720000	-2.5644100000	-0.8906820000
H	0.1067350000	-1.0869930000	2.6859290000
C	1.9885530000	0.4144880000	-0.8671020000
H	0.5453410000	-2.6717110000	0.8660780000
C	3.0564450000	0.7069880000	0.0183520000
C	-0.5359680000	-2.7966440000	0.9596930000
H	-2.7607740000	-3.5445340000	-0.6050770000
H	1.0270210000	-1.1792170000	-1.9601340000
H	-0.8344400000	-3.6373720000	0.3363670000
C	1.8442110000	-0.9311070000	-1.2900160000
H	-0.7646670000	-3.0525180000	1.9983400000
C	3.9165040000	-0.2891700000	0.4514390000
H	4.7283030000	-0.0386660000	1.1248000000
C	2.7058180000	-1.9184360000	-0.8488100000
C	3.7485340000	-1.6083690000	0.0290630000
H	2.5708370000	-2.9396490000	-1.1877610000
H	4.4245360000	-2.3820990000	0.3717150000

Zero-point correction=(Hartree/Particle)	0.315586
Thermal correction to Energy=	0.334491
Thermal correction to Enthalpy=	0.335435
Thermal correction to Gibbs Free Energy=	0.266527
Sum of electronic and zero-point Energies=	-1148.782710
Sum of electronic and thermal Energies=	-1148.763804
Sum of electronic and thermal Enthalpies=	-1148.762860
Sum of electronic and thermal Free Energies=	-1148.831768

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	209.896	72.270	145.028

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	0.5311540000	0.8403230000	-2.0974190000
H	-1.3459080000	-0.6899530000	-1.6470960000
C	-0.3182910000	1.1957600000	-1.5215100000
O	-0.5674170000	-2.8449140000	-0.5927530000
H	-2.9096710000	-2.0788260000	-0.7669820000
C	-1.3309010000	0.2865880000	-1.1796350000
H	0.4384300000	3.1945330000	-1.3642700000
C	-0.3681970000	2.5132500000	-1.1203500000
S	1.8248660000	-1.5297930000	-0.7403470000
C	-3.1411330000	-1.5827080000	0.1844370000
C	-0.6332400000	-1.9468330000	0.2512630000
C	-2.4887140000	0.7375350000	-0.4458630000
H	-3.9879290000	-2.1042450000	0.6302080000
H	-1.9885320000	-2.8320710000	1.5501820000
C	4.1748350000	-0.0088270000	-0.7737980000
C	-3.4169640000	-0.1401710000	0.0758640000
C	0.5308930000	-1.0441810000	0.2993480000
C	-1.5366830000	2.9964930000	-0.4658550000
C	-1.8563550000	-1.8464020000	1.0994960000
C	2.8189340000	-0.2108160000	-0.1765040000
C	-2.5645780000	2.1534240000	-0.1633270000
H	-1.6087030000	4.0480340000	-0.2098500000
H	-4.2634280000	0.2679320000	0.6192410000
N	0.9020680000	0.0094140000	1.0649170000
H	-1.8135330000	-1.1036770000	1.8886430000
C	2.1769940000	0.5086600000	0.7697220000
H	-3.4527720000	2.5267060000	0.3366040000
H	2.0382860000	2.5992340000	1.1901260000
C	2.6691060000	1.7436680000	1.4504100000
H	-0.9153650000	0.9773150000	1.4254650000
H	3.6848010000	1.9642350000	1.1306340000
C	-0.0187640000	0.6809360000	1.9722990000
H	-0.2814520000	0.0194500000	2.7992930000
H	2.6755420000	1.6332350000	2.5370730000
H	0.4566460000	1.5700620000	2.3723000000
H	4.7630210000	-0.9277850000	-0.7200090000
H	4.7261650000	0.7710190000	-0.2506800000
H	4.0986080000	0.2763410000	-1.8262860000

Zero-point correction=  
(Hartree/Particle)

0.315866

Thermal correction to Energy=

0.334233

Thermal correction to Enthalpy=

0.335177

Thermal correction to Gibbs Free Energy=

0.270568

Sum of electronic and zero-point Energies=

-1148.768941

Sum of electronic and thermal Energies=

-1148.750573

Sum of electronic and thermal Enthalpies=

-1148.749629

Sum of electronic and thermal Free Energies=

-1148.814238

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	209.735	72.028	135.982

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

```

H      -0.9593520000      3.0801060000     -1.0741070000
H      0.9597660000       1.5867540000     -1.3125890000
C     -1.1284160000       2.0386540000     -1.3267000000
O      2.7397730000       1.5234710000      0.7089460000
H      2.3546660000       0.3332460000     -2.3395300000
C     -0.0362630000       1.1879460000     -1.4704840000
H     -3.2698820000       2.2457190000     -1.4145130000
C     -2.4257000000       1.5742800000     -1.5183930000
S      0.7063490000       -1.7594540000     0.3721980000
C      2.3046780000       -0.6476150000     -1.8582710000
C      2.3815950000       0.3610370000      0.4955510000
C     -0.2184390000       -0.1641920000     -1.8185950000
H      2.8785110000       -1.3326870000     -2.4845270000
H      4.0665930000       -0.0636910000     -0.7147520000
C     -1.9504230000       -2.6124380000     0.7982240000
C      0.8707600000       -1.1185690000     -1.8042500000
C      1.2013530000       -0.2475370000      1.0221700000
C     -2.6244340000       0.2375760000     -1.8687870000
C      3.0998910000       -0.5182590000     -0.5021390000
C     -0.9009090000       -1.5511170000     0.9568790000
C     -1.5414870000       -0.6134730000     -2.0104940000
H     -3.6289010000       -0.1371660000     -2.0327760000
H      0.6643060000       -2.0548560000     -2.3161820000
N      0.1154400000       0.3907350000      1.6318090000
H      3.2732580000       -1.5185530000     -0.0947300000
C     -1.0327060000       -0.3117410000     1.5469140000
H     -1.7061950000       -1.6541130000     -2.2767130000
H     -2.2606070000       0.4747880000      3.1316680000
C     -2.3223080000       0.2372050000      2.0670880000
H      1.1670900000       1.9500290000      2.5245900000
H     -3.1174150000       -0.4925630000      1.9235150000
C      0.2026210000       1.7812780000      2.0542530000
H      0.1252090000       2.4420700000      1.1861970000
H     -2.5896910000       1.1452780000      1.5199690000
H     -0.6021600000       1.9904840000      2.7562780000
H     -1.5403420000       -3.4809010000      0.2798180000
H     -2.7980580000       -2.2523260000      0.2090340000
H     -2.3235230000       -2.9592330000      1.7656140000

```

Zero-point correction=

0.316196

(Hartree/Particle)

Thermal correction to Energy=

0.334878

Thermal correction to Enthalpy=

0.335822

Thermal correction to Gibbs Free Energy=

0.269745

Sum of electronic and zero-point Energies=

-1148.785228

Sum of electronic and thermal Energies=

-1148.766547

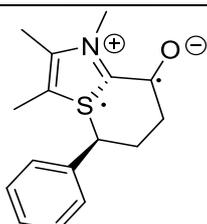
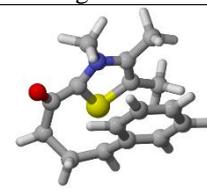
Sum of electronic and thermal Enthalpies=

-1148.765602

Sum of electronic and thermal Free Energies=

-1148.831679

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	210.139	71.520	139.070

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.9593580000	3.0801010000	-1.0741340000
H	0.9597710000	1.5867420000	-1.3126000000
C	-1.1284210000	2.0386480000	-1.3267120000
O	2.7397730000	1.5234770000	0.7089290000
H	2.3546600000	0.3332290000	-2.3395370000
C	-0.0362630000	1.1879410000	-1.4704940000
H	-3.2698820000	2.2457130000	-1.4145310000
C	-2.4256980000	1.5742710000	-1.5184070000
S	0.7063480000	-1.7594450000	0.3722140000
C	2.3046740000	-0.6476280000	-1.8582670000
C	2.3815990000	0.3610390000	0.4955470000
C	-0.2184410000	-0.1642100000	-1.8185940000
H	2.8785070000	-1.3327070000	-2.4845210000
H	4.0665920000	-0.0636900000	-0.7147540000
C	-1.9504210000	-2.6124310000	0.7982450000
C	0.8707590000	-1.1185830000	-1.8042380000
C	1.2013530000	-0.2475310000	1.0221760000
C	-2.6244310000	0.2375650000	-1.8687880000
C	3.0998850000	-0.5182620000	-0.5021400000
C	-0.9009070000	-1.5511120000	0.9568940000
C	-1.5414900000	-0.6134850000	-2.0104880000
H	-3.6289040000	-0.1371880000	-2.0327710000
H	0.6643050000	-2.0548790000	-2.3161640000
N	0.1154450000	0.3907460000	1.6318070000
H	3.2732610000	-1.5185530000	-0.0947220000
C	-1.0327040000	-0.3117290000	1.5469170000
H	-1.7061960000	-1.6541260000	-2.2767000000
H	-2.2606060000	0.4748090000	3.1316690000
C	-2.3223080000	0.2372210000	2.0670860000
H	1.1670940000	1.9500460000	2.5245740000
H	-3.1174170000	-0.4925460000	1.9235300000
C	0.2026250000	1.7813010000	2.0542350000
H	0.1252100000	2.4420790000	1.1861750000
H	-2.5896880000	1.1452920000	1.5199620000
H	-0.6021560000	1.9905090000	2.7562620000
H	-1.5403430000	-3.4808960000	0.2798490000
H	-2.7980570000	-2.2523220000	0.2090530000
H	-2.3235230000	-2.9592170000	1.7656450000

Zero-point correction=  
(Hartree/Particle)

0.316196

Thermal correction to Energy=

0.334877

Thermal correction to Enthalpy=

0.335822

Thermal correction to Gibbs Free Energy=

0.269746

Sum of electronic and zero-point Energies=

-1148.785228

Sum of electronic and thermal Energies=

-1148.766547

Sum of electronic and thermal Enthalpies=

-1148.765603

Sum of electronic and thermal Free Energies=

-1148.831678

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	210.139	71.520	139.068

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 guess=(mix,always)	

38

XYZ file generated by gabedit : coordinates in Angstrom

```

H      -0.9593580000      3.0801010000     -1.0741340000
H      0.9597710000      1.5867420000     -1.3126000000
C     -1.1284210000      2.0386480000     -1.3267120000
O      2.7397730000      1.5234770000      0.7089290000
H      2.3546600000      0.3332290000     -2.3395370000
C     -0.0362630000      1.1879410000     -1.4704940000
H     -3.2698820000      2.2457130000     -1.4145310000
C     -2.4256980000      1.5742710000     -1.5184070000
S      0.7063480000     -1.7594450000      0.3722140000
C      2.3046740000     -0.6476280000     -1.8582670000
C      2.3815990000      0.3610390000      0.4955470000
C     -0.2184410000     -0.1642100000     -1.8185940000
H      2.8785070000     -1.3327070000     -2.4845210000
H      4.0665920000     -0.0636900000     -0.7147540000
C     -1.9504210000     -2.6124310000      0.7982450000
C      0.8707590000     -1.1185830000     -1.8042380000
C      1.2013530000     -0.2475310000      1.0221760000
C     -2.6244310000      0.2375650000     -1.8687880000
C      3.0998850000     -0.5182620000     -0.5021400000
C     -0.9009070000     -1.5511120000      0.9568940000
C     -1.5414900000     -0.6134850000     -2.0104880000
H     -3.6289040000     -0.1371880000     -2.0327710000
H      0.6643050000     -2.0548790000     -2.3161640000
N      0.1154450000      0.3907460000      1.6318070000
H      3.2732610000     -1.5185530000     -0.0947220000
C     -1.0327040000     -0.3117290000      1.5469170000
H     -1.7061960000     -1.6541260000     -2.2767000000
H     -2.2606060000      0.4748090000      3.1316690000
C     -2.3223080000      0.2372210000      2.0670860000
H      1.1670940000      1.9500460000      2.5245740000
H     -3.1174170000     -0.4925460000      1.9235300000
C      0.2026250000      1.7813010000      2.0542350000
H      0.1252100000      2.4420790000      1.1861750000
H     -2.5896880000      1.1452920000      1.5199620000
H     -0.6021560000      1.9905090000      2.7562620000
H     -1.5403430000     -3.4808960000      0.2798490000
H     -2.7980570000     -2.2523220000      0.2090530000
H     -2.3235230000     -2.9592170000      1.7656450000

```

Zero-point correction=  
(Hartree/Particle)

0.316196

Thermal correction to Energy=

0.334877

Thermal correction to Enthalpy=

0.335822

Thermal correction to Gibbs Free Energy=

0.269746

Sum of electronic and zero-point Energies=

-1148.785228

Sum of electronic and thermal Energies=

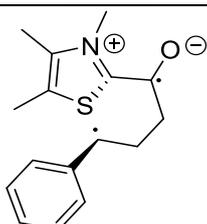
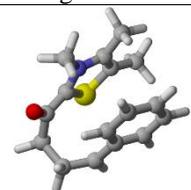
-1148.766547

Sum of electronic and thermal Enthalpies=

-1148.765603

Sum of electronic and thermal Free Energies=

-1148.831678

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	0.4884880000	2.8712970000	1.5866910000
H	-1.5564030000	1.6585010000	0.9908960000
C	0.4480400000	1.7958320000	1.7239070000
O	-2.2797510000	1.5956400000	-1.5191820000
H	-3.3773550000	0.4855420000	0.7314420000
C	-0.7148740000	1.1141740000	1.4052930000
H	2.4681390000	1.6610110000	2.4690840000
C	1.5636450000	1.1184110000	2.2204240000
S	-0.0106270000	-1.6539760000	-1.4938930000
C	-3.1464840000	-0.5538310000	0.4826970000
C	-1.9286470000	0.4030050000	-1.4707100000
C	-0.8047960000	-0.2891110000	1.5844650000
H	-4.0180440000	-1.1540190000	0.7565060000
H	-3.8974680000	-0.3770710000	-1.5485310000
C	2.7010440000	-2.1100790000	-0.9633060000
C	-1.9500450000	-1.0501000000	1.2278360000
C	-0.5752300000	-0.0065450000	-1.6347580000
C	1.4962470000	-0.2639500000	2.4069340000
C	-2.9566580000	-0.6355000000	-1.0582660000
C	1.6420490000	-1.1087000000	-1.2884190000
C	0.3366380000	-0.9529570000	2.1022690000
H	2.3545530000	-0.8000880000	2.7965510000
H	-1.8962960000	-2.1190380000	1.4117120000
N	0.5062320000	0.8473170000	-1.6886000000
H	-2.6846510000	-1.6536210000	-1.3477520000
C	1.7249210000	0.2336680000	-1.4155280000
H	0.2910930000	-2.0281110000	2.2445020000
H	3.2493850000	1.5392750000	-2.2010230000
C	2.9557420000	1.0676440000	-1.2595000000
H	-0.3631780000	2.4657360000	-2.6822490000
H	3.7834410000	0.4505670000	-0.9169120000
C	0.3675000000	2.2856250000	-1.8992530000
H	0.0180510000	2.7773980000	-0.9898530000
H	2.7906850000	1.8516170000	-0.5160160000
H	1.3335570000	2.6882640000	-2.1952610000
H	2.6637590000	-2.9562320000	-1.6539820000
H	2.5670190000	-2.4979850000	0.0510840000
H	3.6951020000	-1.6698680000	-1.0335950000

Zero-point correction=  
(Hartree/Particle)

0.314996

Thermal correction to Energy=

0.333969

Thermal correction to Enthalpy=

0.334913

Thermal correction to Gibbs Free Energy=

0.266553

Sum of electronic and zero-point Energies=

-1148.792165

Sum of electronic and thermal Energies=

-1148.773192

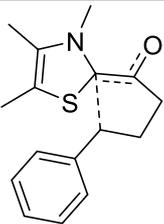
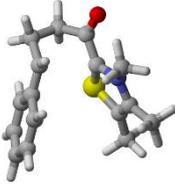
Sum of electronic and thermal Enthalpies=

-1148.772248

Sum of electronic and thermal Free Energies=

-1148.840608

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	209.569	72.571	143.878

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1  Guess=(mix,always)	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	0.0260340000	2.2591060000	-1.9966360000
H	0.7641490000	3.7655450000	-1.4346710000
H	1.2458010000	-3.1400550000	-2.6340340000
C	0.3515070000	2.8094750000	-1.1077640000
S	0.5612730000	-0.3185990000	-1.6155070000
C	0.8141540000	-3.1197910000	-1.6278260000
H	-1.7534900000	3.1795370000	-0.6379760000
H	-0.2664250000	-3.2599440000	-1.7293720000
C	1.4278390000	2.0391480000	-0.3467820000
C	1.1288620000	-1.8387500000	-0.9231070000
C	-0.8156900000	2.9779080000	-0.1096260000
C	1.2427810000	0.5978410000	-0.2812490000
O	2.3267270000	2.6299740000	0.2572320000
H	1.2102770000	-3.9769420000	-1.0821930000
H	-0.6154220000	3.8541650000	0.5135440000
C	1.8109730000	-1.6132700000	0.2248370000
N	1.9209740000	-0.2603000000	0.5640050000
C	-0.9298350000	1.7620570000	0.7934820000
H	2.2535710000	-3.6449580000	0.7161420000
H	3.5190940000	-2.5098690000	1.1832570000
H	2.6736990000	1.2246200000	1.8152540000
C	2.4356460000	-2.6469540000	1.1105600000
H	-0.5003370000	1.8615730000	1.7850980000
C	2.4076310000	0.1739560000	1.8766080000
H	3.2923500000	-0.4001670000	2.1478760000
H	2.0269280000	-2.6097770000	2.1245760000
H	1.6346310000	0.0280520000	2.6391430000
C	-1.8594300000	0.7038260000	0.6144670000
C	-2.5950240000	0.5133280000	-0.5863760000
C	-3.4996790000	-0.5352340000	-0.7207330000
C	-3.6970250000	-1.4453790000	0.3163310000
C	-2.9725000000	-1.2891920000	1.5078270000
C	-2.0771160000	-0.2464480000	1.6535660000
H	-2.4723000000	1.2109280000	-1.4063730000
H	-4.0554690000	-0.6431230000	-1.6464490000
H	-4.4042110000	-2.2594800000	0.2070320000
H	-3.1227660000	-1.9866220000	2.3254680000
H	-1.5356990000	-0.1278080000	2.5872370000

Zero-point correction=  
(Hartree/Particle)

0.311336

Thermal correction to Energy=

0.330086

Thermal correction to Enthalpy=

0.331030

Thermal correction to Gibbs Free Energy=

0.264031

Sum of electronic and zero-point Energies=

-1149.149993

Sum of electronic and thermal Energies=

-1149.131243

Sum of electronic and thermal Enthalpies=

-1149.130299

Sum of electronic and thermal Free Energies=

-1149.197298

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	207.132	71.489	141.011

Relaxierte PES-scans der Primäraddukte 41:

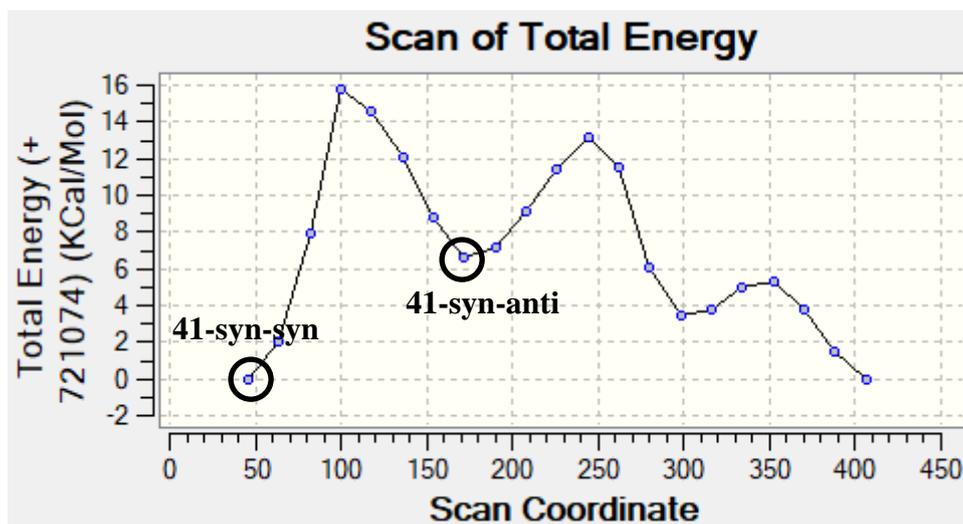


Abbildung A 139: Ergebnis des relaxierten PES-scans von **41-syn** um Diederwinkel 2

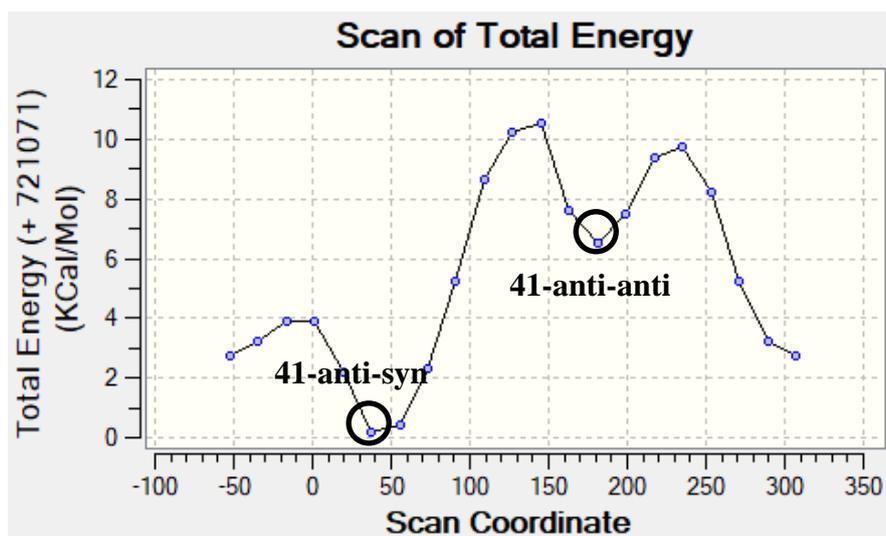


Abbildung A 140: Ergebnis des relaxierten PES-scans von **41-anti** um Diederwinkel 2

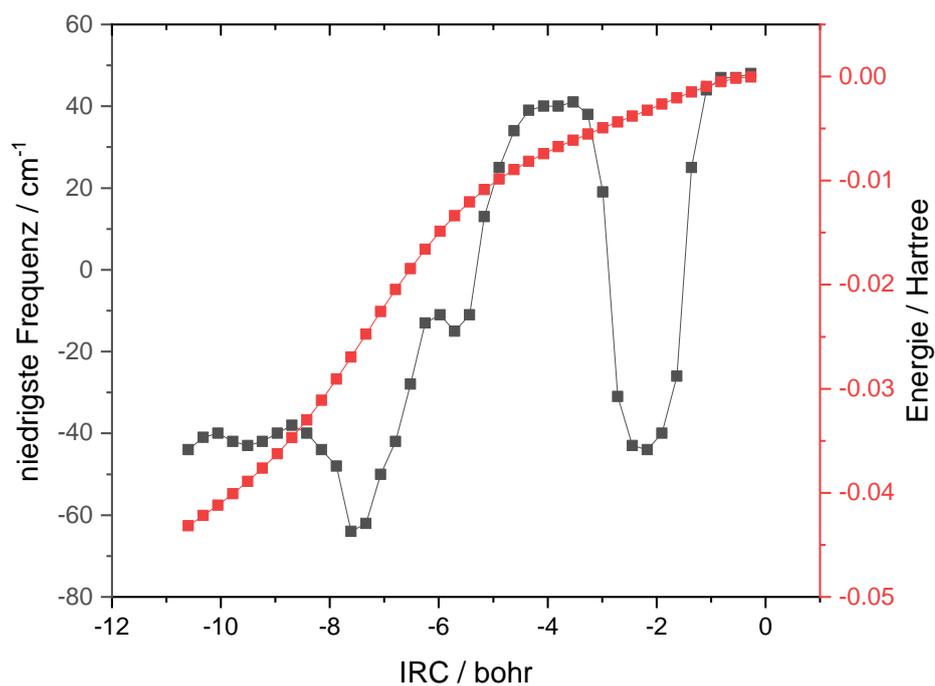


Abbildung A 141: IRC-Verlauf (Energie, rot) und Analyse nach *Harabuchi* (niedrigste orthogonale Frequenz, schwarz) von **42-syn-anti** auf der Methode M062X/6-311+G\*\*, in der Gasphase.

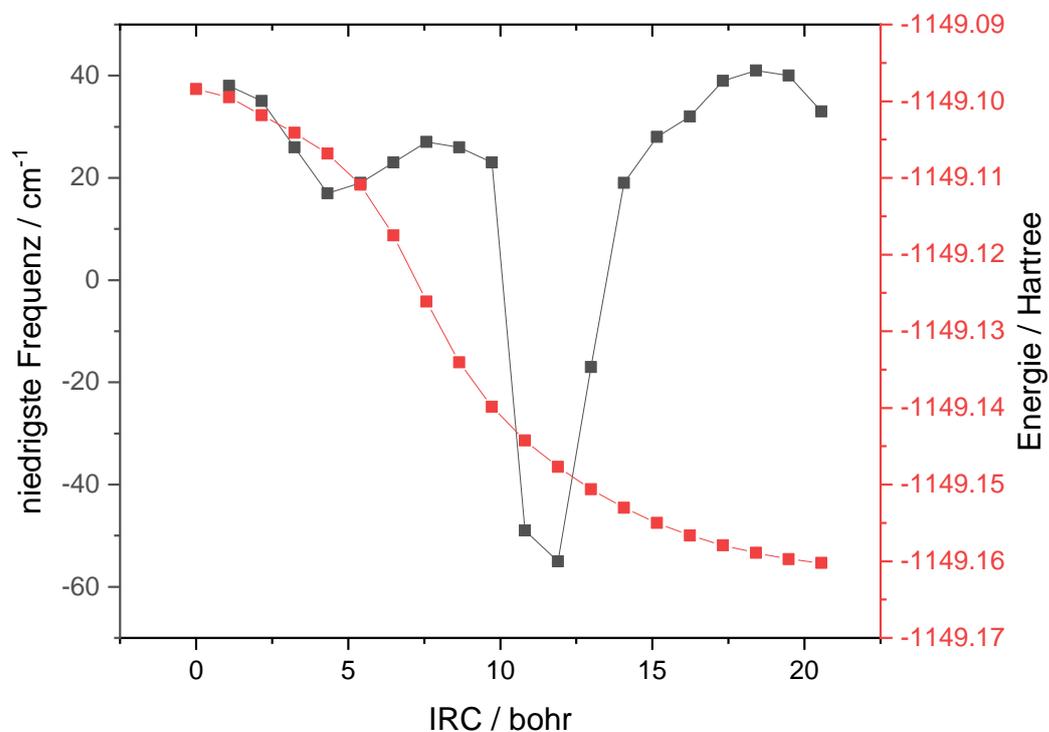


Abbildung A 142: IRC-Verlauf (Energie, rot) und Analyse nach *Harabuchi* (niedrigste orthogonale Frequenz, schwarz) von **42-anti-syn** auf der Methode M062X/6-311+G\*\*, in der Gasphase.

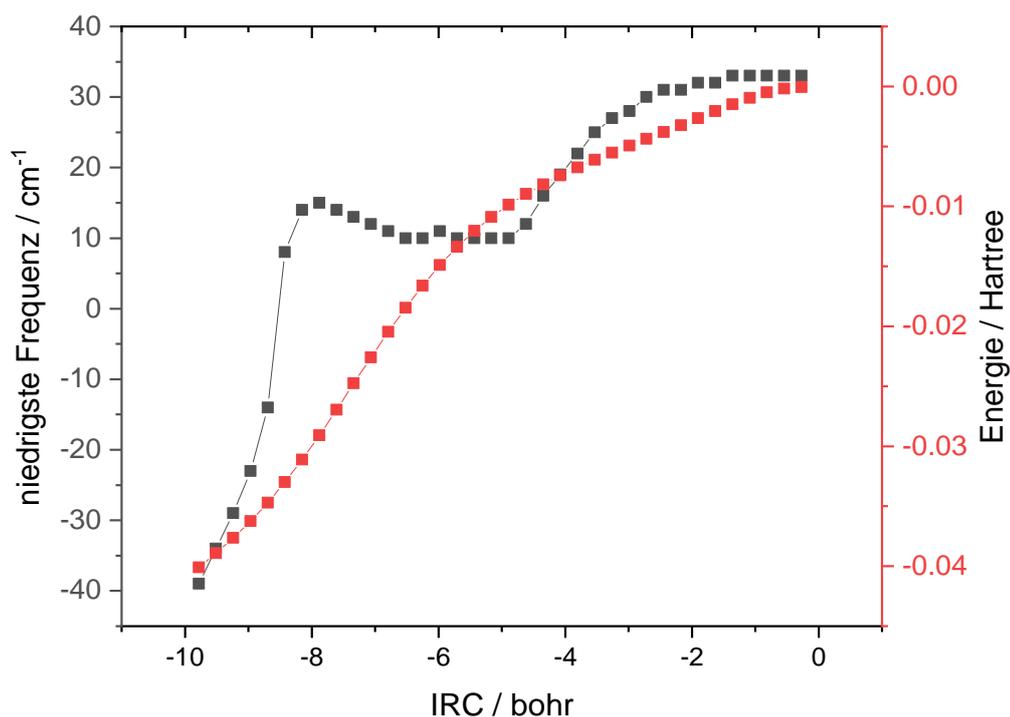
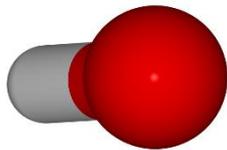


Abbildung A 143: IRC-Verlauf (Energie, rot) und Analyse nach *Harabuchi* (niedrigste orthogonale Frequenz, schwarz) von **42-anti-anti** auf der Methode M062X/6-311+G\*\*, in der Gasphase.

Die aus den Analysen nach *Harabuchi* erhaltenen negativen Frequenzen treten zum größten Teil sehr spät entlang des IRC-Pfades auf. Zu diesem Zeitpunkt ist die Struktur **38** bereits nahezu vollständig gebildet. Bei allen Schwingungen handelt es sich um Rotationsschwingungen von Methylgruppen oder Gerüstschwingungen- Den Gerüstschwingungen entlang des IRCs von **42-syn-anti** (Abbildung A 141, spät entlang des IRC) könnten einen minimalen Anteil einer Schwingung beinhalten, welche auf einen TS **43** hindeutet. Es konnte jedoch keine Schwingung eindeutig mit einer möglichen Bifurkation in Zusammenhang gebracht werden.

## Fragmentierung:

#M062X/6-311+G**	<b>(OH<sup>-</sup>)</b>
------------------	-------------------------

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
$\ominus$ OH	-1 1	

2

XYZ file generated by gabedit : coordinates in Angstrom

O	0.0000000000	-0.4814230000	-0.3744390000
H	0.0000000000	0.4814230000	-0.3744400000

Zero-point correction=	0.008773
(Hartree/Particle)	
Thermal correction to Energy=	0.011133
Thermal correction to Enthalpy=	0.012077
Thermal correction to Gibbs Free Energy=	-0.007476
Sum of electronic and zero-point Energies=	-75.775838
Sum of electronic and thermal Energies=	-75.773478
Sum of electronic and thermal Enthalpies=	-75.772533
Sum of electronic and thermal Free Energies=	-75.792087

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	6.986	4.968	41.153

#M062X/6-311+G**	<b>(H<sub>2</sub>O)</b>
------------------	-------------------------

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
H <sub>2</sub> O	0 1	

3

XYZ file generated by gabedit : coordinates in Angstrom

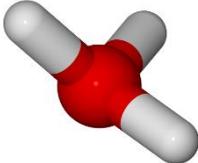
O	0.0000000000	0.1166230000	0.0000000000
H	0.7615700000	-0.4666790000	0.0000000000
H	-0.7615700000	-0.4663080000	0.0000000000

Zero-point correction=	0.021620
(Hartree/Particle)	
Thermal correction to Energy=	0.024456
Thermal correction to Enthalpy=	0.025400
Thermal correction to Gibbs Free Energy=	0.003332
Sum of electronic and zero-point Energies=	-76.399196
Sum of electronic and thermal Energies=	-76.396360
Sum of electronic and thermal Enthalpies=	-76.395416
Sum of electronic and thermal Free Energies=	-76.417485

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	15.346	6.015	46.447

#M062X/6-311+G\*\*

(H<sub>3</sub>O<sup>+</sup>)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
⊕ OH <sub>3</sub>	+1 1	

4

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.9005510000	0.2955150000	0.1794780000
H	0.1939210000	-0.9271470000	0.1793900000
H	0.7065250000	0.6311450000	0.1795390000
O	0.0000130000	0.0000610000	-0.0673010000

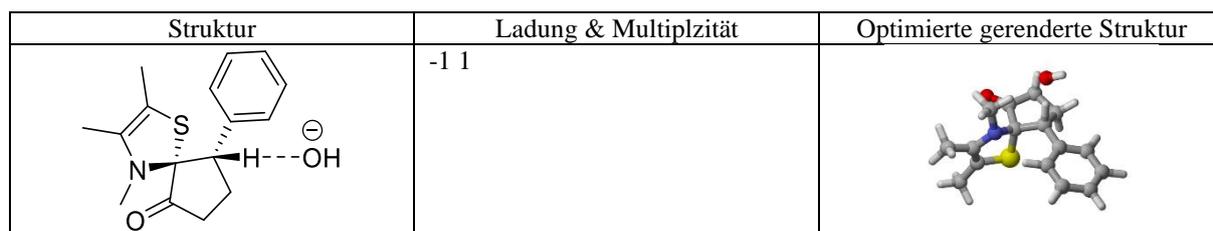
Zero-point correction= 0.034455  
(Hartree/Particle)

Thermal correction to Energy=	0.037384
Thermal correction to Enthalpy=	0.038328
Thermal correction to Gibbs Free Energy=	0.015314
Sum of electronic and zero-point Energies=	-76.659471
Sum of electronic and thermal Energies=	-76.656542
Sum of electronic and thermal Enthalpies=	-76.655598
Sum of electronic and thermal Free Energies=	-76.678612

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	23.459	6.767	48.437

#M062X/6-311+G\*\*

(49-s)



40

XYZ file generated by gabedit : coordinates in Angstrom

H	4.8504850000	-2.6983020000	0.3841000000
H	2.6418010000	-3.0863590000	1.4600750000
C	4.0522160000	-1.9719770000	0.2784970000
O	0.9374950000	2.8645690000	1.7416150000
H	1.7982930000	3.0645240000	2.1167960000
H	5.1971650000	-0.6243780000	-0.9428480000
C	2.8133360000	-2.1842060000	0.8814290000
H	-2.4231050000	-3.2865770000	-1.7507600000
C	4.2421700000	-0.8109520000	-0.4616340000
H	-3.7565640000	-2.9190620000	-0.6498790000
H	-2.5414770000	-1.9749010000	2.5246350000
C	-3.0314890000	-2.4755390000	-1.3341550000
H	-3.8194400000	-2.2380990000	1.3262420000
C	1.7893470000	-1.2562820000	0.7501470000
C	3.2134440000	0.1171650000	-0.5988260000
H	0.8315340000	-1.4357850000	1.2224160000
C	-3.1045520000	-1.5114540000	1.7083810000
H	-3.5819870000	-2.0219110000	-2.1648780000
C	-2.1753740000	-1.4649780000	-0.6459320000
C	-2.1757560000	-1.0505200000	0.6288580000
C	1.9605620000	-0.0760770000	0.0042860000
H	3.3894980000	1.0097650000	-1.1875670000
S	-0.8504950000	-0.7137060000	-1.5719530000
H	-3.6591320000	-0.6679520000	2.1278150000
N	-1.1527110000	-0.1605300000	0.9946640000
H	-1.3788580000	0.0763600000	3.0669950000
C	-0.5486640000	0.4933380000	-0.1622190000
C	-1.3276500000	0.6963720000	2.1686160000
C	0.8959960000	0.9527950000	-0.0922580000
H	-0.4686670000	1.3692760000	2.2569790000
H	1.1080040000	1.4352200000	-2.2282490000
H	0.9881100000	1.7491300000	0.8676760000
H	-2.2340460000	1.3096540000	2.0973910000
C	1.0082950000	1.9470850000	-1.2594550000
C	-1.3030470000	1.7762910000	-0.5820800000
H	1.8664390000	2.6091930000	-1.1273790000
O	-2.4789430000	1.9679720000	-0.4059820000
C	-0.3009910000	2.7385160000	-1.1777640000
H	-0.6625510000	3.1725540000	-2.1110990000
H	-0.1840830000	3.5228660000	-0.4202870000

Zero-point correction=  
(Hartree/Particle)

0.323827

Thermal correction to Energy=

0.344261

Thermal correction to Enthalpy=

0.345205

Thermal correction to Gibbs Free Energy=

0.275167

Sum of electronic and zero-point Energies=

-1224.678544

Sum of electronic and thermal Energies=

-1224.658110

Sum of electronic and thermal Enthalpies=

-1224.657166

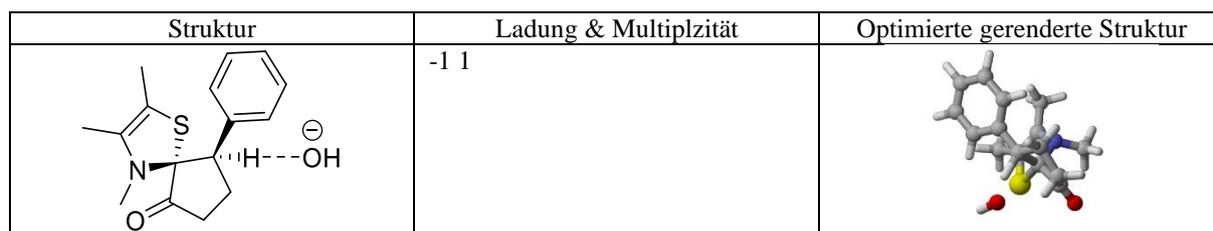
Sum of electronic and thermal Free Energies=

-1224.727204

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	216.027	78.043	147.407

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(49-r)



40

XYZ file generated by gabedit : coordinates in Angstrom

H	1.9565350000	2.0297090000	2.0954180000
H	0.8309430000	3.3848750000	2.2389100000
H	-1.3019180000	-2.1204360000	2.9193940000
C	1.3438150000	2.7350590000	1.5238620000
H	2.0057220000	3.3503110000	0.9130150000
O	-1.6373190000	-2.3574020000	2.0514930000
S	-0.9612700000	1.1276240000	1.5083310000
C	0.3534840000	1.9925740000	0.6866550000
H	-0.8732550000	-1.8062500000	1.1171230000
C	-0.4127350000	-1.2566190000	0.0268580000
H	2.1091410000	2.9172760000	-1.1930040000
C	0.3801300000	1.7599610000	-0.6305180000
C	-1.1501810000	0.0795610000	-0.0175100000
C	1.4307840000	2.1735780000	-1.6115070000
H	-2.8995320000	-2.4237190000	0.1068790000
C	-2.6178090000	-0.3787860000	-0.2217430000
O	-3.5912210000	0.2972090000	-0.0189270000
N	-0.6876560000	0.9415390000	-1.1313810000
H	2.0121570000	1.2911280000	-1.8997190000
H	-0.8651160000	-3.1125010000	-1.0225000000
H	-2.2355250000	2.4206650000	-1.0570010000
C	-1.1253800000	-2.0522510000	-1.0730630000
C	-2.6002170000	-1.7989400000	-0.7417900000
H	0.9854400000	2.5886840000	-2.5205540000
C	-1.7082630000	1.7782800000	-1.7741870000
H	-0.9023410000	-1.6845840000	-2.0858930000
H	-1.2158620000	2.4034820000	-2.5219050000
H	-3.3115930000	-1.9133000000	-1.5625040000
H	-2.4397830000	1.1523060000	-2.2872170000
C	1.0693020000	-1.2016400000	-0.0364390000
C	1.8167560000	-0.8199770000	1.0948470000
C	3.2004900000	-0.7374070000	1.0590850000
C	3.9016490000	-1.0668750000	-0.1032730000
C	3.1878650000	-1.4866430000	-1.2189920000
C	1.7949700000	-1.5490550000	-1.1854290000
H	1.2765840000	-0.5871820000	2.0061910000
H	3.7434010000	-0.4324470000	1.9486900000
H	4.9845420000	-1.0129950000	-0.1280980000
H	3.7153750000	-1.7591200000	-2.1280670000
H	1.2593540000	-1.8620210000	-2.0744510000

Zero-point correction=  
(Hartree/Particle)

0.323235

Thermal correction to Energy=

0.343621

Thermal correction to Enthalpy=

0.344565

Thermal correction to Gibbs Free Energy=

0.274946

Sum of electronic and zero-point Energies=

-1224.666056

Sum of electronic and thermal Energies=

-1224.645670

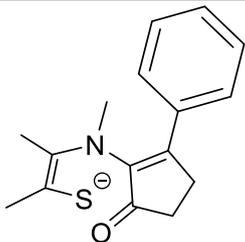
Sum of electronic and thermal Enthalpies=

-1224.644726

Sum of electronic and thermal Free Energies=

-1224.714344

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	215.625	78.038	146.525

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	-1 1	

37

XYZ file generated by gabedit : coordinates in Angstrom

H	-5.2958470000	-2.0702270000	-0.0735400000
C	-4.4207280000	-1.4296360000	-0.0589190000
H	-3.0991420000	-2.9655160000	0.6649280000
H	-5.4830810000	0.3128330000	-0.7413740000
C	-3.1862400000	-1.9320760000	0.3469730000
C	-4.5255400000	-0.0921100000	-0.4312170000
H	4.0312350000	-2.5918570000	0.8189450000
C	-2.0594690000	-1.1180860000	0.3671910000
C	-3.4023340000	0.7274220000	-0.4078980000
H	-1.0989540000	-1.4860360000	0.7244120000
H	-3.4897340000	1.7690160000	-0.7006500000
C	-2.1495990000	0.2239750000	-0.0304660000
C	3.9572900000	-1.5034100000	0.7361170000
H	4.6910430000	-1.1462570000	0.0108440000
S	1.3705740000	-1.4587050000	1.6796050000
H	4.2106970000	-1.0945420000	1.7163270000
C	2.5292010000	-1.1160800000	0.4084860000
H	-1.7762610000	2.3756480000	1.6045740000
H	2.6875850000	-0.4168210000	-2.8763250000
C	-0.9774160000	1.1075740000	0.0497990000
C	2.2396290000	-0.5429480000	-0.7828020000
H	4.0679470000	-0.9182060000	-1.9077340000
C	0.3142030000	0.8604250000	-0.3096840000
N	0.8919390000	-0.1113660000	-1.0739880000
C	3.1948040000	-0.2656760000	-1.9166760000
C	-1.1328880000	2.4582770000	0.7240880000
H	-1.5906890000	3.2011800000	0.0585820000
H	-0.1531030000	-1.9472980000	-1.2379520000
C	0.0975320000	-1.0580250000	-1.8283980000
H	3.5278370000	0.7783220000	-1.8915640000
H	-0.8242460000	-0.5875680000	-2.1771820000
C	1.1484990000	2.0335000000	0.1217930000
C	0.3035010000	2.8621310000	1.0684400000
H	0.5527770000	2.5362430000	2.0823490000
H	0.6815810000	-1.3760300000	-2.6968240000
O	2.2586640000	2.3164900000	-0.2552550000
H	0.5356160000	3.9224980000	0.9674950000

Zero-point correction=  
(Hartree/Particle)

0.304407

Thermal correction to Energy=

0.323107

Thermal correction to Enthalpy=

0.324052

Thermal correction to Gibbs Free Energy=

0.256794

Sum of electronic and zero-point Energies=

-1148.304163

Sum of electronic and thermal Energies=

-1148.285463

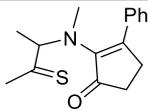
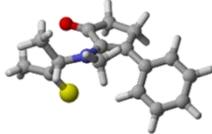
Sum of electronic and thermal Enthalpies=

-1148.284519

Sum of electronic and thermal Free Energies=

-1148.351777

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	202.753	70.185	141.556

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

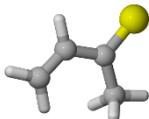
XYZ file generated by gabedit : coordinates in Angstrom

H	5.4385350000	-1.8435450000	-0.3517030000
C	4.5343990000	-1.2543050000	-0.2546390000
H	3.2598890000	-2.7722080000	-1.0891130000
H	5.5446810000	0.4493550000	0.5808610000
C	3.3099000000	-1.7773250000	-0.6618620000
C	4.5939030000	0.0340080000	0.2676940000
H	-4.5624510000	-1.6149940000	-0.2817270000
C	2.1490710000	-1.0258870000	-0.5316950000
C	3.4357920000	0.7932280000	0.3859290000
H	1.1943480000	-1.4147640000	-0.8720780000
H	3.4906850000	1.7992250000	0.7877970000
C	2.1964480000	0.2673870000	0.0041990000
C	-4.0549200000	-0.7510910000	-0.7242390000
H	-4.3642340000	0.1352620000	-0.1640470000
S	-1.6118650000	-1.0069410000	-1.9239830000
H	-4.3507160000	-0.6568900000	-1.7657650000
C	-2.5701590000	-0.9152380000	-0.6112520000
H	1.5999500000	2.6759590000	-1.2324550000
H	-2.4713890000	-0.9415990000	2.8968640000
C	0.9740930000	1.0810910000	0.0730570000
C	-2.0115480000	-1.0943490000	0.8008070000
H	-3.8697280000	-1.3659150000	1.9152620000
C	-0.2805610000	0.6696640000	0.4001240000
N	-0.6884030000	-0.5032990000	0.9938040000
C	-2.9710590000	-0.7470150000	1.9459110000
C	1.0114440000	2.5414940000	-0.3219140000
H	1.4847780000	3.1487680000	0.4567850000
H	0.6514200000	-2.1253650000	1.3266490000
C	0.2061340000	-1.2659300000	1.8424130000
H	-3.2508720000	0.3040540000	1.9090670000
H	1.0136350000	-0.6267770000	2.1979030000
C	-1.2375020000	1.7703110000	0.1008060000
C	-0.4606440000	2.9212500000	-0.5025710000
H	-0.7281990000	2.9813140000	-1.5609220000
H	-0.3488590000	-1.6327750000	2.7109400000
O	-2.4334270000	1.7469090000	0.2841900000
H	-0.7598560000	3.8581820000	-0.0319670000
H	-1.8442870000	-2.1821750000	0.8446500000

Zero-point correction= 0.317813  
(Hartree/Particle)

Thermal correction to Energy= 0.336261  
 Thermal correction to Enthalpy= 0.337205  
 Thermal correction to Gibbs Free Energy= 0.271346  
 Sum of electronic and zero-point Energies= -1148.831620  
 Sum of electronic and thermal Energies= -1148.813172  
 Sum of electronic and thermal Enthalpies= -1148.812228  
 Sum of electronic and thermal Free Energies= -1148.878087

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	211.007	70.446	138.612

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

11

XYZ file generated by gabedit : coordinates in Angstrom

H	-2.5759270000	-0.6100540000	0.0000070000
S	1.6737550000	0.4198240000	0.0000300000
H	-0.7584580000	-1.8753220000	-0.8816210000
C	-2.2699150000	0.4300830000	0.0000520000
C	-0.9861930000	0.7971340000	-0.0000430000
C	0.1439850000	-0.1425630000	-0.0000790000
C	-0.1653850000	-1.6146880000	-0.0000690000
H	-0.7163070000	1.8478900000	-0.0003510000
H	-3.0590700000	1.1721590000	0.0002300000
H	-0.7575480000	-1.8749390000	0.8823090000
H	0.7522800000	-2.1967110000	-0.0002180000

Zero-point correction= 0.088413  
(Hartree/Particle)

Thermal correction to Energy= 0.094180

Thermal correction to Enthalpy= 0.095124

Thermal correction to Gibbs Free Energy= 0.059123

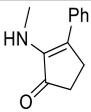
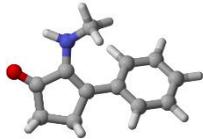
Sum of electronic and zero-point Energies= -554.057606

Sum of electronic and thermal Energies= -554.051839

Sum of electronic and thermal Enthalpies= -554.050895

Sum of electronic and thermal Free Energies= -554.086896

	E (Thermal) kCal/Mol	CV cal/Mol-Kelvin	S cal/Mol-kelvin
Total	59.099	19.887	75.770

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

27

XYZ file generated by gabedit : coordinates in Angstrom

H	4.8721320000	0.1499050000	-0.2247080000
H	3.9170930000	-1.6988870000	1.1223970000
H	-0.8561660000	-2.4171300000	0.9965020000
C	3.7986470000	0.0130920000	-0.1723320000
C	3.2617660000	-1.0252720000	0.5827750000
H	3.3609810000	1.6636670000	-1.4783140000
C	2.9491340000	0.8671540000	-0.8695980000
C	1.8855750000	-1.2040010000	0.6465030000
H	1.4763880000	-2.0176660000	1.2349620000
C	-0.4321910000	2.4705730000	0.8888520000
C	1.5728180000	0.6955970000	-0.7985800000
C	1.0191770000	-0.3348620000	-0.0274380000
H	0.9105050000	1.3413140000	-1.3652130000
C	-0.4340670000	-0.5406650000	0.0043730000
C	-1.0226640000	-1.9395050000	0.0258800000
C	-1.4037460000	0.4048460000	-0.0431640000
N	-1.3755750000	1.7757640000	0.0237000000
H	-0.5406510000	-2.5706450000	-0.7251670000
H	-3.1778970000	-2.2501440000	0.4710370000
C	-2.7342370000	-0.2461730000	-0.1565000000
C	-2.5225680000	-1.7435540000	-0.2382550000
H	-2.3187810000	2.1443040000	0.0396560000
O	-3.7832380000	0.3520840000	-0.1765330000
H	-2.8045680000	-2.0752420000	-1.2403940000
H	0.5000520000	2.7072710000	0.3726350000
H	-0.1848460000	1.8676770000	1.7693740000
H	-0.8851690000	3.4051680000	1.2185070000

Zero-point correction=  
(Hartree/Particle)

0.226258

Thermal correction to Energy=

0.238654

Thermal correction to Enthalpy=

0.239598

Thermal correction to Gibbs Free Energy=

0.187145

Sum of electronic and zero-point Energies=

-594.753373

Sum of electronic and thermal Energies=

-594.740978

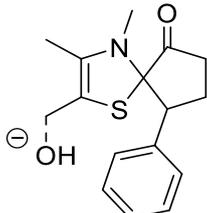
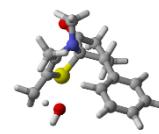
Sum of electronic and thermal Enthalpies=

-594.740033

Sum of electronic and thermal Free Energies=

-594.792487

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	149.758	47.517	110.397

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	-1 1	

40

XYZ file generated by gabedit : coordinates in Angstrom

H	2.5502960000	-2.9671040000	-1.5925210000
H	2.4047980000	-3.4865770000	0.0857710000
C	2.0444910000	-2.7586360000	-0.6483780000
H	0.0642120000	-3.7023630000	-0.5152720000
O	3.5720000000	-1.0261410000	0.0861980000
C	0.5133970000	-2.7323340000	-0.7288750000
C	2.4443450000	-1.3786950000	-0.1353390000
H	0.1778520000	-2.4215780000	-1.7222040000
H	0.3138440000	-2.0376010000	1.2958750000
C	0.1002620000	-1.6474990000	0.2857690000
C	1.1670120000	-0.5492280000	0.0667310000
H	3.1739840000	0.6658400000	1.8983540000
H	-1.9644900000	-3.3447040000	0.4336080000
S	0.9848320000	0.3225250000	-1.5722760000
H	2.1919920000	-0.6800780000	2.5148440000
C	2.1579730000	0.3570250000	2.1717050000
H	0.2937930000	2.8367450000	-2.6154480000
C	-2.3067020000	-2.3173880000	0.3481860000
C	-1.3697650000	-1.2802790000	0.2511190000
N	1.2003050000	0.4801660000	1.0837430000
C	0.8277780000	1.9126960000	-0.7620570000
C	0.9728800000	1.7908930000	0.5654780000
C	0.2958730000	3.0453690000	-1.5433570000
H	1.5470250000	3.2599160000	2.0615600000
H	1.8073700000	0.9681750000	3.0063910000
H	-4.3770630000	-2.8786510000	0.4219310000
C	-3.6723610000	-2.0569600000	0.3450720000
C	-1.8434780000	0.0292470000	0.1629820000
H	-1.1876900000	0.8871750000	0.0971820000
O	-2.0515840000	3.1887010000	-0.3573180000
H	-0.9335480000	3.1798930000	-1.0429190000
H	0.8690020000	3.9594800000	-1.3604460000
C	0.6593430000	2.8776190000	1.5431530000
H	0.1568610000	3.6919300000	1.0195860000
H	-2.5776360000	3.8971550000	-0.7367540000
H	-0.0429120000	2.4974840000	2.2939540000
C	-4.1296670000	-0.7444780000	0.2423720000
C	-3.2114780000	0.2948260000	0.1521630000
H	-5.1950970000	-0.5394690000	0.2339910000
H	-3.4947940000	1.3392350000	0.0613500000

Zero-point correction=  
(Hartree/Particle)

0.322938

Thermal correction to Energy=

0.343182

Thermal correction to Enthalpy=

0.344126

Thermal correction to Gibbs Free Energy=

0.274939

Sum of electronic and zero-point Energies=

-1224.656767

Sum of electronic and thermal Energies=

-1224.636523

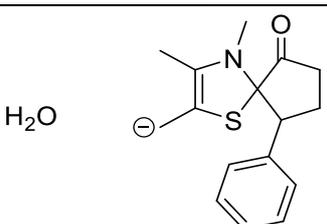
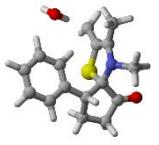
Sum of electronic and thermal Enthalpies=

-1224.635579

Sum of electronic and thermal Free Energies=

-1224.704766

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	215.350	77.897	145.616

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
 <p>H<sub>2</sub>O</p>	-1 1	

40

XYZ file generated by gabedit : coordinates in Angstrom

H	2.3142460000	-3.0202110000	-1.7210000000
H	2.1472410000	-3.6485810000	-0.0818740000
C	1.8291150000	-2.8494390000	-0.7586310000
H	-0.2070860000	-3.6717320000	-0.6543910000
O	3.4713350000	-1.2889890000	0.0957610000
C	0.3020160000	-2.7225430000	-0.8257650000
C	2.3213330000	-1.5346390000	-0.1550980000
H	-0.0181200000	-2.3425130000	-1.7997630000
H	0.1515460000	-2.1199490000	1.2320810000
C	-0.0325150000	-1.6648610000	0.2440810000
C	1.1013120000	-0.6286760000	0.0811220000
H	3.1763320000	0.3608100000	1.9165530000
H	-2.2016370000	-3.2166350000	0.3776250000
S	1.0108850000	0.2959080000	-1.5353600000
H	2.1062140000	-0.9313470000	2.5130120000
C	2.1460410000	0.1169070000	2.2028780000
H	0.8534430000	2.8986910000	-2.5737420000
C	-2.4760140000	-2.1671180000	0.3214290000
C	-1.4709230000	-1.1960030000	0.2370200000
N	1.1765850000	0.3559440000	1.1408650000
C	1.0472610000	1.8914010000	-0.6976720000
C	1.1412540000	1.7093240000	0.6425670000
C	0.7871920000	3.0482710000	-1.4989880000
H	1.7789890000	3.1007500000	2.2036650000
H	1.8602450000	0.7249170000	3.0647520000
H	-4.5791730000	-2.5888600000	0.4137650000
C	-3.8205990000	-1.8160670000	0.3451480000
C	-1.8505440000	0.1463970000	0.1862910000
H	-1.1181170000	0.9422070000	0.1317110000
O	-1.9375420000	3.3957230000	-0.5584760000
H	-0.9934310000	3.2690710000	-0.8956340000
H	1.2834530000	3.9580680000	-1.1662650000
C	0.8885290000	2.7915990000	1.6396940000
H	0.4929430000	3.6690940000	1.1213620000
H	-2.3644460000	3.8044900000	-1.3142770000
H	0.1329270000	2.4600590000	2.3651760000
C	-4.1862920000	-0.4738330000	0.2829310000
C	-3.1980040000	0.5006640000	0.2039060000
H	-5.2341170000	-0.1929340000	0.2969590000
H	-3.4370110000	1.5562880000	0.1462380000

Zero-point correction= 0.326205  
(Hartree/Particle)

Thermal correction to Energy= 0.347266

Thermal correction to Enthalpy= 0.348210

Thermal correction to Gibbs Free Energy= 0.276613

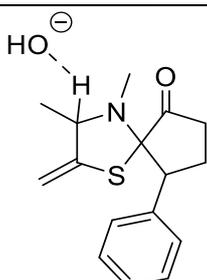
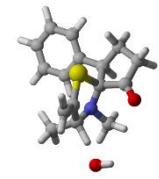
Sum of electronic and zero-point Energies= -1224.660363

Sum of electronic and thermal Energies= -1224.639302

Sum of electronic and thermal Enthalpies= -1224.638358

Sum of electronic and thermal Free Energies= -1224.709956

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	217.913	79.994	150.689

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	-1 1	

40

XYZ file generated by gabedit : coordinates in Angstrom

H	-4.9957510000	-2.4262670000	0.2259300000
H	-5.1580620000	-0.1532010000	1.2087590000
C	-4.2119810000	-1.6975440000	0.0515420000
C	-4.3012830000	-0.4250890000	0.6017730000
H	-3.0168610000	-3.0212530000	-1.1524210000
C	-3.1037850000	-2.0286640000	-0.7244360000
C	-3.2884130000	0.5062460000	0.3827340000
H	-3.3770550000	1.4906610000	0.8272140000
C	-2.0983910000	-1.0972810000	-0.9492730000
C	-2.1723700000	0.1844010000	-0.3903130000
H	-2.0225500000	3.1390670000	-0.5570500000
H	-1.2204230000	-1.3614990000	-1.5267360000
H	-1.4675360000	2.5065980000	0.9984730000
C	-1.0574880000	1.1673260000	-0.6511140000
C	-1.2244500000	2.5781270000	-0.0653820000
H	-0.9575870000	1.2717010000	-1.7407340000
S	0.3013550000	0.2982320000	1.6338070000
C	0.3486700000	0.7283140000	-0.1564790000
H	0.3732100000	-2.8290810000	0.3247690000
C	0.1576540000	3.2169090000	-0.2330050000
H	0.6596050000	0.2385080000	-2.8089590000
N	0.9173160000	-0.4104130000	-0.8201570000
H	0.4147460000	3.9591680000	0.5232920000
H	0.2654290000	3.6901710000	-1.2150630000
C	1.7700340000	-0.7140040000	1.4041920000
H	2.4439450000	-0.5774160000	3.4109360000
C	1.1439050000	2.0499620000	-0.1999070000
C	1.3960430000	-2.6889920000	-0.0538960000
C	1.4521930000	-0.1398990000	-2.1507960000
C	1.8362890000	-1.2261620000	0.0194960000
C	2.5954740000	-0.9822900000	2.4179640000
H	1.4363120000	-3.0259950000	-1.0949680000
H	1.8277390000	-1.0784180000	-2.5599750000
H	2.0861730000	-3.3144110000	0.5170320000
H	2.2964560000	0.5588380000	-2.1442000000
H	3.4562700000	-1.6153230000	2.2325660000
O	2.3387140000	2.1562120000	-0.2408810000
H	3.0331150000	-1.2199830000	-0.4426960000
H	4.7218580000	-0.6079860000	-0.9195850000
O	4.2244690000	-1.4200700000	-1.0497450000

Zero-point correction= 0.323217  
(Hartree/Particle)

Thermal correction to Energy= 0.343497

Thermal correction to Enthalpy= 0.344441

Thermal correction to Gibbs Free Energy= 0.273891

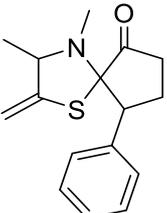
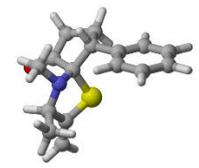
Sum of electronic and zero-point Energies= -1224.648436

Sum of electronic and thermal Energies= -1224.628156

Sum of electronic and thermal Enthalpies= -1224.627212

Sum of electronic and thermal Free Energies= -1224.697762

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	215.547	77.598	148.485

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

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XYZ file generated by gabedit : coordinates in Angstrom

H	-2.7252710000	-1.2664740000	-3.1476040000
H	-3.6664440000	-2.1631620000	-1.8259300000
C	-2.8461740000	-1.5098410000	-2.1001510000
H	-3.1173640000	-0.8943200000	0.6449900000
C	-2.0279840000	-1.0323710000	-1.1686720000
H	-2.8822330000	-3.3258050000	0.1602060000
S	-0.6170650000	-0.0320790000	-1.5258170000
H	-2.1152160000	-2.9691580000	1.7088320000
C	-2.1464760000	-1.2951120000	0.3219950000
C	-2.0591810000	-2.7876200000	0.6335630000
H	1.2792370000	-1.2940130000	1.5341480000
O	-2.7352920000	1.7302640000	0.3823220000
H	-1.1130860000	-3.1819140000	0.2577560000
H	-1.0985450000	3.6888630000	-0.7096760000
H	3.2386520000	-2.7357410000	1.1171160000
C	-0.6074640000	0.5672340000	0.2136250000
H	-2.1466030000	0.4574600000	2.5159250000
C	-1.5453710000	1.7906470000	0.2266130000
N	-1.0523560000	-0.5685230000	0.9895480000
H	0.9055800000	2.4187830000	-1.2078340000
C	2.0767440000	-0.9493440000	0.8871700000
C	3.1750730000	-1.7630520000	0.6430810000
C	-0.7092290000	3.0504880000	0.0835150000
C	-1.3351020000	-0.2718970000	2.3884660000
C	0.7216550000	2.5474850000	-0.1377800000
H	-1.6185240000	-1.1951550000	2.8944100000
C	0.7659050000	1.1771990000	0.5668730000
C	1.9689450000	0.3066310000	0.2801150000
H	-0.8031470000	3.6013290000	1.0253580000
C	4.1918470000	-1.3353180000	-0.2065170000
H	-0.4360520000	0.1003150000	2.8838400000
H	5.0485620000	-1.9708150000	-0.3971830000
H	1.4788630000	3.2285970000	0.2517390000
H	0.7417090000	1.3721880000	1.6473710000
C	2.9963960000	0.7279890000	-0.5629430000
C	4.0999750000	-0.0863700000	-0.8056620000
H	2.9476640000	1.6992300000	-1.0400230000
H	4.8867400000	0.2601130000	-1.4655470000

Zero-point correction= 0.318428  
(Hartree/Particle)

Thermal correction to Energy= 0.336055

Thermal correction to Enthalpy= 0.336999

Thermal correction to Gibbs Free Energy= 0.272517

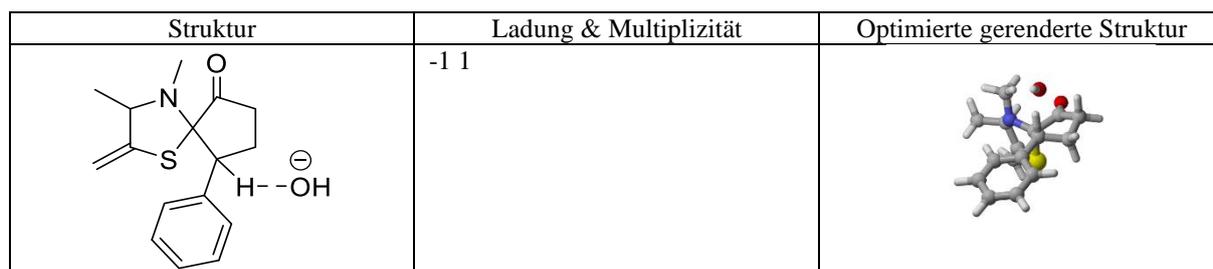
Sum of electronic and zero-point Energies= -1148.837331

Sum of electronic and thermal Energies= -1148.819704

Sum of electronic and thermal Enthalpies= -1148.818760

Sum of electronic and thermal Free Energies= -1148.883242

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	210.878	69.244	135.713



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XYZ file generated by gabedit : coordinates in Angstrom

H	4.8380930000	-2.6633190000	0.1966090000
H	5.1247890000	-0.5590130000	-1.0952710000
C	4.0336470000	-1.9383740000	0.1398690000
C	4.1906600000	-0.7603650000	-0.5804980000
H	2.6783200000	-3.0843560000	1.3548450000
C	2.8215390000	-2.1691080000	0.7892620000
C	3.1539840000	0.1663240000	-0.6548880000
H	3.3015560000	1.0721060000	-1.2310150000
C	1.7912220000	-1.2415700000	0.7237880000
C	1.9282900000	-0.0469940000	-0.0060860000
H	1.8191750000	2.7001820000	-0.9490680000
H	0.8519460000	-1.4285700000	1.2298480000
H	1.0594060000	1.6173790000	-2.1424120000
C	0.8511690000	0.9747240000	-0.0425620000
C	0.9626210000	2.0493870000	-1.1350050000
H	0.9465410000	1.7147920000	0.9587920000
S	-0.8215070000	-0.6915760000	-1.5725670000
C	-0.5897600000	0.4988130000	-0.1482970000
H	-1.8284210000	-2.7489820000	1.6170030000
C	-0.3488880000	2.8230270000	-0.9818500000
H	-0.4862920000	1.2930490000	2.2975820000
N	-1.1696790000	-0.2145830000	0.9823800000
H	-0.6937010000	3.3827880000	-1.8522300000
H	-0.2406460000	3.4941970000	-0.1188830000
C	-2.2122440000	-1.4415700000	-0.8081930000
H	-2.8314490000	-2.6403250000	-2.4341840000
C	-1.3540290000	1.7819380000	-0.5570560000
C	-2.6744320000	-2.0581420000	1.5999820000
C	-1.3396270000	0.6192580000	2.1741630000
C	-2.3925100000	-0.9292920000	0.6110860000
C	-2.9898710000	-2.3473240000	-1.4039400000
H	-2.8279460000	-1.6592070000	2.6043330000
H	-1.4058780000	-0.0223410000	3.0562160000
H	-3.5758240000	-2.6054460000	1.3178050000
H	-2.2542620000	1.2289380000	2.1108700000
H	-3.8101180000	-2.8129410000	-0.8707280000
O	-2.5519520000	1.9117310000	-0.4938070000
H	-3.2482510000	-0.2363220000	0.5947090000
H	1.7915470000	2.9030840000	2.3096670000
O	0.9435340000	2.8054200000	1.8702160000

Zero-point correction= 0.323871  
(Hartree/Particle)

Thermal correction to Energy= 0.343818

Thermal correction to Enthalpy= 0.344763

Thermal correction to Gibbs Free Energy= 0.273350

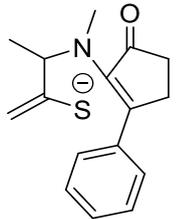
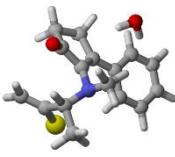
Sum of electronic and zero-point Energies= -1224.673487

Sum of electronic and thermal Energies= -1224.653539

Sum of electronic and thermal Enthalpies= -1224.652595

Sum of electronic and thermal Free Energies= -1224.724007

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	215.749	77.105	150.300

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
H <sub>2</sub> O 	-1 1	

40

XYZ file generated by gabedit : coordinates in Angstrom

H	4.8832710000	-2.4876170000	0.1998330000
H	5.2337090000	-0.1479950000	-0.5538780000
C	4.0335110000	-1.8325010000	0.0419860000
C	4.2312260000	-0.5227250000	-0.3802830000
H	2.5768130000	-3.3326100000	0.5467690000
C	2.7375670000	-2.3034410000	0.2457730000
C	3.1351080000	0.3089370000	-0.5895690000
H	3.2963020000	1.3258750000	-0.9326910000
C	1.6385040000	-1.4760820000	0.0553570000
C	1.8307930000	-0.1493450000	-0.3586820000
H	1.5083720000	2.6552830000	-1.2222680000
H	0.6235600000	-1.8445540000	0.1671330000
H	1.1068810000	1.5344670000	-2.5270370000
C	0.6937190000	0.7649370000	-0.5610620000
C	0.7792990000	1.9075630000	-1.5536470000
H	1.1575960000	2.6632500000	1.4756320000
S	-1.6061970000	-2.2756820000	-1.2701340000
C	-0.4802510000	0.7639730000	0.1036320000
H	-1.8400520000	-2.5711560000	1.6233170000
C	-0.6369750000	2.4993920000	-1.5709610000
H	0.4408100000	0.5965920000	2.5141270000
N	-0.9021550000	-0.1466880000	1.0954050000
H	-1.2210180000	2.0763130000	-2.3934400000
H	-0.6845250000	3.5870480000	-1.6201210000
C	-2.5165390000	-0.9513260000	-0.5926100000
H	-3.6321420000	-0.4056960000	-2.3077760000
C	-1.2582800000	1.9745640000	-0.2897790000
C	-2.5989030000	-1.8024810000	1.7794050000
C	-0.6175200000	0.3307680000	2.4430830000
C	-2.2998370000	-0.6020510000	0.8842220000
C	-3.4091100000	-0.1936930000	-1.2682350000
H	-2.6454570000	-1.5264310000	2.8364310000
H	-0.7976320000	-0.4692550000	3.1619550000
H	-3.5660310000	-2.2190930000	1.4907490000
H	-1.2262750000	1.2048770000	2.7247810000
H	-3.9215300000	0.6350330000	-0.7877350000
O	-2.1478080000	2.4947630000	0.3459190000
H	-2.9887650000	0.2160140000	1.1426170000
H	2.4268020000	1.8555140000	1.3301540000
O	2.1115170000	2.7293520000	1.5858290000

Zero-point correction=  
(Hartree/Particle)

0.329124

Thermal correction to Energy=

0.350804

Thermal correction to Enthalpy=

0.351748

Thermal correction to Gibbs Free Energy=

0.277676

Sum of electronic and zero-point Energies=

-1224.705083

Sum of electronic and thermal Energies=

-1224.683403

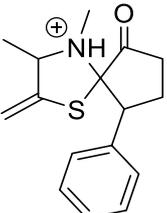
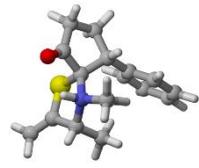
Sum of electronic and thermal Enthalpies=

-1224.682459

Sum of electronic and thermal Free Energies=

-1224.756531

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	220.133	80.215	155.898

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	+1 1	

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XYZ file generated by gabedit : coordinates in Angstrom

```

H      -2.0633890000      3.0972720000     -1.3768490000
H      -1.5860980000      3.6860130000      0.2084890000
C      -1.4730010000      2.8541130000     -0.4916790000
H       0.6678270000      3.3623820000     -0.6427520000
H       0.1223800000      2.1726240000     -1.8160720000
C      -0.0000510000      2.5147610000     -0.7858260000
O      -3.0523510000      1.4399250000      0.7549450000
C      -2.0159270000      1.6169630000      0.1778140000
H       2.2724450000      0.9514180000      2.0527950000
C       0.3622280000      1.3728910000      0.1979690000
H       0.3666650000      1.8231630000      1.1997870000
H      -2.2829840000     -0.2918420000      1.3315230000
C      -0.9251610000      0.5248490000      0.1233910000
C       2.5537240000      0.5457390000      1.0851660000
S      -1.1469090000     -0.3659040000     -1.4801740000
H      -0.9159150000      0.7690020000      2.8695930000
H       4.4330130000     -0.1980760000      1.8091100000
C       1.6989440000      0.7028490000     -0.0087120000
H      -2.9647510000     -2.5807730000     -2.2256820000
C       3.7814200000     -0.0932200000      0.9501780000
H       0.4495930000     -0.3039220000      2.4233310000
C      -1.7560560000     -1.8200270000     -0.6731990000
C      -0.6286170000     -0.2240160000      2.5265720000
N      -1.2688540000     -0.4721750000      1.2034530000
H      -1.8051360000     -2.4975100000      1.3604370000
C      -2.5761970000     -2.7051850000     -1.2230160000
C      -1.1608260000     -1.9058440000      0.7054860000
C       2.1232300000      0.2465220000     -1.2596650000
H      -2.8607830000     -3.5986110000     -0.6783740000
H      -1.0025680000     -0.9730850000      3.2236070000
C       4.1758340000     -0.5777920000     -0.2917850000
H       1.5068640000      0.3892580000     -2.1376950000
C       3.3500560000     -0.3948070000     -1.3960390000
H       5.1322910000     -1.0735140000     -0.4042370000
C       0.2680130000     -2.4268520000      0.7313590000
H       0.9375510000     -1.8028010000      0.1364230000
H       0.2599710000     -3.4287990000      0.3007550000
H       0.6530550000     -2.5047590000      1.7488520000
H       3.6656240000     -0.7428100000     -2.3720660000

```

Zero-point correction= 0.334238  
(Hartree/Particle)

Thermal correction to Energy= 0.351338

Thermal correction to Enthalpy= 0.352283

Thermal correction to Gibbs Free Energy= 0.290361

Sum of electronic and zero-point Energies= -1149.198271

Sum of electronic and thermal Energies= -1149.181171

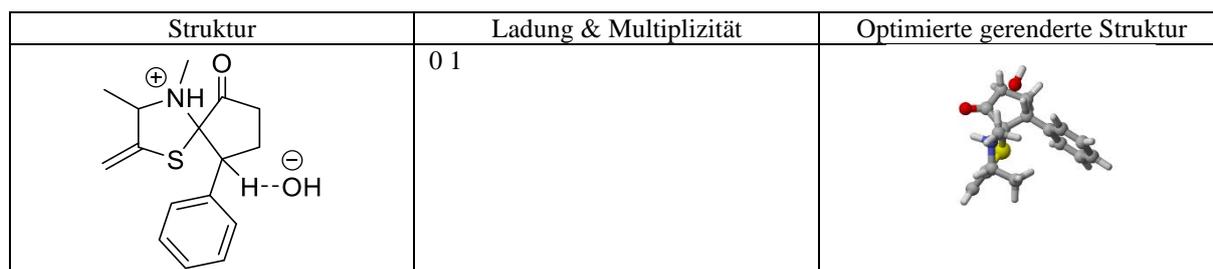
Sum of electronic and thermal Enthalpies= -1149.180226

Sum of electronic and thermal Free Energies= -1149.242148

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-kelvin
Total	220.468	68.931	130.325

#M062X/6-311+G\*\*

(TS-56-58)



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XYZ file generated by gabedit : coordinates in Angstrom

H	-2.0038310000	2.5932590000	-2.2361630000
H	-1.3663190000	3.4252610000	-0.7967890000
C	-1.3777840000	2.4824800000	-1.3494650000
H	0.7627180000	2.7928270000	-1.7173270000
H	0.0900220000	1.3683440000	-2.5186690000
C	0.0513220000	1.9741180000	-1.6026290000
O	-3.0325560000	1.4401190000	0.1393810000
C	-1.9608190000	1.4684180000	-0.4046940000
H	2.2743130000	1.3190900000	1.5296490000
C	0.3828320000	1.1588020000	-0.3361030000
H	0.3475720000	2.0735700000	0.5571380000
H	-2.2488360000	0.0235480000	1.2661170000
C	-0.8868480000	0.3889640000	-0.1447500000
C	2.5651440000	0.6171000000	0.7526870000
S	-1.2491470000	-0.9849100000	-1.3983660000
H	-0.7080030000	1.4608530000	2.3576150000
H	4.4376850000	0.0999540000	1.6699350000
C	1.6974590000	0.4338400000	-0.3302680000
H	-3.0500700000	-3.3518020000	-1.3382370000
C	3.7804480000	-0.0576940000	0.8222590000
H	0.4950960000	0.1644660000	2.3107950000
C	-1.8253280000	-2.0982680000	-0.1633320000
C	-0.5679200000	0.3749640000	2.3779210000
N	-1.2478520000	-0.2350390000	1.1934470000
H	-1.8444170000	-2.0800180000	1.9806430000
C	-2.6410960000	-3.1283600000	-0.3616750000
C	-1.2041950000	-1.7420840000	1.1615380000
C	2.1108670000	-0.4080390000	-1.3701880000
H	-2.9027000000	-3.7846380000	0.4609440000
H	-0.9993810000	-0.0886570000	3.2659930000
C	4.1591510000	-0.9205480000	-0.2015370000
H	1.4771400000	-0.5443910000	-2.2385420000
C	3.3256620000	-1.0833690000	-1.3041840000
H	5.1048940000	-1.4474130000	-0.1505380000
C	0.2075930000	-2.2903940000	1.3238510000
H	0.8828870000	-1.8827630000	0.5691860000
H	0.1613730000	-3.3729910000	1.2001820000
H	0.6084610000	-2.0751800000	2.3144950000
H	3.6239390000	-1.7349440000	-2.1176970000
O	0.0612480000	3.0033650000	1.4862270000
H	0.4503140000	3.8780040000	1.4295450000

Zero-point correction= 0.339760  
(Hartree/Particle)

Thermal correction to Energy= 0.359268

Thermal correction to Enthalpy= 0.360212

Thermal correction to Gibbs Free Energy= 0.292981

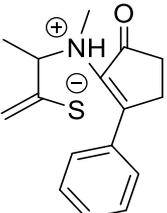
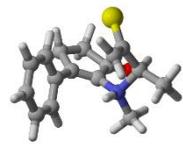
Sum of electronic and zero-point Energies= -1225.162316

Sum of electronic and thermal Energies= -1225.142809

Sum of electronic and thermal Enthalpies= -1225.141864

Sum of electronic and thermal Free Energies= -1225.209095

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	225.444	76.811	141.500

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

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XYZ file generated by gabedit : coordinates in Angstrom

H	1.9455180000	3.6135480000	-0.3241760000
H	2.1313360000	2.7918080000	1.2342200000
C	1.6312110000	2.7503430000	0.2655040000
O	3.2051300000	1.1645130000	-0.7357850000
C	2.0818890000	1.4789020000	-0.4250520000
H	-0.4436230000	3.4485610000	-0.0612780000
C	0.1069110000	2.6250270000	0.3995350000
H	-0.1976100000	2.5563100000	1.4484220000
H	-0.6691360000	-2.9662070000	0.4424480000
C	0.8577910000	0.6876230000	-0.6747620000
H	2.6670060000	-0.6062910000	-2.2855960000
C	-0.2451640000	1.3129590000	-0.2523500000
H	2.5006560000	-1.0383080000	0.2893570000
C	-0.5012650000	-2.2096340000	1.2040120000
H	-1.2471370000	-2.1267290000	1.9839510000
H	-0.0258790000	-1.0533660000	-1.1554220000
H	1.1533670000	-0.1458280000	-3.1096870000
H	-1.8465470000	0.8513030000	1.8398110000
C	1.6147370000	-0.8484310000	-2.4171660000
N	0.9402470000	-0.7042440000	-1.0922770000
C	1.5688070000	-1.5509980000	0.0545400000
C	0.6025510000	-1.4316120000	1.2354130000
C	-1.6136000000	0.7749400000	-0.2933880000
C	-2.3262370000	0.6075670000	0.8971590000
H	1.4859880000	-1.8679100000	-2.7711870000
H	2.6639660000	-2.9978410000	-1.1541940000
H	-1.6386830000	0.5446270000	-2.4331090000
C	1.8421190000	-2.9632550000	-0.4371100000
C	-2.1833820000	0.3827600000	-1.5072470000
S	1.0022160000	-0.2386050000	2.4304290000
H	2.1245150000	-3.5564800000	0.4327330000
C	-3.5927600000	0.0415870000	0.8641470000
H	-4.1338590000	-0.1103990000	1.7902980000
H	0.9601000000	-3.4310590000	-0.8811470000
C	-3.4568940000	-0.1767650000	-1.5332310000
C	-4.1599380000	-0.3497970000	-0.3464700000
H	-3.8991200000	-0.4716110000	-2.4773880000
H	-5.1497380000	-0.7901370000	-0.3639000000

Zero-point correction= 0.319658  
(Hartree/Particle)

Thermal correction to Energy= 0.337748

Thermal correction to Enthalpy= 0.338692

Thermal correction to Gibbs Free Energy= 0.273676

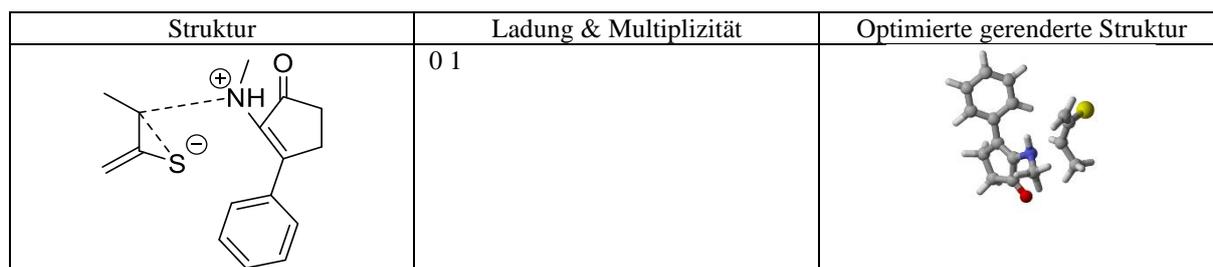
Sum of electronic and zero-point Energies= -1148.789530

Sum of electronic and thermal Energies= -1148.771440

Sum of electronic and thermal Enthalpies= -1148.770496

Sum of electronic and thermal Free Energies= -1148.835512

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	211.940	70.111	136.839



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XYZ file generated by gabedit : coordinates in Angstrom

H	-1.6270550000	3.4351340000	-0.4096690000
H	3.7646090000	-0.1872500000	0.8893190000
H	4.0408810000	-0.0830290000	-0.8503140000
H	-0.3871190000	1.3607980000	-0.7343660000
C	-2.1189110000	2.4917590000	-0.2046260000
H	3.1372570000	-1.4624230000	-0.1992190000
C	3.3265750000	-0.3939730000	-0.0885310000
H	-0.4082840000	-3.7921890000	-1.9239110000
C	-1.4069590000	1.3083830000	-0.3692110000
H	-3.9959990000	3.3791640000	0.3443660000
H	-2.0372820000	-2.0510350000	-2.0728190000
C	-3.4434960000	2.4565360000	0.2130810000
S	2.5041790000	2.4797110000	-1.3375560000
C	-2.0171970000	0.0749780000	-0.1151570000
C	-0.7610220000	-3.4452160000	-0.9520140000
C	-1.8348230000	-2.3557840000	-1.0425490000
C	-1.2710790000	-1.1851790000	-0.2694790000
C	-4.0640340000	1.2322620000	0.4538710000
C	2.0582110000	0.3933840000	-0.2730200000
C	1.9815690000	1.7899350000	0.1587270000
C	-0.0456800000	-1.4575640000	0.2279270000
C	-3.3602660000	0.0487570000	0.2822490000
H	-1.0907510000	-4.3236950000	-0.3931400000
H	0.6731270000	-1.5431070000	2.8740490000
C	0.3958200000	-2.8091520000	-0.2003740000
H	-5.0982630000	1.2011810000	0.7754070000
C	1.6919620000	2.3054790000	1.3609090000
H	1.7386830000	3.3753500000	1.5153820000
H	1.4317390000	0.1194300000	-1.1144630000
N	0.7837350000	-0.5932810000	0.9766510000
H	-2.7904490000	-2.6720020000	-0.6167170000
H	-3.8468430000	-0.9002710000	0.4775770000
H	1.4342770000	1.6891040000	2.2156400000
C	1.4258330000	-1.1875340000	2.1654240000
H	2.0549300000	-2.0180890000	1.8562620000
O	1.4773260000	-3.3085620000	-0.0037730000
H	2.0404080000	-0.4227330000	2.6385730000
H	0.2555090000	0.2393260000	1.2391900000

Zero-point correction=  
(Hartree/Particle)

0.316122

Thermal correction to Energy=

0.334868

Thermal correction to Enthalpy=

0.335812

Thermal correction to Gibbs Free Energy=

0.268207

Sum of electronic and zero-point Energies=

-1148.767734

Sum of electronic and thermal Energies=

-1148.748988

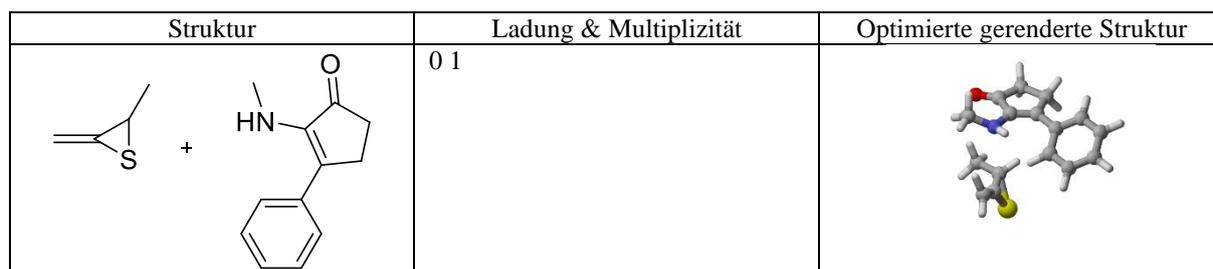
Sum of electronic and thermal Enthalpies=

-1148.748044

Sum of electronic and thermal Free Energies=

-1148.815650

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	210.133	70.610	142.288



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XYZ file generated by gabedit : coordinates in Angstrom

H	2.0040000000	-3.2056780000	0.8893280000
H	-4.0364570000	-0.3964010000	-0.6725790000
H	-3.1005350000	0.5022500000	-1.8854200000
H	0.4768370000	-1.3264400000	0.5676890000
C	2.4003980000	-2.2520590000	0.5604660000
H	-2.9050230000	0.8775350000	-0.1644190000
C	-3.0735510000	0.0705970000	-0.8833450000
H	-0.4216370000	3.1557960000	-2.2043290000
C	1.5363640000	-1.1761770000	0.3930770000
H	4.4311630000	-2.9492110000	0.4281180000
H	1.4741260000	1.7233510000	-2.3195410000
C	3.7578700000	-2.1109980000	0.2953540000
S	-2.2461850000	-2.6780860000	-1.3643480000
C	2.0143910000	0.0669130000	-0.0490540000
C	0.1849850000	3.1787730000	-1.2967790000
C	1.3780680000	2.2216820000	-1.3507610000
C	1.1148080000	1.2108130000	-0.2543200000
C	4.2444060000	-0.8870700000	-0.1559250000
C	-1.9636740000	-0.9411790000	-0.7585300000
C	-2.0433520000	-1.9984080000	0.2296490000
C	-0.0013860000	1.5064680000	0.4616120000
C	3.3824050000	0.1859860000	-0.3345250000
H	0.4644700000	4.2193810000	-1.1216290000
H	-0.8340330000	2.4112570000	2.9412870000
C	-0.6677900000	2.6975500000	-0.1369520000
H	5.2995130000	-0.7694480000	-0.3733330000
C	-2.0390220000	-2.2957150000	1.5172170000
H	-2.1896820000	-3.3081330000	1.8678030000
H	-0.9677840000	-0.5849480000	-1.0101160000
N	-0.5440570000	0.8237030000	1.5333540000
H	2.3197320000	2.7491090000	-1.1741430000
H	3.7764920000	1.1305370000	-0.6905860000
H	-1.8941440000	-1.5031290000	2.2423650000
C	-1.3421750000	1.5276160000	2.5404720000
H	-2.2953010000	1.8415800000	2.1222110000
O	-1.7168950000	3.1854520000	0.2106470000
H	-1.5282590000	0.8307490000	3.3578910000
H	0.1125690000	0.1729290000	1.9443660000

Zero-point correction=  
(Hartree/Particle)

0.315291

Thermal correction to Energy=

0.335343

Thermal correction to Enthalpy=

0.336287

Thermal correction to Gibbs Free Energy=

0.264026

Sum of electronic and zero-point Energies=

-1148.805218

Sum of electronic and thermal Energies=

-1148.785166

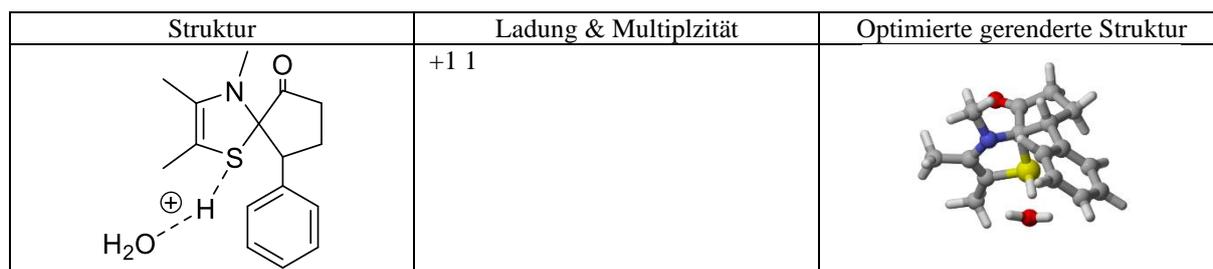
Sum of electronic and thermal Enthalpies=

-1148.784222

Sum of electronic and thermal Free Energies=

-1148.856484

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	210.431	73.219	152.087



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XYZ file generated by gabedit : coordinates in Angstrom

```

H      0.7110650000      2.3183940000     -1.6823420000
H     -1.4005940000      3.4717300000     -1.5119920000
H      2.5546310000      1.2994700000     -1.6526380000
H      4.5452210000     -0.1321430000     -1.6561100000
H     -3.2791210000     -2.9175290000     -1.2465840000
H     -3.1951860000     -1.6630140000     -2.4844840000
S     -0.6211010000     -0.2552300000     -1.4507500000
H      1.1845990000      3.4740590000     -0.4412990000
C      0.4916410000      2.6654030000     -0.6698280000
C     -0.9805680000      3.0902410000     -0.5807020000
C     -2.6039350000     -2.2452200000     -1.7741090000
C      2.7497030000      0.6722400000     -0.7910830000
C      3.8851480000     -0.1397400000     -0.7969760000
H     -1.1392880000      3.8589220000      0.1821440000
H     -1.9012290000     -2.8605870000     -2.3430440000
C     -1.8958530000     -1.3560490000     -0.8063870000
C     -1.7222100000      1.8507980000     -0.1232010000
C      0.6270420000      1.5091420000      0.3414320000
C     -0.6746150000      0.7143960000      0.1260680000
C      1.8935790000      0.6875840000      0.3108860000
O     -2.8874320000      1.7199750000      0.1000870000
C      4.1805490000     -0.9405340000      0.3030730000
H      5.0712250000     -1.5574640000      0.3043290000
H      0.5361700000      1.9503860000      1.3418680000
C     -1.9845240000     -1.1961590000      0.5229500000
N     -1.0958340000     -0.2655390000      1.1037190000
C      2.2085110000     -0.1099470000      1.4173520000
H      1.0962350000     -2.6523060000      0.0170150000
O      1.3373910000     -2.2579860000     -0.8316360000
C      3.3407810000     -0.9161940000      1.4179490000
H     -3.5003750000     -2.6687030000      0.8520770000
C     -2.9193230000     -1.9442360000      1.4162910000
H      1.5624180000     -0.0949040000      2.2887390000
H     -2.2791730000      0.9218770000      2.4318810000
H      3.5798940000     -1.5139700000      2.2896890000
C     -1.4020970000      0.2678380000      2.4345540000
H     -3.6108470000     -1.2507510000      1.9007800000
H     -0.5418950000      0.8234200000      2.8062470000
H     -2.3683480000     -2.4773520000      2.1947890000
H     -1.5708620000     -0.5586810000      3.1212310000
H      2.2602180000     -1.9593010000     -0.7455690000
H      0.5310590000     -1.2223710000     -1.1179800000

```

Zero-point correction= 0.350514  
(Hartree/Particle)

Thermal correction to Energy= 0.371081

Thermal correction to Enthalpy= 0.372025

Thermal correction to Gibbs Free Energy= 0.302521

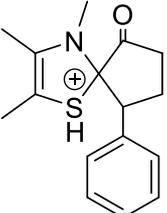
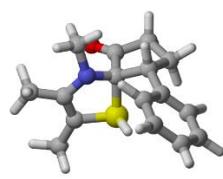
Sum of electronic and zero-point Energies= -1225.596848

Sum of electronic and thermal Energies= -1225.576280

Sum of electronic and thermal Enthalpies= -1225.575336

Sum of electronic and thermal Free Energies= -1225.644841

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	232.857	79.663	146.285

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	+1 1	

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XYZ file generated by gabedit : coordinates in Angstrom

```

H      1.0153760000      2.3339260000     -1.4189670000
H      -0.9729770000      3.6962090000     -1.1082780000
H       2.9260800000      1.3740500000     -1.3201720000
H       4.7596440000     -0.2366060000     -1.5405030000
H      -3.2178790000     -2.7859720000     -1.6245500000
H      -2.7951200000     -1.6196990000     -2.8694510000
S      -0.4960430000     -0.2118720000     -1.4881620000
H       1.5532790000      3.2696650000     -0.0288440000
C       0.7969180000      2.5655080000     -0.3726620000
C      -0.6303430000      3.1123840000     -0.2534650000
C      -2.3917210000     -2.2186120000     -2.0505020000
C       2.9586320000      0.5214780000     -0.6521320000
C       4.0067430000     -0.3890230000     -0.7767020000
H      -0.7506490000      3.7419610000      0.6351240000
H      -1.6764330000     -2.9339940000     -2.4650830000
C      -1.7750830000     -1.3557450000     -0.9973040000
C      -1.5011850000      1.8940990000     -0.0485440000
C       0.8045010000      1.2790860000      0.4770360000
C      -0.5643850000      0.6451620000      0.1484350000
C       1.9857080000      0.3474750000      0.3341430000
O      -2.6878130000      1.8187420000      0.0395230000
C       4.0942810000     -1.4782780000      0.0806040000
H       4.9120090000     -2.1817890000     -0.0157830000
H       0.7295920000      1.5858550000      1.5279590000
C      -1.9498970000     -1.2560050000      0.3373320000
N      -1.1355340000     -0.3575220000      1.0187460000
C       2.0894290000     -0.7478250000      1.1995310000
C       3.1344940000     -1.6539240000      1.0744930000
H      -3.4604400000     -2.7642450000      0.4739900000
C      -2.9263150000     -2.0721620000      1.1184100000
H       1.3479950000     -0.8884400000      1.9789230000
H      -2.3272550000      0.7814750000      2.3745150000
H       3.2054690000     -2.4921830000      1.7568010000
C      -1.4826440000      0.0862790000      2.3709760000
H      -3.6526600000     -1.4216680000      1.6107450000
H      -0.6149890000      0.5647180000      2.8241080000
H      -2.4050690000     -2.6508000000      1.8845940000
H      -1.7238020000     -0.7816220000      2.9803550000
H       0.6409460000     -0.9275650000     -1.2301940000

```

Zero-point correction= 0.328004  
(Hartree/Particle)

Thermal correction to Energy= 0.346575

Thermal correction to Enthalpy= 0.347520

Thermal correction to Gibbs Free Energy= 0.281215

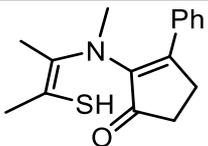
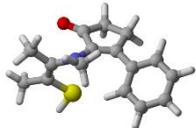
Sum of electronic and zero-point Energies= -1149.176523

Sum of electronic and thermal Energies= -1149.157951

Sum of electronic and thermal Enthalpies= -1149.157007

Sum of electronic and thermal Free Energies= -1149.223312

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	217.479	71.804	139.550

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.8569300000	0.1462250000	1.7450080000
H	-2.5611130000	-0.2917950000	2.8381920000
H	-0.5541710000	3.9785680000	-0.4000840000
H	-3.5929470000	-1.5617380000	2.1618920000
C	-3.0973680000	-0.6126370000	1.9461750000
O	-2.3044310000	2.1021950000	0.4214540000
H	-4.3513610000	-0.5385020000	-1.5071750000
C	-1.1628150000	1.9648510000	0.0592710000
C	-0.3388030000	2.9624870000	-0.7287720000
H	1.6180190000	3.1400280000	0.2035500000
H	-0.6757790000	-1.2669320000	2.8558180000
H	-4.6251610000	-1.3249740000	0.0540030000
C	-3.9835000000	-1.3110670000	-0.8256750000
C	-2.1486650000	-0.7013100000	0.7716020000
H	-0.6326210000	2.8746870000	-1.7784190000
C	-0.2830590000	0.7873120000	0.3448220000
H	0.7989520000	-0.4234500000	2.3407490000
N	-0.8007000000	-0.3097860000	1.0048590000
C	1.1097130000	2.5037900000	-0.5285390000
C	-0.0349960000	-1.0383200000	2.0011480000
H	-4.0798220000	-2.2759870000	-1.3320760000
C	-2.5538850000	-1.0405030000	-0.4598860000
C	0.9913420000	1.0803740000	-0.0198100000
H	3.5564060000	1.7979450000	0.4177580000
H	1.7009810000	2.5357800000	-1.4466360000
H	0.3652160000	-1.9806790000	1.6134740000
C	2.1697220000	0.2030110000	0.0012470000
C	3.4459260000	0.7374000000	0.2209010000
S	-1.3882150000	-1.0365000000	-1.8121750000
H	5.5493990000	0.3533800000	0.3868660000
C	4.5716620000	-0.0767170000	0.2032450000
C	2.0576010000	-1.1671830000	-0.2721350000
H	1.0820450000	-1.5834360000	-0.4957310000
C	4.4452850000	-1.4382420000	-0.0539110000
C	3.1856540000	-1.9770300000	-0.3003330000
H	5.3233930000	-2.0729140000	-0.0715170000
H	3.0815690000	-3.0324190000	-0.5240480000
H	-2.1371700000	-1.7959430000	-2.6285830000

Zero-point correction=  
(Hartree/Particle)

0.314491

Thermal correction to Energy=

0.333857

Thermal correction to Enthalpy=

0.334802

Thermal correction to Gibbs Free Energy=

0.266702

Sum of electronic and zero-point Energies=

-1148.836015

Sum of electronic and thermal Energies=

-1148.816648

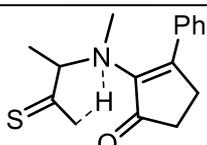
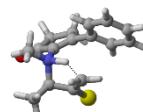
Sum of electronic and thermal Enthalpies=

-1148.815704

Sum of electronic and thermal Free Energies=

-1148.883804

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	209.499	72.648	143.328

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.7555720000	3.8187580000	-0.3633510000
H	-2.0083770000	2.9216820000	-1.8577190000
C	-1.5206610000	2.8874860000	-0.8826980000
O	-3.2534900000	1.5018780000	0.1462140000
C	-2.0901080000	1.7250870000	-0.0867210000
H	0.5977350000	3.4509420000	-0.5976400000
C	-0.0112120000	2.6187140000	-0.9576130000
H	0.3173540000	2.3992240000	-1.9779430000
H	0.1437930000	-2.8285460000	1.1819680000
C	-0.9437060000	0.8946030000	0.3499070000
H	-2.8400410000	0.1118420000	2.1971450000
C	0.2166140000	1.3922880000	-0.1059080000
H	-2.3258240000	-0.7960640000	-0.7264220000
C	0.4856690000	-2.2629460000	0.3140790000
H	1.5090250000	-2.4490920000	0.0130830000
H	-0.0484580000	-1.0113970000	0.9809320000
H	-1.2521870000	0.4880990000	2.9130390000
H	2.0329750000	0.6192740000	-1.9480290000
C	-1.8133650000	-0.2345440000	2.3201290000
N	-1.1422670000	-0.3662910000	1.0128020000
C	-1.7372970000	-1.3542380000	-0.0006420000
C	-0.4500780000	-1.8869430000	-0.6608530000
C	1.5648810000	0.8540060000	0.1388840000
C	2.3918870000	0.5085890000	-0.9316240000
H	-1.7964740000	-1.1987400000	2.8259410000
H	-3.4962610000	-2.0105810000	1.0903030000
H	1.3736850000	0.9494730000	2.2783480000
C	-2.5968690000	-2.4324530000	0.6380660000
C	2.0148670000	0.6690040000	1.4489090000
S	-0.2190430000	-1.6389300000	-2.2927160000
H	-2.9043190000	-3.1135480000	-0.1572690000
C	3.6430960000	-0.0446320000	-0.6881900000
H	4.2685270000	-0.3392270000	-1.5221420000
H	-2.0552110000	-3.0146380000	1.3849640000
C	3.2741460000	0.1354140000	1.6872470000
C	4.0863110000	-0.2300480000	0.6175190000
H	3.6189830000	-0.0022630000	2.7049560000
H	5.0640760000	-0.6596260000	0.8010120000

Zero-point correction= 0.313378

(Hartree/Particle)

Thermal correction to Energy= 0.331217

Thermal correction to Enthalpy= 0.332161

Thermal correction to Gibbs Free Energy= 0.267339

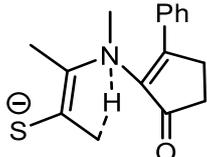
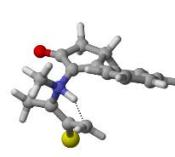
Sum of electronic and zero-point Energies= -1148.775131

Sum of electronic and thermal Energies= -1148.757292

Sum of electronic and thermal Enthalpies= -1148.756348

Sum of electronic and thermal Free Energies= -1148.821170

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	207.842	69.127	136.429

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	-1 1	

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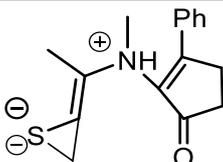
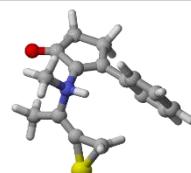
XYZ file generated by gabedit : coordinates in Angstrom

H	-0.5952940000	3.6831090000	-1.3814040000
H	-1.5252640000	2.4782930000	-2.2746120000
C	-0.7761110000	2.6114430000	-1.4917280000
O	-2.3382600000	2.4999910000	0.3754320000
C	-1.3556670000	2.0640800000	-0.1909780000
H	1.3836710000	2.4593570000	-1.8931030000
C	0.5145420000	1.8134400000	-1.7357700000
H	0.4199720000	1.1721180000	-2.6183280000
H	-0.0177090000	-2.5227110000	1.2474310000
C	-0.4513320000	1.0123230000	0.2624720000
H	-1.7757450000	1.1660940000	2.7263130000
C	0.6881780000	0.9578170000	-0.4945460000
C	-0.2133560000	-2.2609350000	0.2019000000
H	0.2844050000	-2.9092450000	-0.5079300000
H	-0.0992030000	-0.7876670000	1.0402760000
H	-0.0284130000	0.9391120000	2.9619170000
H	2.5666160000	0.1846150000	-2.2605640000
C	-0.9532400000	0.4547210000	2.6428190000
N	-0.8338020000	0.0228070000	1.2454460000
C	-1.9780670000	-0.6932400000	0.6288490000
C	-1.5286430000	-1.7996210000	-0.1188680000
C	1.9638160000	0.3207500000	-0.1970800000
C	2.8646180000	0.0152380000	-1.2324110000
H	-1.1617760000	-0.4298360000	3.2471900000
H	-3.6453300000	0.5175420000	-0.0954530000
H	1.7566260000	0.3760940000	1.9505950000
C	-3.3684960000	-0.1647550000	0.7171060000
C	2.3997720000	0.0978930000	1.1242910000
S	-2.4889750000	-2.4203460000	-1.4178980000
H	-4.0397490000	-1.0239350000	0.6543660000
C	4.1024510000	-0.5527270000	-0.9633340000
H	4.7624830000	-0.8042100000	-1.7865820000
H	-3.5534150000	0.3668190000	1.6559020000
C	3.6346080000	-0.4665340000	1.3891930000
C	4.4967260000	-0.8106860000	0.3460770000
H	3.9345900000	-0.6354580000	2.4178040000
H	5.4610290000	-1.2593780000	0.5530330000

Zero-point correction= 0.298870  
(Hartree/Particle)

Thermal correction to Energy=	0.317200
Thermal correction to Enthalpy=	0.318144
Thermal correction to Gibbs Free Energy=	0.251488
Sum of electronic and zero-point Energies=	-1148.190405
Sum of electronic and thermal Energies=	-1148.172075
Sum of electronic and thermal Enthalpies=	-1148.171131
Sum of electronic and thermal Free Energies=	-1148.237787

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	199.046	69.785	140.290

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	-1 1	

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XYZ file generated by gabedit : coordinates in Angstrom

H	-3.5249990000	2.7774030000	-0.3730220000
H	-3.3506310000	1.9114750000	-1.8916080000
C	-2.8880190000	2.0776990000	-0.9176560000
O	-3.7696280000	0.0229480000	0.0812580000
C	-2.8526370000	0.7638310000	-0.1561230000
H	-1.2712760000	3.5419290000	-0.5709670000
C	-1.4284500000	2.5508170000	-1.0028790000
H	-1.0586130000	2.5961350000	-2.0312800000
H	2.2994400000	-2.1207670000	1.2940550000
C	-1.4338620000	0.5564980000	0.2320770000
H	-2.8040620000	-1.2441700000	1.7800960000
C	-0.6341400000	1.5294540000	-0.2258280000
C	1.9637910000	-1.8012090000	0.3127910000
H	2.4448770000	-0.9181360000	-0.0971190000
H	-0.0265470000	-0.3732640000	1.3159510000
H	-1.8503160000	-0.1313740000	2.7929070000
H	1.2651950000	1.6817930000	-2.1371680000
C	-1.8077500000	-0.9966140000	2.1324970000
N	-0.9511560000	-0.6287480000	0.9489970000
C	-0.6832650000	-1.7768850000	0.0279010000
C	0.5925060000	-2.1015710000	-0.0940540000
C	0.8239210000	1.6073360000	-0.0285140000
C	1.6764140000	1.6719310000	-1.1341440000
H	-1.3346450000	-1.8441100000	2.6247510000
H	-2.3200380000	-1.6985140000	-1.3646750000
H	0.7058370000	1.6212190000	2.1274260000
C	-1.8506130000	-2.3936460000	-0.6651650000
C	1.3650850000	1.6000340000	1.2630450000
S	1.6787660000	-3.1673200000	-0.8859600000
H	-1.4975070000	-3.2592020000	-1.2243390000
C	3.0535280000	1.7040610000	-0.9470880000
H	3.7105620000	1.7476190000	-1.8071650000
H	-2.6177960000	-2.7274470000	0.0362790000
C	2.7435290000	1.6439880000	1.4444490000
C	3.5881130000	1.6886190000	0.3390510000
H	3.1550380000	1.6617070000	2.4462880000
H	4.6614170000	1.7264220000	0.4797420000

Zero-point correction= 0.308736

(Hartree/Particle)

Thermal correction to Energy= 0.326803

Thermal correction to Enthalpy= 0.327747

Thermal correction to Gibbs Free Energy= 0.262032

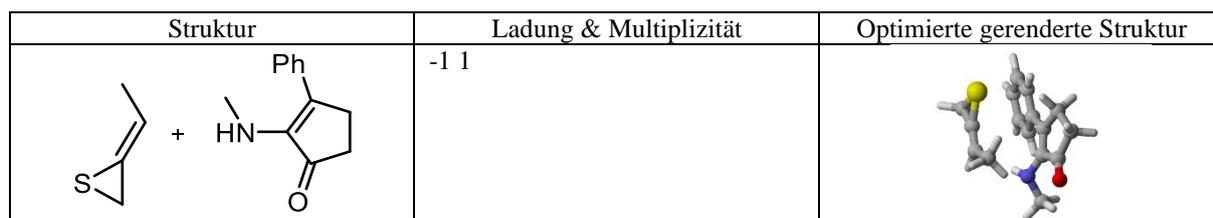
Sum of electronic and zero-point Energies= -1147.977769

Sum of electronic and thermal Energies= -1147.959703

Sum of electronic and thermal Enthalpies= -1147.958758

Sum of electronic and thermal Free Energies= -1148.024473

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	205.072	68.822	138.308



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XYZ file generated by gabedit : coordinates in Angstrom

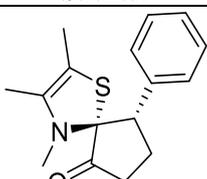
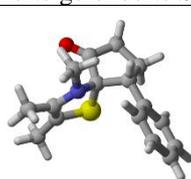
H	2.6159050000	-1.3674280000	-2.7873560000
H	2.6990040000	0.3917110000	-2.7396620000
C	2.2479690000	-0.4803310000	-2.2655700000
O	3.8207780000	-0.4201690000	-0.4083670000
C	2.6933790000	-0.5627030000	-0.8174820000
H	0.2515000000	-1.1449870000	-2.9126660000
C	0.7174100000	-0.4552230000	-2.2044070000
H	0.3297130000	0.5459040000	-2.4225930000
H	-2.5511960000	2.7763920000	1.5484070000
C	1.4863370000	-0.8365970000	0.0126640000
H	3.4972480000	-1.7504110000	1.5408150000
C	0.3829270000	-0.8345890000	-0.7769500000
C	-1.9905350000	2.0348420000	0.9895240000
H	-2.4299730000	1.0429160000	0.9333740000
H	0.7033210000	-0.8389390000	1.8597580000
H	2.1802110000	-2.9092940000	1.8430320000
H	-1.8474260000	-0.0466900000	-2.0508130000
C	2.5117260000	-1.8722740000	1.9862800000
N	1.5953340000	-0.9030960000	1.3908120000
C	0.6315350000	2.0609230000	1.4843470000
C	-0.5503390000	2.1638290000	0.9060010000
C	-1.0055940000	-1.1223560000	-0.3881290000
C	-2.0625100000	-0.6501490000	-1.1783820000
H	2.5908110000	-1.6719240000	3.0548940000
H	1.7787490000	2.5091940000	-0.2671980000
H	-0.5311820000	-2.3793610000	1.3029570000
C	1.9283070000	2.3783540000	0.8072520000
C	-1.3234870000	-1.9215690000	0.7228190000
S	-1.2914340000	2.6535360000	-0.6063860000
H	2.3585130000	3.3026840000	1.2045450000
C	-3.3847120000	-0.9186110000	-0.8436800000
H	-4.1831710000	-0.5305570000	-1.4651290000
H	2.6519240000	1.5767300000	0.9691790000
C	-2.6441370000	-2.1893420000	1.0570000000
C	-3.6827190000	-1.6782250000	0.2826750000
H	-2.8644260000	-2.8120180000	1.9162180000
H	-4.7131500000	-1.8868290000	0.5449090000
H	0.6596730000	1.7234980000	2.5169930000

Zero-point correction= 0.315590  
(Hartree/Particle)

Thermal correction to Energy=	0.335388
Thermal correction to Enthalpy=	0.336332
Thermal correction to Gibbs Free Energy=	0.265802
Sum of electronic and zero-point Energies=	-1148.806470
Sum of electronic and thermal Energies=	-1148.786672
Sum of electronic and thermal Enthalpies=	-1148.785728
Sum of electronic and thermal Free Energies=	-1148.856257

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	210.459	72.858	148.441

Mit, durch das PCModel genäherten, Lösungsmiteleinflüssen berechnete Strukturen der Fragmentierung.

#M062X/6-311+G**	(38-s)	
Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 Scrf=(pcm, solvent=water)	

38

XYZ file generated by gabedit : coordinates in Angstrom

```

H      -4.9579120000      -2.1195830000      0.1773590000
H      -3.4360200000      -2.3390980000     -1.7730620000
C      -4.1286280000     -1.4334030000      0.0525250000
C      -3.2737740000     -1.5569500000     -1.0404710000
H      -4.5772480000     -0.3095880000      1.8286140000
C      -3.9134720000     -0.4184440000      0.9787210000
C      -2.2135160000     -0.6723320000     -1.1975340000
H      -1.5535090000     -0.7710140000     -2.0527010000
C      -2.8462160000      0.4643880000      0.8206670000
C      -1.9805400000      0.3454290000     -0.2668000000
H      -2.6992030000      1.2476550000      1.5548070000
H      2.0025930000      -2.9966070000     -1.6348820000
H      0.4696900000      0.3547650000     -2.8129450000
H      1.3629980000     -1.1485860000     -2.9403160000
H      -0.7770980000     1.5290350000     -1.5410060000
C      -0.7966900000      1.2549240000     -0.4784290000
N      1.0032950000     -0.5051460000     -0.9819410000
C      1.2942940000     -0.2147930000     -2.3839660000
C      2.6684010000     -2.3615290000     -1.0435860000
C      1.8765880000     -1.3592810000     -0.2657420000
H      3.2459500000     -2.9990080000     -0.3782930000
H      -1.5022160000      3.2739660000     -0.0069250000
C      0.5805160000      0.6218200000     -0.1786970000
S      0.6690510000      0.0198440000      1.5688840000
C      1.8418240000     -1.2362500000      1.0667850000
C      -0.7385550000      2.5690980000      0.3206330000
H      -0.8937770000      2.3766670000      1.3849560000
H      3.3589450000     -1.8704910000     -1.7336880000
C      2.5142620000     -2.0240560000      2.1425460000
H      2.2203700000      0.3542360000     -2.5174860000
C      1.5161790000      1.8481670000     -0.2053830000
C      0.6887740000      3.0856160000      0.0884030000
H      0.7449810000      3.7170030000     -0.8041740000
O      2.6942040000      1.8102130000     -0.4553090000
H      1.1093640000      3.6524420000      0.9193850000
H      1.7784410000     -2.4992550000      2.7987730000
H      3.1425330000     -1.3821650000      2.7661180000
H      3.1429130000     -2.8079840000      1.7213400000

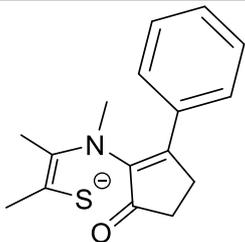
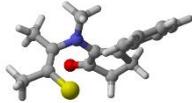
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Zero-point correction=                0.318149
(Hartree/Particle)
Thermal correction to Energy=          0.336279
Thermal correction to Enthalpy=        0.337223
Thermal correction to Gibbs Free Energy= 0.272149
Sum of electronic and zero-point Energies= -1148.857913
Sum of electronic and thermal Energies= -1148.839782
Sum of electronic and thermal Enthalpies= -1148.838838
Sum of electronic and thermal Free Energies= -1148.903912

```

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	211.018	70.231	136.960

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	-1 1  Scrf=(pcm, solvent=water)	

37

XYZ file generated by gabedit : coordinates in Angstrom

H	5.2441750000	-2.1990760000	-0.0748780000
C	4.3881850000	-1.5348520000	-0.0516170000
H	2.9741910000	-3.0699410000	-0.5723090000
H	5.5489980000	0.2084640000	0.4413580000
C	3.1117560000	-2.0236020000	-0.3236150000
C	4.5587110000	-0.1828790000	0.2381620000
H	-4.0872730000	-2.4053960000	-1.1636670000
C	2.0113710000	-1.1746730000	-0.2878100000
C	3.4611280000	0.6705010000	0.2644430000
H	1.0194760000	-1.5384410000	-0.5361820000
H	3.6066010000	1.7222440000	0.4863550000
C	2.1682730000	0.1849680000	0.0205350000
C	-4.0171150000	-1.4137240000	-0.7097970000
H	-4.6204080000	-1.4072920000	0.1985490000
S	-1.5273310000	-1.1781700000	-1.9041210000
H	-4.4609360000	-0.7094820000	-1.4209930000
C	-2.5667460000	-1.0553410000	-0.4723290000
H	1.8217910000	2.5183630000	-1.4260540000
H	-2.5731650000	-0.1410430000	2.8039400000
C	1.0194970000	1.0985140000	-0.0083960000
C	-2.1738200000	-0.6399060000	0.7502090000
H	-3.5439800000	-1.4993340000	2.2313240000
C	-0.2753800000	0.8340610000	0.3244450000
N	-0.8324860000	-0.2132100000	1.0128800000
C	-3.1096170000	-0.5384360000	1.9416010000
C	1.1940350000	2.5094640000	-0.5317980000
H	1.6799980000	3.1534020000	0.2084880000
H	0.2954740000	-1.9433190000	1.5339170000
C	-0.0665040000	-1.0003860000	1.9599340000
H	-3.9327960000	0.1502300000	1.7330560000
H	0.7934610000	-0.4261750000	2.3081330000
C	-1.1044900000	2.0271920000	-0.0201500000
C	-0.2359200000	2.9868730000	-0.8022500000
H	-0.4845680000	2.8734420000	-1.8616300000
H	-0.6985690000	-1.2394860000	2.8189250000
O	-2.2566840000	2.2240540000	0.3039880000
H	-0.4444940000	4.0169480000	-0.5138720000

Zero-point correction= 0.304917

(Hartree/Particle)

Thermal correction to Energy= 0.323492

Thermal correction to Enthalpy= 0.324436

Thermal correction to Gibbs Free Energy= 0.257646

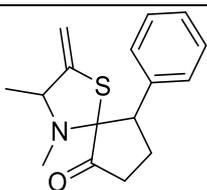
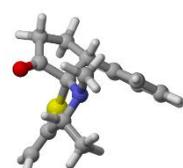
Sum of electronic and zero-point Energies= -1148.392372

Sum of electronic and thermal Energies= -1148.373797

Sum of electronic and thermal Enthalpies= -1148.372853

Sum of electronic and thermal Free Energies= -1148.439643

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	202.994	70.166	140.571

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 Scrf=(pcm, solvent=water)	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-2.6738970000	-1.3613330000	-3.1401120000
H	-3.5743220000	-2.2947180000	-1.8134970000
C	-2.7854380000	-1.6047010000	-2.0910580000
H	-3.0654190000	-0.9746160000	0.6630520000
C	-1.9870230000	-1.0897490000	-1.1607810000
H	-2.7932230000	-3.3898040000	0.1926040000
S	-0.6220820000	-0.0261990000	-1.5281880000
H	-2.0133140000	-3.0110840000	1.7287130000
C	-2.0870790000	-1.3497030000	0.3320670000
C	-1.9714030000	-2.8380510000	0.6520080000
H	1.5607960000	-0.9699860000	1.9116800000
O	-2.7815030000	1.6656110000	0.3304140000
H	-1.0248030000	-3.2249990000	0.2686860000
H	-1.1959060000	3.7216640000	-0.6111170000
H	3.5086480000	-2.4200730000	1.4687330000
C	-0.6134530000	0.5659960000	0.2164990000
H	-2.1600690000	0.3755930000	2.5114940000
C	-1.5835670000	1.7650530000	0.2278740000
N	-1.0083060000	-0.5895940000	0.9898220000
H	0.8147590000	2.4873330000	-1.2015200000
C	2.2230700000	-0.7454950000	1.0828500000
C	3.3191800000	-1.5634500000	0.8320930000
C	-0.7822550000	3.0462870000	0.1378380000
C	-1.3029440000	-0.3008000000	2.3914130000
C	0.6568640000	2.5884780000	-0.1250110000
H	-1.5255780000	-1.2351190000	2.9059400000
C	0.7438060000	1.2155530000	0.5666890000
C	1.9570450000	0.3653790000	0.2750260000
H	-0.8689450000	3.5377380000	1.1134100000
C	4.1757490000	-1.2796160000	-0.2297000000
H	-0.4331180000	0.1384840000	2.8806500000
H	5.0320210000	-1.9144160000	-0.4253480000
H	1.4028920000	3.2829120000	0.2603310000
H	0.7180210000	1.4020670000	1.6469760000
C	2.8270620000	0.6455670000	-0.7792030000
C	3.9281120000	-0.1706280000	-1.0307860000
H	2.6563000000	1.5059930000	-1.4144230000
H	4.5922840000	0.0650980000	-1.8542140000

Zero-point correction=  
(Hartree/Particle)

0.317907

Thermal correction to Energy=

0.335608

Thermal correction to Enthalpy=

0.336552

Thermal correction to Gibbs Free Energy=

0.271635

Sum of electronic and zero-point Energies=

-1148.850100

Sum of electronic and thermal Energies=

-1148.832398

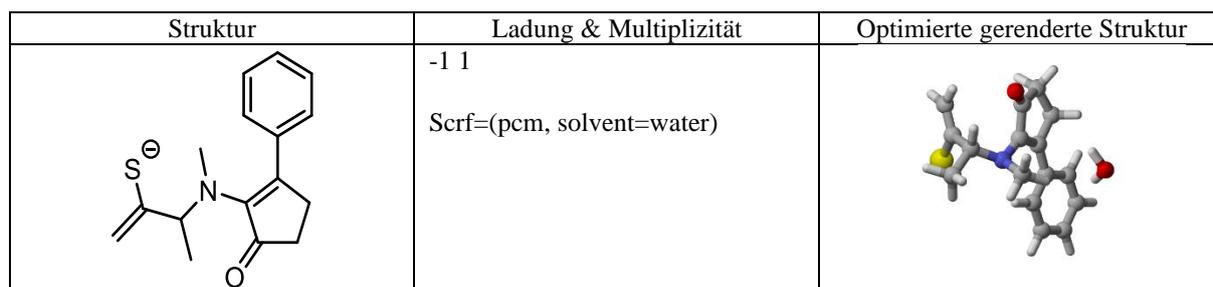
Sum of electronic and thermal Enthalpies=

-1148.831454

Sum of electronic and thermal Free Energies=

-1148.896372

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	210.597	69.369	136.630



40

XYZ file generated by gabedit : coordinates in Angstrom

H	4.9706670000	-2.4539390000	-0.1658090000
H	5.1075110000	-0.3302290000	-1.4445630000
C	4.1065650000	-1.8041250000	-0.2384620000
C	4.1838270000	-0.6136710000	-0.9544050000
H	2.8422170000	-3.0792570000	0.9431520000
C	2.9110100000	-2.1525580000	0.3855360000
C	3.0745960000	0.2193720000	-1.0440210000
H	3.1596570000	1.1413940000	-1.6056260000
C	1.8025820000	-1.3186440000	0.3076720000
C	1.8629520000	-0.1122240000	-0.4134500000
H	1.6291210000	2.7386180000	-0.9746930000
H	0.8775840000	-1.5974440000	0.7926930000
H	1.1316770000	1.8104280000	-2.3821310000
C	0.7299720000	0.8273080000	-0.5033270000
C	0.8496070000	2.0742010000	-1.3606160000
H	1.8456740000	2.2168020000	1.7530140000
S	-2.0375660000	-2.1646040000	-1.4578020000
C	-0.4675030000	0.7740340000	0.1325560000
H	-2.0571360000	-2.5693310000	1.5471950000
C	-0.5257890000	2.7422770000	-1.2826670000
H	0.5598260000	0.2425090000	2.3944880000
N	-0.9375740000	-0.2263650000	1.0076240000
H	-1.1157940000	2.5384560000	-2.1814900000
H	-0.4980350000	3.8204940000	-1.1304310000
C	-2.7317610000	-0.7753820000	-0.6133150000
H	-3.9246210000	-0.0569470000	-2.2139090000
C	-1.2043560000	2.0440640000	-0.1272880000
C	-2.7486140000	-1.7427490000	1.7198740000
C	-0.4981460000	-0.0272460000	2.3897610000
C	-2.3758000000	-0.5374490000	0.8566040000
C	-3.5991980000	0.0766620000	-1.1881960000
H	-2.7464770000	-1.4894470000	2.7815620000
H	-0.6046490000	-0.9535610000	2.9554920000
H	-3.7551800000	-2.0729730000	1.4557460000
H	-1.0642410000	0.7666020000	2.8980710000
H	-3.9906620000	0.9273730000	-0.6396670000
O	-2.1341830000	2.4743480000	0.5238180000
H	-2.9745640000	0.3181090000	1.1949740000
H	2.9356870000	1.2134010000	1.4063020000
O	2.7112020000	1.9061480000	2.0373770000

Zero-point correction=  
(Hartree/Particle)

0.329557

Thermal correction to Energy=

0.351282

Thermal correction to Enthalpy=

0.352226

Thermal correction to Gibbs Free Energy=

0.278623

Sum of electronic and zero-point Energies=

-1224.797152

Sum of electronic and thermal Energies=

-1224.775427

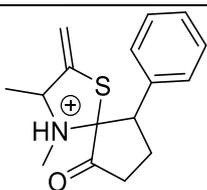
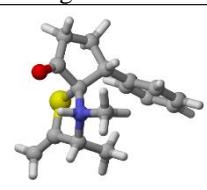
Sum of electronic and thermal Enthalpies=

-1224.774483

Sum of electronic and thermal Free Energies=

-1224.848086

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	220.433	80.356	154.911

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	+1 1  Scrf=(pcm, solvent=water)	

39

XYZ file generated by gabedit : coordinates in Angstrom

H	-2.0604690000	3.1537320000	-1.3325150000
H	-1.5851340000	3.6536560000	0.2893880000
C	-1.4808010000	2.8609100000	-0.4562940000
H	0.6544080000	3.3718240000	-0.5893660000
H	0.1111500000	2.1970760000	-1.7844800000
C	-0.0108200000	2.5257510000	-0.7499380000
O	-3.1197210000	1.4054900000	0.6470850000
C	-2.0427190000	1.6030810000	0.1524150000
H	2.2485770000	0.9110900000	2.0724670000
C	0.3430970000	1.3746450000	0.2231800000
H	0.3450060000	1.8113830000	1.2289800000
H	-2.2990530000	-0.3349910000	1.3297710000
C	-0.9404460000	0.5210480000	0.1336980000
C	2.5395290000	0.5402930000	1.0948210000
S	-1.1354020000	-0.3694710000	-1.4764430000
H	-0.9424320000	0.7698590000	2.8718560000
H	4.4168840000	-0.2181050000	1.8066300000
C	1.6842440000	0.7157680000	0.0041370000
H	-2.8285110000	-2.6592100000	-2.2674900000
C	3.7711290000	-0.0896410000	0.9463240000
H	0.4204190000	-0.3121050000	2.4502360000
C	-1.7043420000	-1.8459560000	-0.6796140000
C	-0.6574810000	-0.2258510000	2.5385670000
N	-1.2816850000	-0.4812540000	1.2064820000
H	-1.7782320000	-2.5162450000	1.3557910000
C	-2.4678740000	-2.7663280000	-1.2527380000
C	-1.1379240000	-1.9124000000	0.7114030000
C	2.1139690000	0.2905940000	-1.2567690000
H	-2.7271440000	-3.6675150000	-0.7090120000
H	-1.0453420000	-0.9708700000	3.2302230000
C	4.1711970000	-0.5445500000	-0.3057770000
H	1.4961310000	0.4468110000	-2.1312580000
C	3.3446190000	-0.3413640000	-1.4069240000
H	5.1282370000	-1.0378450000	-0.4269360000
C	0.2985160000	-2.4096890000	0.7566940000
H	0.9624660000	-1.7857310000	0.1559910000
H	0.3033470000	-3.4182570000	0.3427570000
H	0.6730640000	-2.4652230000	1.7788460000
H	3.6592690000	-0.6708030000	-2.3899380000

Zero-point correction=  
(Hartree/Particle)

0.334399

Thermal correction to Energy=

0.351570

Thermal correction to Enthalpy=

0.352514

Thermal correction to Gibbs Free Energy=

0.290137

Sum of electronic and zero-point Energies=

-1149.269554

Sum of electronic and thermal Energies=

-1149.252383

Sum of electronic and thermal Enthalpies=

-1149.251439

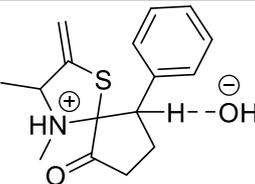
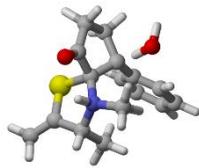
Sum of electronic and thermal Free Energies=

-1149.313816

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	220.613	68.977	131.284

#M062X/6-311+G\*\*

(TS-56-58)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 Scrf=(pcm, solvent=water)	

41

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.9791500000	2.5088030000	-2.2717540000
H	-1.4253940000	3.4652120000	-0.8934610000
C	-1.3776750000	2.4790050000	-1.3610870000
H	0.7684330000	2.8230460000	-1.6498610000
H	0.1396150000	1.3951940000	-2.4739720000
C	0.0664640000	1.9925330000	-1.5552710000
O	-3.0252680000	1.5169240000	0.1775720000
C	-1.9597440000	1.4926900000	-0.3865150000
H	2.2709110000	1.1526950000	1.6186680000
C	0.3664870000	1.1688870000	-0.2852930000
H	0.3835300000	2.1517380000	0.6668120000
H	-2.2807370000	-0.0091900000	1.2873600000
C	-0.9079270000	0.4018410000	-0.1228110000
C	2.5421820000	0.5072330000	0.7894960000
S	-1.2741550000	-0.9602510000	-1.3970140000
H	-0.7898450000	1.4405880000	2.3768570000
H	4.3927740000	-0.1208930000	1.6837690000
C	1.6719870000	0.4218550000	-0.3043580000
H	-3.0202630000	-3.3613220000	-1.3724840000
C	3.7416320000	-0.1999010000	0.8204470000
H	0.4567740000	0.1804980000	2.3280130000
C	-1.8300280000	-2.1011960000	-0.1694230000
C	-0.6097090000	0.3676690000	2.3901350000
N	-1.2773340000	-0.2421080000	1.2025950000
H	-1.8526190000	-2.1016520000	1.9754390000
C	-2.6243840000	-3.1429070000	-0.3889690000
C	-1.2153720000	-1.7534360000	1.1605360000
C	2.0765860000	-0.3596090000	-1.3966340000
H	-2.8749450000	-3.8143410000	0.4246530000
H	-1.0349030000	-0.0990350000	3.2772810000
C	4.1071770000	-1.0010610000	-0.2574520000
H	1.4470300000	-0.4246640000	-2.2760290000
C	3.2746550000	-1.0676720000	-1.3723140000
H	5.0376580000	-1.5563940000	-0.2364910000
C	0.1999090000	-2.2895840000	1.3208900000
H	0.8644990000	-1.9035800000	0.5461140000
H	0.1504530000	-3.3751910000	1.2316960000
H	0.6087770000	-2.0496800000	2.3024790000
H	3.5593300000	-1.6724950000	-2.2261240000
O	0.3735720000	3.1107860000	1.4886420000
H	0.5860120000	3.9096680000	0.9971240000

Zero-point correction=  
(Hartree/Particle)

0.339422

Thermal correction to Energy=

0.359174

Thermal correction to Enthalpy=

0.360118

Thermal correction to Gibbs Free Energy=

0.292294

Sum of electronic and zero-point Energies=

-1225.187738

Sum of electronic and thermal Energies=

-1225.167986

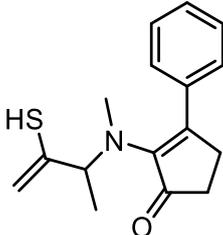
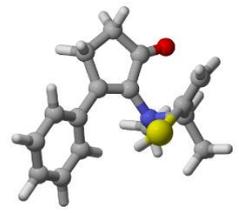
Sum of electronic and thermal Enthalpies=

-1225.167042

Sum of electronic and thermal Free Energies=

-1225.234866

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	225.385	77.225	142.748

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 Scrf=(pcm, solvent=water)	

38

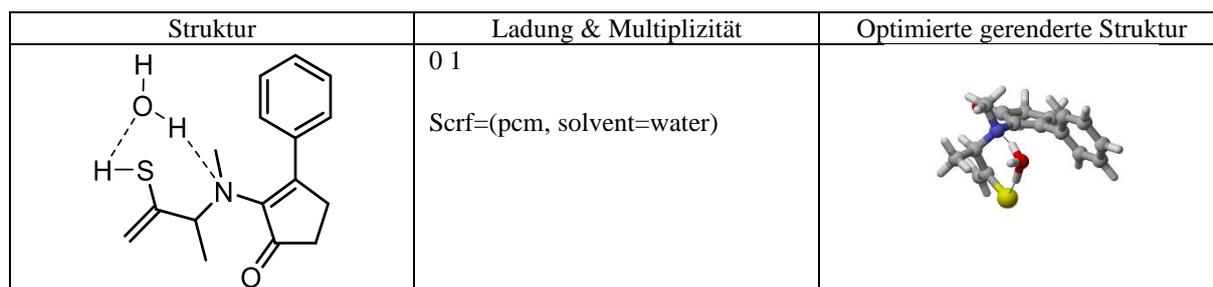
XYZ file generated by gabedit : coordinates in Angstrom

H	5.1967310000	-1.3271540000	0.2836300000
H	4.7609100000	0.3036750000	-1.5340480000
C	4.2553910000	-0.7918250000	0.2465180000
C	4.0109330000	0.1240420000	-0.7728760000
H	3.4770830000	-1.7085870000	2.0296240000
C	3.2877650000	-1.0088600000	1.2242400000
C	2.8045940000	0.8131740000	-0.8175850000
H	2.6307110000	1.5211670000	-1.6187680000
C	2.0758690000	-0.3304230000	1.1750670000
C	1.8117230000	0.5840190000	0.1447450000
H	1.1169820000	3.3605170000	-0.0889770000
H	1.3332290000	-0.5060590000	1.9406140000
H	0.7525980000	2.6088470000	-1.6329150000
C	0.5271480000	1.2962370000	0.0542480000
C	0.4394390000	2.6631540000	-0.5876470000
S	-0.2143400000	-1.9191360000	-1.6399470000
C	-0.6820700000	0.8621990000	0.4767730000
H	-1.2250870000	-3.0336810000	1.0001840000
C	-1.0317800000	3.0725380000	-0.4616930000
H	-0.4922380000	0.3937300000	2.9477900000
N	-0.9754770000	-0.3970090000	1.0693480000
H	-1.5129430000	3.2396450000	-1.4275060000
H	-1.1729770000	3.9746480000	0.1363580000
C	-1.7449600000	-1.1665140000	-1.1258310000
H	-2.4044020000	-0.7751550000	-3.0998740000
C	-1.7049040000	1.9052510000	0.2299710000
C	-2.1963640000	-2.5387780000	0.9306770000
C	-1.2303580000	-0.2801220000	2.5110370000
C	-2.0460210000	-1.1276750000	0.3589120000
C	-2.6099480000	-0.7251340000	-2.0370410000
H	-2.6471930000	-2.5119720000	1.9231310000
H	-1.1246260000	-1.2545820000	2.9892990000
H	-2.8454620000	-3.1279470000	0.2810320000
H	-2.2312440000	0.1184850000	2.7235270000
H	-3.5592260000	-0.3064370000	-1.7216280000
O	-2.8779750000	1.8419290000	0.5419060000
H	-3.0019600000	-0.5988330000	0.4647730000
H	0.4319470000	-1.7282030000	-0.4748780000

Zero-point correction= 0.315157  
(Hartree/Particle)

Thermal correction to Energy= 0.333795  
 Thermal correction to Enthalpy= 0.334739  
 Thermal correction to Gibbs Free Energy= 0.267669  
 Sum of electronic and zero-point Energies= -1148.841860  
 Sum of electronic and thermal Energies= -1148.823222  
 Sum of electronic and thermal Enthalpies= -1148.822277  
 Sum of electronic and thermal Free Energies= -1148.889348

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	209.460	71.425	141.163



41

XYZ file generated by gabedit : coordinates in Angstrom

H	5.3374200000	-1.0136090000	0.1555640000
H	4.3153070000	-0.5503780000	-2.0553350000
C	4.3662140000	-0.5367610000	0.0954380000
C	3.7933440000	-0.2739760000	-1.1470120000
H	4.1379470000	-0.3737820000	2.2281950000
C	3.6924150000	-0.1799240000	1.2596150000
C	2.5541720000	0.3509150000	-1.2255890000
H	2.1096720000	0.5536770000	-2.1938430000
C	2.4431400000	0.4254690000	1.1836460000
C	1.8637690000	0.6913550000	-0.0588530000
H	1.1339860000	3.4155360000	-0.4424350000
H	1.9203230000	0.7061460000	2.0910020000
H	0.7415230000	2.5561350000	-1.9219350000
C	0.5597980000	1.3745200000	-0.1432480000
C	0.4439860000	2.6886420000	-0.8784090000
H	0.1806640000	-1.2716340000	0.9711300000
S	-0.7436730000	-2.1153790000	-1.7059200000
C	-0.6101740000	0.9958430000	0.4021890000
H	-1.6309920000	-2.9396410000	1.0946520000
C	-1.0213930000	3.1021610000	-0.7228830000
H	-0.2939830000	0.6581040000	2.9032920000
N	-0.8968870000	-0.2332000000	1.0951070000
H	-1.5669550000	3.0724370000	-1.6694810000
H	-1.1528980000	4.0961820000	-0.2945500000
C	-1.9723420000	-1.0264870000	-1.0246540000
H	-2.7866010000	-0.4453550000	-2.8906720000
C	-1.6259260000	2.0596960000	0.1946790000
C	-2.4467580000	-2.2196020000	1.1580800000
C	-1.0913780000	0.0083630000	2.5467250000
C	-2.1188580000	-0.8884170000	0.4852780000
C	-2.8223300000	-0.3548670000	-1.8111640000
H	-2.7203440000	-2.0825410000	2.2043520000
H	-1.0338260000	-0.9384630000	3.0825960000
H	-3.3063030000	-2.6525470000	0.6437850000
H	-2.0568000000	0.4831280000	2.7409640000
H	-3.5746290000	0.2985140000	-1.3814580000
O	-2.7333090000	2.1030120000	0.6885640000
H	-2.9587040000	-0.2123430000	0.6620900000
H	0.2262690000	-2.2725040000	-0.3509530000
O	0.7886100000	-2.1100570000	0.6729010000
H	0.6674140000	-2.8538180000	1.2772580000

Zero-point correction=  
(Hartree/Particle)

0.336888

Thermal correction to Energy=

0.356847

Thermal correction to Enthalpy=

0.357791

Thermal correction to Gibbs Free Energy=

0.287813

Sum of electronic and zero-point Energies=

-1225.238103

Sum of electronic and thermal Energies=

-1225.218145

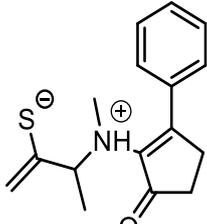
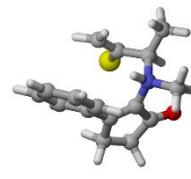
Sum of electronic and thermal Enthalpies=

-1225.217201

Sum of electronic and thermal Free Energies=

-1225.287178

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	223.925	76.934	147.280

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1  Scrf=(pcm, solvent=water)	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.5832850000	-3.7036150000	-0.5895420000
H	-1.9494360000	-3.0957020000	1.0260050000
C	-1.3937550000	-2.8876600000	0.1108160000
O	-3.0535090000	-1.3386310000	-0.7930790000
C	-1.9090810000	-1.6002760000	-0.4960110000
H	0.7377620000	-3.4057580000	-0.1275340000
C	0.1031650000	-2.6561610000	0.3490950000
H	0.3496750000	-2.6529080000	1.4146460000
H	0.6649430000	2.6692340000	0.4729420000
C	-0.7372320000	-0.7201190000	-0.6714640000
H	-2.5144280000	0.4278950000	-2.4587160000
C	0.3903920000	-1.2909520000	-0.2233470000
H	-2.6145970000	0.9770000000	-0.0069360000
C	0.2891200000	2.0541660000	1.2865660000
H	0.9072070000	1.9874540000	2.1733600000
H	0.0596840000	1.0599090000	-1.1749340000
H	-0.9249660000	-0.0153550000	-3.1445410000
H	2.0791550000	-1.1459760000	1.8670890000
C	-1.4644880000	0.6999530000	-2.5275150000
N	-0.8826200000	0.6499010000	-1.1450820000
C	-1.6601230000	1.4898170000	-0.1075980000
C	-0.8831500000	1.4025780000	1.2063830000
C	1.7321530000	-0.6903140000	-0.2107200000
C	2.4829880000	-0.6918660000	0.9695110000
H	-1.3418170000	1.7043890000	-2.9211740000
H	-2.5542130000	2.9289020000	-1.4746750000
H	1.7047100000	-0.1350730000	-2.2953610000
C	-1.8703430000	2.9033610000	-0.6264210000
C	2.2563940000	-0.0922270000	-1.3612460000
S	-1.5877560000	0.3974560000	2.4590330000
H	-2.3148950000	3.4851820000	0.1815770000
C	3.7251540000	-0.0723260000	1.0024320000
H	4.2949980000	-0.0608860000	1.9236760000
H	-0.9311560000	3.3838610000	-0.9089830000
C	3.5058970000	0.5173740000	-1.3259460000
C	4.2370610000	0.5356410000	-0.1421620000
H	3.9081970000	0.9707850000	-2.2235470000
H	5.2080520000	1.0151560000	-0.1119280000

Zero-point correction= 0.320142  
(Hartree/Particle)

Thermal correction to Energy= 0.338332

Thermal correction to Enthalpy= 0.339276

Thermal correction to Gibbs Free Energy= 0.272577

Sum of electronic and zero-point Energies= -1148.824420

Sum of electronic and thermal Energies= -1148.806230

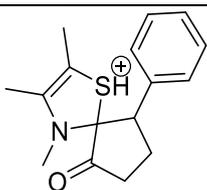
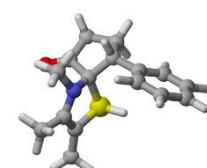
Sum of electronic and thermal Enthalpies= -1148.805286

Sum of electronic and thermal Free Energies= -1148.871985

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	212.306	69.861	140.380

#M062X/6-311+G\*\*

(60)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	+1 1 Scrf=(pcm, solvent=water)	

39

XYZ file generated by gabedit : coordinates in Angstrom

H	0.9569100000	2.3770520000	-1.4180150000
H	-1.0244470000	3.7262280000	-1.0250950000
H	2.8484250000	1.3413700000	-1.3927910000
H	4.7041320000	-0.2497720000	-1.6004600000
H	-3.1015160000	-2.8949720000	-1.6183630000
H	-2.8016290000	-1.6842640000	-2.8629280000
S	-0.5828790000	-0.1230440000	-1.5329200000
H	1.5274980000	3.2823680000	-0.0178710000
C	0.7653910000	2.5855260000	-0.3623360000
C	-0.6577120000	3.1297520000	-0.1897950000
C	-2.3357310000	-2.2598150000	-2.0609220000
C	2.9142920000	0.5148770000	-0.6951670000
C	3.9714560000	-0.3865310000	-0.8141810000
H	-0.7450880000	3.7381160000	0.7166650000
H	-1.5728450000	-2.9071430000	-2.5008670000
C	-1.7596400000	-1.3618950000	-1.0155730000
C	-1.5245680000	1.9122670000	0.0195990000
C	0.7827230000	1.2878780000	0.4651990000
C	-0.5912350000	0.6585170000	0.1465510000
C	1.9623980000	0.3577250000	0.3136590000
O	-2.7133930000	1.8467260000	0.1410000000
C	4.0884330000	-1.4505390000	0.0717670000
H	4.9105400000	-2.1497290000	-0.0225130000
H	0.7171750000	1.5819470000	1.5194700000
C	-1.8825390000	-1.3142870000	0.3267170000
N	-1.1112440000	-0.3786820000	1.0041910000
C	2.0942390000	-0.7123940000	1.2064700000
C	3.1470590000	-1.6102100000	1.0867740000
H	-3.2712070000	-2.9321880000	0.4816670000
C	-2.7516580000	-2.2286630000	1.1254200000
H	1.3672950000	-0.8402980000	2.0010570000
H	-2.3627350000	0.6117030000	2.4189050000
H	3.2355920000	-2.4317130000	1.7874380000
C	-1.4489540000	0.0129780000	2.3746800000
H	-3.4891960000	-1.6559510000	1.6911060000
H	-0.6246010000	0.5849620000	2.7974340000
H	-2.1408560000	-2.7929130000	1.8337640000
H	-1.5659290000	-0.8822490000	2.9811430000
H	0.6006790000	-0.7880010000	-1.3935200000

Zero-point correction=  
(Hartree/Particle)

0.327987

Thermal correction to Energy=

0.346574

Thermal correction to Enthalpy=

0.347518

Thermal correction to Gibbs Free Energy=

0.281166

Sum of electronic and zero-point Energies=

-1149.245435

Sum of electronic and thermal Energies=

-1149.226848

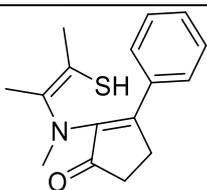
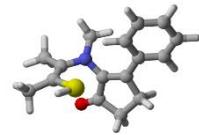
Sum of electronic and thermal Enthalpies=

-1149.225904

Sum of electronic and thermal Free Energies=

-1149.292257

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-kelvin	Cal/Mol-kelvin
Total	217.478	71.742	139.650

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 Scrf=(pcm, solvent=water)	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-4.0763030000	-1.1538680000	1.5780380000
H	-3.1013690000	0.0935870000	2.3708000000
H	-0.5040900000	4.0028720000	-0.1634160000
H	-2.7069850000	-1.6150240000	2.5773300000
C	-3.0663120000	-0.8727160000	1.8601720000
O	-2.3087980000	2.1171410000	0.5386980000
H	-4.2145170000	-0.5378040000	-1.7807020000
C	-1.1635650000	1.9812970000	0.1643500000
C	-0.3389390000	3.0084280000	-0.5773050000
H	1.6649210000	3.0917050000	0.2641800000
H	-0.7025060000	-0.3275930000	3.1028320000
H	-4.6133550000	-1.3804140000	-0.2810240000
C	-3.8874160000	-1.3184270000	-1.0878970000
C	-2.1394590000	-0.7799060000	0.6782740000
H	-0.6715270000	3.0174850000	-1.6192310000
C	-0.3070470000	0.7836510000	0.3844340000
H	0.8349060000	-0.5553380000	2.2523730000
N	-0.8103020000	-0.3768350000	0.9769640000
C	1.1004450000	2.4992640000	-0.4620110000
C	-0.2232180000	-0.8090660000	2.2441110000
H	-3.9092340000	-2.2666230000	-1.6328550000
C	-2.4983360000	-1.0269090000	-0.5941260000
C	0.9678150000	1.0666370000	0.0103250000
H	3.5572280000	1.8009200000	0.0040470000
H	1.6450860000	2.5451540000	-1.4074210000
H	-0.3130280000	-1.8925640000	2.3461260000
C	2.1369720000	0.1762440000	0.0116020000
C	3.4273860000	0.7252230000	-0.0106750000
S	-1.2659970000	-0.9103740000	-1.8914200000
H	5.5392440000	0.3511910000	-0.0471900000
C	4.5508820000	-0.0928480000	-0.0416100000
C	2.0058530000	-1.2216540000	-0.0196800000
H	1.0167980000	-1.6624530000	-0.0256890000
C	4.4063250000	-1.4767110000	-0.0691300000
C	3.1300910000	-2.0360630000	-0.0662980000
H	5.2813850000	-2.1154410000	-0.0946250000
H	3.0097890000	-3.1126330000	-0.0983520000
H	-1.9468480000	-1.6551190000	-2.7780400000

Zero-point correction= 0.314799  
 (Hartree/Particle)

Thermal correction to Energy= 0.333970

Thermal correction to Enthalpy= 0.334914

Thermal correction to Gibbs Free Energy= 0.266902

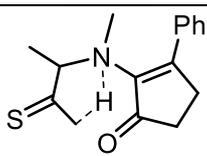
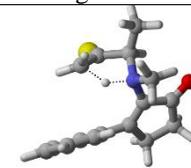
Sum of electronic and zero-point Energies= -1148.847347

Sum of electronic and thermal Energies= -1148.828177

Sum of electronic and thermal Enthalpies= -1148.827232

Sum of electronic and thermal Free Energies= -1148.895244

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	209.569	72.322	143.143

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 Scrf=(pcm, solvent=water)	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	1.3864440000	3.9989510000	0.4597100000
H	1.6718870000	3.1227330000	1.9610700000
C	1.2113550000	3.0521940000	0.9745130000
O	3.0596530000	1.8082890000	-0.0324820000
C	1.8752800000	1.9394490000	0.1900130000
H	-0.9245460000	3.4551590000	0.6092680000
C	-0.2757570000	2.6782750000	1.0192250000
H	-0.6217490000	2.4795560000	2.0370400000
H	0.1485630000	-2.6814070000	-1.4250730000
C	0.8085810000	1.0157250000	-0.2573540000
H	2.6251940000	0.5504610000	-2.2880350000
C	-0.3934180000	1.4235160000	0.1878150000
H	2.3939580000	-0.5803710000	0.6710510000
C	-0.2003280000	-2.3316410000	-0.4512810000
H	-1.1530500000	-2.7350950000	-0.1316660000
H	0.0507890000	-1.0096270000	-0.9243490000
H	0.9479960000	0.7828260000	-2.8352220000
H	-2.2636270000	0.7396570000	2.0105770000
C	1.6350200000	0.0963980000	-2.3416600000
N	1.1025780000	-0.1830010000	-0.9917580000
C	1.8864220000	-1.1468290000	-0.1080490000
C	0.7592870000	-1.9914500000	0.5136620000
C	-1.6923340000	0.7792850000	-0.0668860000
C	-2.5512550000	0.4863170000	0.9962790000
H	1.6783580000	-0.8314450000	-2.9093900000
H	3.6804180000	-1.3696470000	-1.3042660000
H	-1.4192170000	0.6941040000	-2.2005490000
C	2.9023520000	-1.9931980000	-0.8624020000
C	-2.0737540000	0.4486960000	-1.3712170000
S	0.6619100000	-2.1541890000	2.1764680000
H	3.3724260000	-2.6669350000	-0.1440260000
C	-3.7589150000	-0.1607420000	0.7583780000
H	-4.4110210000	-0.4024230000	1.5890540000
H	2.4411080000	-2.5994990000	-1.6426920000
C	-3.2907150000	-0.1780610000	-1.6073120000
C	-4.1305950000	-0.4930220000	-0.5417060000
H	-3.5813700000	-0.4244480000	-2.6215160000
H	-5.0757240000	-0.9903120000	-0.7244140000

Zero-point correction=  
(Hartree/Particle)

0.313097

Thermal correction to Energy=

0.331038

Thermal correction to Enthalpy=

0.331982

Thermal correction to Gibbs Free Energy=

0.266094

Sum of electronic and zero-point Energies=

-1148.796499

Sum of electronic and thermal Energies=

-1148.778559

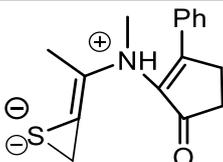
Sum of electronic and thermal Enthalpies=

-1148.777615

Sum of electronic and thermal Free Energies=

-1148.843503

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	207.729	69.144	138.672

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	-1 1 Scrf=(pcm, solvent=water)	

37

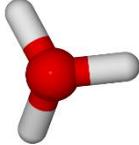
XYZ file generated by gabedit : coordinates in Angstrom

H	2.1328120000	-3.5003040000	-0.7233980000
H	2.7802260000	-2.4796010000	-2.0129360000
C	2.0728030000	-2.5047300000	-1.1810240000
O	3.6625830000	-1.1182010000	0.1041240000
C	2.4549810000	-1.4319400000	-0.1434540000
H	0.0414990000	-3.0446820000	-1.8652940000
C	0.6210130000	-2.1598940000	-1.5866000000
H	0.6420640000	-1.4946100000	-2.4654190000
H	-1.9119460000	2.3593000000	0.7203570000
C	1.2529600000	-0.9479750000	0.3425530000
H	3.0641980000	0.2580610000	1.9224900000
C	0.0786000000	-1.4525770000	-0.3592200000
C	-1.4009240000	1.9368120000	-0.1376450000
H	-1.9136020000	1.1269940000	-0.6472720000
H	0.1624920000	0.3106070000	1.4823310000
H	1.7862850000	-0.4233670000	2.9583800000
H	-2.1336740000	-1.9638910000	-1.8768800000
C	2.0483660000	0.3900520000	2.2844610000
N	1.1268910000	0.3083750000	1.1141230000
C	1.2024830000	1.4903850000	0.2270300000
C	0.0484090000	1.9876340000	-0.1839170000
C	-1.2353560000	-1.3158770000	0.0171720000
C	-2.3449140000	-1.5394960000	-0.8993140000
H	1.9133040000	1.3550750000	2.7710860000
H	3.1782030000	1.1062440000	-0.4845640000
H	-0.9598610000	-0.9698460000	2.1854100000
C	2.5634120000	1.9542310000	-0.1737780000
C	-1.6530630000	-0.8794620000	1.3505090000
S	-0.6102870000	3.2032520000	-1.2456880000
H	2.4713070000	2.6661570000	-0.9936350000
C	-3.6295550000	-1.1603640000	-0.5912480000
H	-4.4076210000	-1.3109910000	-1.3360690000
H	3.0728720000	2.4526570000	0.6560030000
C	-2.9617060000	-0.5150070000	1.6234420000
C	-3.9742040000	-0.5882580000	0.6595060000
H	-3.2096600000	-0.1939050000	2.6329750000
H	-4.9930320000	-0.3001380000	0.8847490000

Zero-point correction= 0.303337  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.321564  
 Thermal correction to Enthalpy= 0.322508  
 Thermal correction to Gibbs Free Energy= 0.257675  
 Sum of electronic and zero-point Energies= -1148.258075  
 Sum of electronic and thermal Energies= -1148.239848  
 Sum of electronic and thermal Enthalpies= -1148.238904  
 Sum of electronic and thermal Free Energies= -1148.303737

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	201.785	70.698	136.453

#M062X/6-311+G**	<b>(H<sub>3</sub>O<sup>+</sup>)</b>
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Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
$\oplus$ OH <sub>3</sub>	+1 1  Scrf=(pcm, solvent=water)	

4

XYZ file generated by gabedit : coordinates in Angstrom

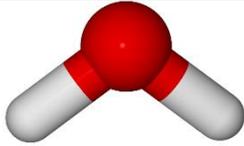
H	0.6433040000	0.6706960000	0.2188530000
H	-0.9030890000	0.2203240000	0.2190840000
H	0.2606770000	-0.8918690000	0.2186240000
O	-0.0001120000	0.0001060000	-0.0820700000

Zero-point correction= 0.035083  
(Hartree/Particle)

Thermal correction to Energy=	0.037967
Thermal correction to Enthalpy=	0.038911
Thermal correction to Gibbs Free Energy=	0.015959
Sum of electronic and zero-point Energies=	-76.782698
Sum of electronic and thermal Energies=	-76.779814
Sum of electronic and thermal Enthalpies=	-76.778869
Sum of electronic and thermal Free Energies=	-76.801822

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	23.825	6.494	48.307

#M062X/6-311+G**	<b>(H<sub>2</sub>O)</b>
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Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
H <sub>2</sub> O	0 1  Scrf=(pcm, solvent=water)	

3

XYZ file generated by gabedit : coordinates in Angstrom

O	0.0000000000	0.1174720000	0.0000000000
H	0.7605520000	-0.4698850000	0.0000000000
H	-0.7605520000	-0.4698880000	0.0000000000

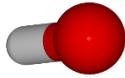
Zero-point correction= 0.021515  
(Hartree/Particle)

Thermal correction to Energy=	0.024351
Thermal correction to Enthalpy=	0.025295
Thermal correction to Gibbs Free Energy=	0.003220
Sum of electronic and zero-point Energies=	-76.407375
Sum of electronic and thermal Energies=	-76.404539
Sum of electronic and thermal Enthalpies=	-76.403595
Sum of electronic and thermal Free Energies=	-76.425670

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	15.281	6.014	46.462

#M062X/6-311+G\*\*

(OH<sup>-</sup>)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
$\ominus$ OH	-1 1  Scrf=(pcm, solvent=water)	

2

XYZ file generated by gabedit : coordinates in Angstrom

O	0.0000000000	-0.4804460000	-0.3736800000
H	0.0000000000	0.4804460000	-0.3736800000

Zero-point correction= 0.008885  
(Hartree/Particle)

Thermal correction to Energy= 0.011245

Thermal correction to Enthalpy= 0.012189

Thermal correction to Gibbs Free Energy= -0.007360

Sum of electronic and zero-point Energies= -75.909114

Sum of electronic and thermal Energies= -75.906753

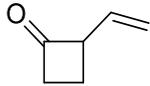
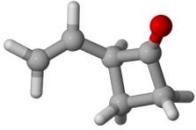
Sum of electronic and thermal Enthalpies= -75.905809

Sum of electronic and thermal Free Energies= -75.925358

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	7.056	4.968	41.145

## CC-Info vinyl:

#M062X/6-311+G**	(21)
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Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

15

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.4331520000	-0.5157690000	-0.6289660000
C	-2.5316150000	0.0238030000	-0.3657660000
H	-2.5043090000	1.0828980000	-0.5993350000
H	-1.5736380000	-1.6526530000	0.4450980000
C	-1.5123480000	-0.5900350000	0.2233740000
H	-0.2980170000	1.6433380000	-0.9176170000
H	0.1238690000	2.2932200000	0.6849290000
C	-0.2283270000	0.0647440000	0.6129400000
C	0.2097780000	1.4335890000	0.0238670000
H	-0.1154600000	0.0655590000	1.7050600000
C	1.0718120000	-0.5118940000	0.0271600000
C	1.6432650000	0.8827760000	-0.2160810000
H	2.1095420000	1.0474690000	-1.1869660000
O	1.4289120000	-1.6173820000	-0.2388500000
H	2.3444850000	1.1570980000	0.5756330000

Zero-point correction=  
(Hartree/Particle)

0.125036

Thermal correction to Energy=

0.131982

Thermal correction to Enthalpy=

0.132927

Thermal correction to Gibbs Free Energy=

0.093797

Sum of electronic and zero-point Energies=

-308.443395

Sum of electronic and thermal Energies=

-308.436449

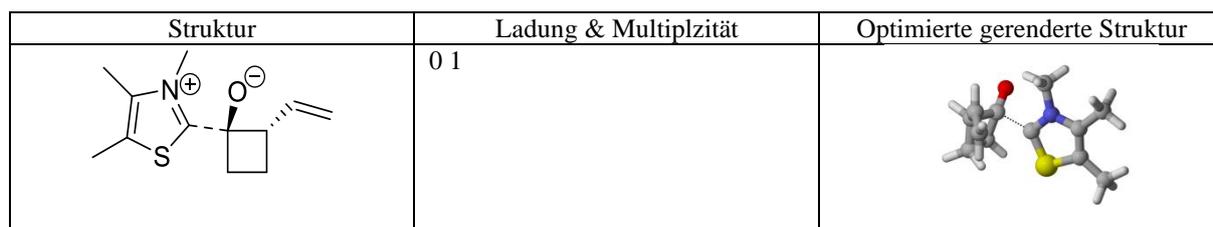
Sum of electronic and thermal Enthalpies=

-308.435505

Sum of electronic and thermal Free Energies=

-308.474634

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.820	25.120	82.356



32

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.5547590000	-0.5372460000	-1.8335110000
C	-2.6327860000	-0.1762330000	-1.3799180000
H	-1.8154580000	-0.8354530000	-1.6725890000
H	-3.1890300000	1.9199330000	-1.7488240000
C	-2.2890970000	1.3171190000	-1.6015590000
H	-3.6859410000	0.4018980000	0.4261440000
H	-1.5526550000	1.5892550000	-2.3575050000
H	-1.4559050000	-2.4238080000	-0.1651650000
C	-2.6806250000	0.0640160000	0.1446800000
C	-1.6112850000	-2.0947060000	0.8567980000
C	-2.2018860000	-0.9346440000	1.1358680000
C	-1.9064260000	1.4192900000	-0.1025460000
S	0.8824070000	0.3010090000	-1.6517560000
C	-0.0251840000	0.6596970000	-0.2456950000
H	3.8935120000	0.7019770000	-2.2650550000
O	-1.8402390000	2.4063250000	0.6246400000
C	2.4033640000	0.2291270000	-0.7992290000
C	3.6850230000	-0.0623390000	-1.5133740000
N	0.8218460000	0.7249800000	0.7748640000
H	4.5236860000	-0.0863410000	-0.8181220000
H	-0.6371780000	1.4411490000	2.0712480000
H	0.2983450000	0.0351020000	2.6864320000
C	2.1823810000	0.4810520000	0.5102440000
C	0.3456160000	0.9791350000	2.1404310000
H	3.6381900000	-1.0282370000	-2.0205360000
H	1.0301110000	1.6640290000	2.6391910000
H	2.8688220000	-0.1238540000	2.4498580000
C	3.1760410000	0.5240850000	1.6259750000
H	4.1500150000	0.1864450000	1.2774090000
H	3.2895960000	1.5375630000	2.0190200000
H	-1.2758730000	-2.7599210000	1.6441190000
H	-2.3458040000	-0.6584980000	2.1796880000

Zero-point correction=  
(Hartree/Particle)

0.266694

Thermal correction to Energy=

0.282649

Thermal correction to Enthalpy=

0.283593

Thermal correction to Gibbs Free Energy=

0.221828

Sum of electronic and zero-point Energies=

-995.190420

Sum of electronic and thermal Energies=

-995.174466

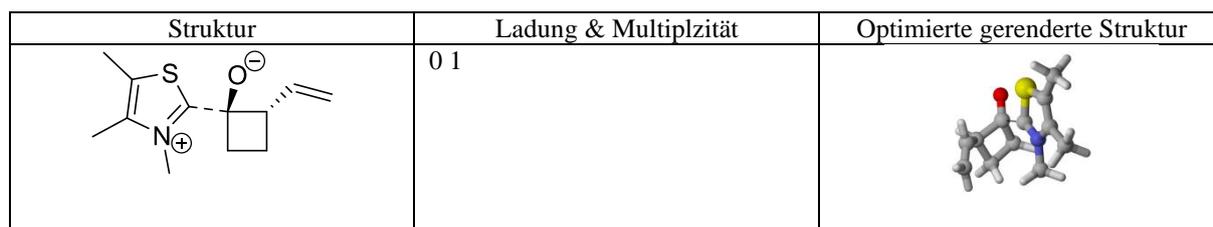
Sum of electronic and thermal Enthalpies=

-995.173521

Sum of electronic and thermal Free Energies=

-995.235286

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.365	59.465	129.994



32

XYZ file generated by gabedit : coordinates in Angstrom

H	-4.1486300000	-0.0271410000	0.3403960000
H	-3.2928620000	1.5928290000	-1.2784950000
H	-2.2604150000	1.9310890000	2.0469960000
C	-3.0696130000	-0.0201820000	0.1909730000
H	-3.3151280000	-1.3643110000	-1.5487610000
C	-2.5192720000	1.1693630000	-0.6280440000
H	-2.5973140000	-0.1135520000	1.1692470000
C	-1.6977950000	2.5197240000	1.3288670000
C	-2.5350480000	-1.0210050000	-0.8663470000
C	-1.7572510000	2.2679830000	0.0222180000
C	-1.7645540000	0.1397280000	-1.5631120000
O	-1.5648120000	0.2861740000	-2.7757270000
H	-1.9645140000	-1.8851030000	-0.5229610000
H	-0.7737190000	-1.0893450000	1.2825870000
C	0.0115530000	0.1253280000	-0.8050140000
H	-0.0994490000	0.2883340000	2.1848910000
C	0.1371850000	-0.5554580000	1.5338060000
N	0.7397050000	-0.0708140000	0.2929060000
H	0.8247920000	-1.2355000000	2.0341380000
S	1.0356400000	0.6959180000	-2.0488080000
C	2.1069730000	0.2425330000	0.2172620000
C	2.4390010000	0.6785190000	-1.0203980000
H	2.5623010000	0.5715020000	2.2891390000
C	2.9838490000	0.0681520000	1.4160550000
H	3.1203910000	-0.9876230000	1.6655150000
H	3.7658610000	2.1483180000	-1.8453270000
C	3.7781960000	1.0998720000	-1.5398320000
H	4.0613190000	0.5026710000	-2.4089620000
H	3.9660470000	0.4967650000	1.2265450000
H	4.5515880000	0.9756900000	-0.7822840000
H	-1.1100270000	3.3431060000	1.7178970000
H	-1.1992660000	2.9036320000	-0.6646830000

Zero-point correction=  
(Hartree/Particle)

0.266822

Thermal correction to Energy=

0.282691

Thermal correction to Enthalpy=

0.283635

Thermal correction to Gibbs Free Energy=

0.223697

Sum of electronic and zero-point Energies=

-995.183342

Sum of electronic and thermal Energies=

-995.167474

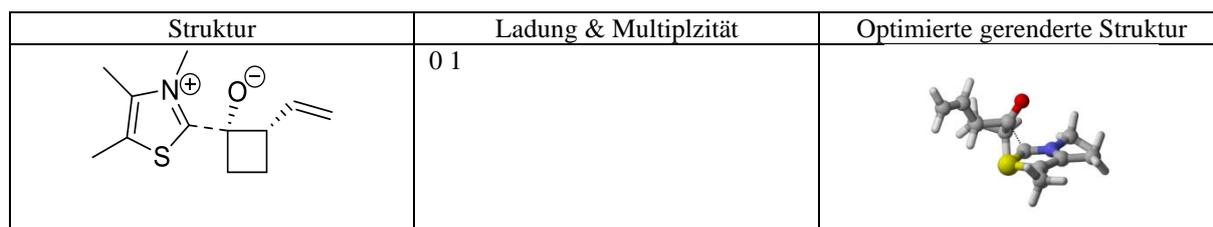
Sum of electronic and thermal Enthalpies=

-995.166530

Sum of electronic and thermal Free Energies=

-995.226467

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.391	59.502	126.149



32

XYZ file generated by gabedit : coordinates in Angstrom

H	4.0193460000	-0.4513540000	-1.6488940000
H	4.1427250000	-1.0318850000	0.0326910000
C	3.4564070000	-0.7158400000	-0.7541210000
H	2.4533550000	-2.7520420000	-0.6222020000
H	1.8406590000	-1.6619100000	-1.9147410000
C	2.2835300000	-1.7165920000	-0.9196480000
H	2.0806450000	0.9448080000	-1.0713340000
C	2.4686990000	0.3682620000	-0.2270660000
C	1.5429450000	-0.8456500000	0.1237460000
C	2.8644470000	1.2473670000	0.9010760000
H	-0.2218100000	-2.8019230000	-0.2142600000
H	2.5978380000	3.1125490000	-0.0464380000
C	2.8776980000	2.5766010000	0.8558980000
O	1.3093680000	-1.2134710000	1.2844220000
C	-0.2386150000	-0.3174280000	-0.5388000000
C	-1.1224470000	-2.4285530000	0.2638990000
H	-1.9904710000	-2.9924930000	-0.0756710000
N	-1.2804740000	-1.0180440000	-0.1006370000
S	-0.7456360000	1.3041290000	-0.7315970000
H	-0.9960500000	-2.5117450000	1.3437610000
C	-2.4841830000	-0.3296730000	0.1168640000
C	-2.3748650000	0.9825170000	-0.1936720000
H	-4.0364090000	-1.8013380000	-0.0928370000
C	-3.6772540000	-1.0669810000	0.6330720000
H	-3.0823560000	2.8619410000	0.5544070000
H	-3.4387600000	-1.5958300000	1.5586070000
C	-3.4018680000	2.0675670000	-0.1232570000
H	-4.3550280000	1.6800340000	0.2359110000
H	-4.4901440000	-0.3739360000	0.8403320000
H	-3.5690940000	2.5119380000	-1.1067630000
H	3.1309410000	0.7294770000	1.8197380000
H	3.1661990000	3.1721240000	1.7143910000

Zero-point correction=  
(Hartree/Particle)

0.266625

Thermal correction to Energy=

0.282744

Thermal correction to Enthalpy=

0.283688

Thermal correction to Gibbs Free Energy=

0.222629

Sum of electronic and zero-point Energies=

-995.184216

Sum of electronic and thermal Energies=

-995.168097

Sum of electronic and thermal Enthalpies=

-995.167153

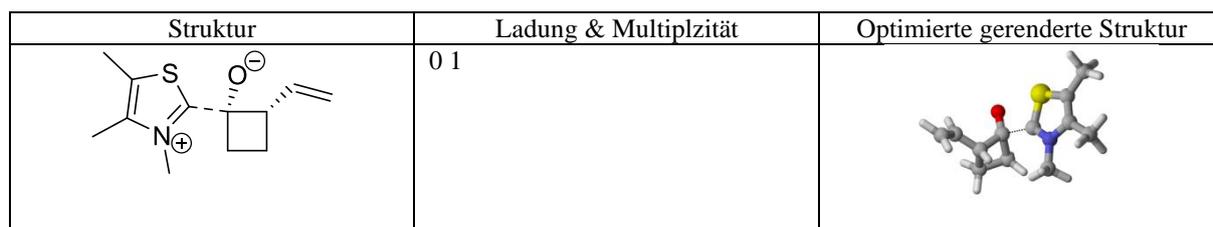
Sum of electronic and thermal Free Energies=

-995.228213

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.425	59.700	128.511

#M062X/6-311+G\*\*

(46-anti-anti)



32

XYZ file generated by gabedit : coordinates in Angstrom

H	3.6702230000	1.3662410000	1.6008360000
H	4.1570830000	1.6251960000	-0.0912660000
C	3.3130360000	1.4343330000	0.5728670000
H	2.3626290000	3.3536360000	-0.1944820000
H	1.5074330000	2.5669960000	1.1636070000
C	2.1359720000	2.4026490000	0.2865010000
H	0.3611630000	0.8864790000	2.1508250000
C	2.4674180000	0.2278430000	0.0634950000
H	1.9302830000	-0.2358960000	0.8953020000
C	3.1069940000	-0.8005660000	-0.7958050000
C	1.6095360000	1.3131750000	-0.6815190000
H	-1.2790750000	1.2684370000	2.7206440000
H	2.7956920000	-2.4863210000	0.4341320000
C	-0.6816750000	0.5830110000	2.1184860000
C	3.1964080000	-2.0933760000	-0.4959550000
H	-0.7784180000	-0.4287290000	2.5149930000
O	1.6086700000	1.4411730000	-1.9137030000
C	-0.2784190000	0.9207910000	-0.2614990000
N	-1.1232010000	0.6225850000	0.7251490000
H	-3.5879250000	0.8268330000	2.1300320000
H	-3.1422020000	-0.8793320000	2.0019370000
C	-2.4529570000	0.3387570000	0.3697110000
S	-1.1246660000	0.8566260000	-1.7409840000
C	-3.4511640000	-0.0010290000	1.4294880000
C	-2.6260170000	0.4286890000	-0.9700530000
H	-4.4177050000	-0.2191740000	0.9795230000
C	-3.8697960000	0.2113890000	-1.7737950000
H	-3.7233660000	-0.5837010000	-2.5076610000
H	-4.1449790000	1.1184930000	-2.3158050000
H	-4.7085570000	-0.0679440000	-1.1367520000
H	3.4995540000	-0.4297820000	-1.7401530000
H	3.6698460000	-2.8013660000	-1.1661940000

Zero-point correction=  
(Hartree/Particle)

0.266068

Thermal correction to Energy=

0.282493

Thermal correction to Enthalpy=

0.283437

Thermal correction to Gibbs Free Energy=

0.220419

Sum of electronic and zero-point Energies=

-995.178813

Sum of electronic and thermal Energies=

-995.162388

Sum of electronic and thermal Enthalpies=

-995.161444

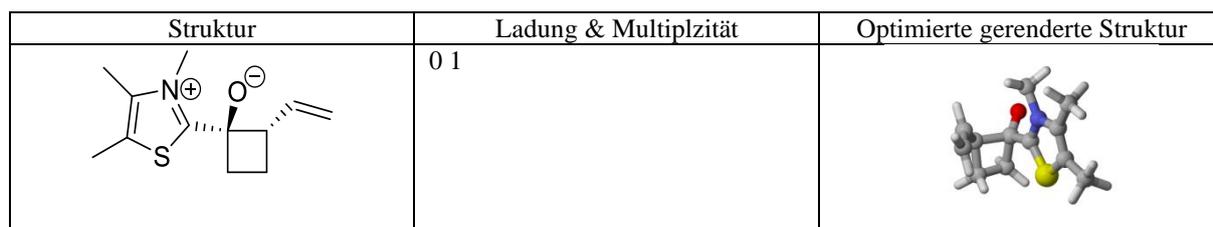
Sum of electronic and thermal Free Energies=

-995.224462

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.267	59.915	132.632

#M062X/6-311+G\*\*

(22-syn-syn)



32

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.5918480000	-0.5537090000	-1.5501280000
H	-1.8492660000	-0.8014050000	-1.7015080000
C	-2.6179010000	-0.1957240000	-1.2169850000
H	-0.8887540000	-2.3350160000	-0.4421700000
H	3.1994540000	-0.8464490000	-2.2635780000
C	-1.0450350000	-2.1869340000	0.6216080000
H	-1.7916950000	1.6845850000	-2.2160740000
C	-2.3399000000	1.3151130000	-1.3440580000
C	-2.4146850000	-0.0971960000	0.3024560000
H	-3.2497770000	1.9035730000	-1.2253860000
S	0.6448250000	0.6180650000	-1.5973980000
C	-1.7834380000	-1.1800010000	1.0951310000
C	3.3910000000	0.0070930000	-1.6106110000
H	-3.3328000000	0.2510520000	0.7814170000
H	3.6994830000	0.8482910000	-2.2351410000
C	2.1737810000	0.3512080000	-0.8116940000
H	4.2232430000	-0.2513670000	-0.9572150000
C	-1.6341000000	1.3397920000	0.0562410000
C	-0.1428070000	0.9456020000	-0.1183070000
C	2.0338410000	0.5248100000	0.5226190000
N	0.7236510000	0.8629700000	0.8809700000
O	-1.7735830000	2.3312730000	0.8766880000
H	4.0073690000	0.0332620000	1.1586440000
H	0.2805960000	0.0613080000	2.7615900000
H	2.7582580000	-0.2938500000	2.3640630000
C	3.0767580000	0.4015810000	1.5847500000
C	0.3269940000	1.0425110000	2.2873950000
H	-0.6441060000	1.5456670000	2.2764790000
H	3.2773880000	1.3675940000	2.0542240000
H	1.0695120000	1.6672690000	2.7815450000
H	-0.5941870000	-2.9135860000	1.2877070000
H	-1.9139960000	-1.1050670000	2.1742100000

Zero-point correction=  
(Hartree/Particle)

0.267889

Thermal correction to Energy=

0.283795

Thermal correction to Enthalpy=

0.284739

Thermal correction to Gibbs Free Energy=

0.225146

Sum of electronic and zero-point Energies=

-995.197485

Sum of electronic and thermal Energies=

-995.181579

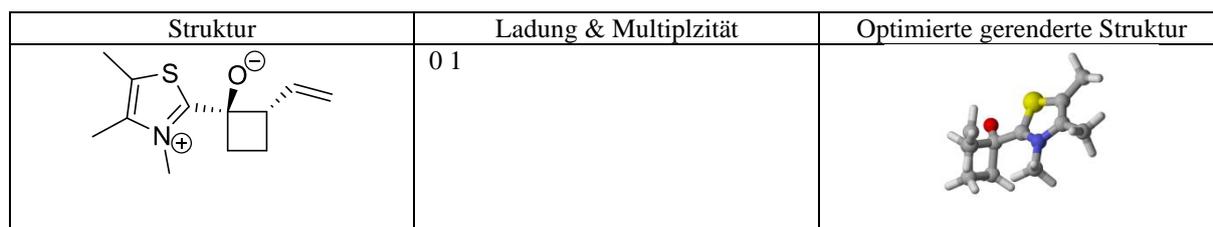
Sum of electronic and thermal Enthalpies=

-995.180635

Sum of electronic and thermal Free Energies=

-995.240228

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.084	60.511	125.423



32

XYZ file generated by gabedit : coordinates in Angstrom

H	2.9365910000	-1.0735580000	1.1533520000
H	4.2273540000	-0.0537620000	-0.6304420000
O	1.2040190000	-2.3632770000	-0.0326040000
H	-3.9064790000	-1.1637380000	1.5603910000
C	2.4089700000	-0.2657130000	0.6418060000
S	-1.1922900000	-1.5848540000	0.2950420000
C	3.1700490000	0.2094280000	-0.6131630000
C	1.3694240000	-1.0929720000	-0.2901630000
H	3.1056750000	1.2832910000	-0.8013650000
C	1.8690210000	0.6942220000	1.6394860000
H	-4.2760700000	-1.4751020000	-0.1363650000
C	-3.8647320000	-0.7373900000	0.5562490000
C	-0.0412380000	-0.4621220000	-0.2557030000
H	2.7475540000	-1.5616150000	-1.8842340000
C	2.2630030000	-0.6577740000	-1.5184640000
C	-2.4568330000	-0.3877820000	0.1863260000
H	-4.5093350000	0.1407400000	0.5390570000
C	2.0819400000	2.0088180000	1.6928450000
H	2.7379630000	2.5116510000	0.9891070000
N	-0.5915660000	0.7203330000	-0.5124820000
H	1.7719910000	-0.1545040000	-2.3562730000
C	-1.9719230000	0.7919410000	-0.2682990000
H	1.1920730000	1.6299400000	-1.0903130000
C	0.1357140000	1.8628120000	-1.0645190000
H	-0.0170030000	2.7325350000	-0.4272020000
H	-3.7610400000	1.9420950000	-0.3450440000
C	-2.6949040000	2.0773600000	-0.5137140000
H	-2.3446010000	2.8657350000	0.1574470000
H	-0.2239910000	2.0674050000	-2.0742630000
H	-2.5608380000	2.4229500000	-1.5413960000
H	1.2221490000	0.2422500000	2.3921430000
H	1.6325160000	2.6202630000	2.4668200000

Zero-point correction=  
(Hartree/Particle)

0.267873

Thermal correction to Energy=

0.283942

Thermal correction to Enthalpy=

0.284887

Thermal correction to Gibbs Free Energy=

0.225078

Sum of electronic and zero-point Energies=

-995.188845

Sum of electronic and thermal Energies=

-995.172776

Sum of electronic and thermal Enthalpies=

-995.171832

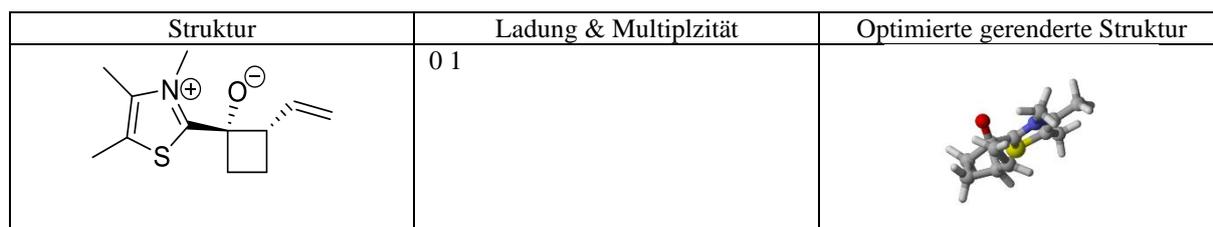
Sum of electronic and thermal Free Energies=

-995.231640

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.177	60.717	125.878

#M062X/6-311+G\*\*

(22-anti-syn)



32

XYZ file generated by gabedit : coordinates in Angstrom

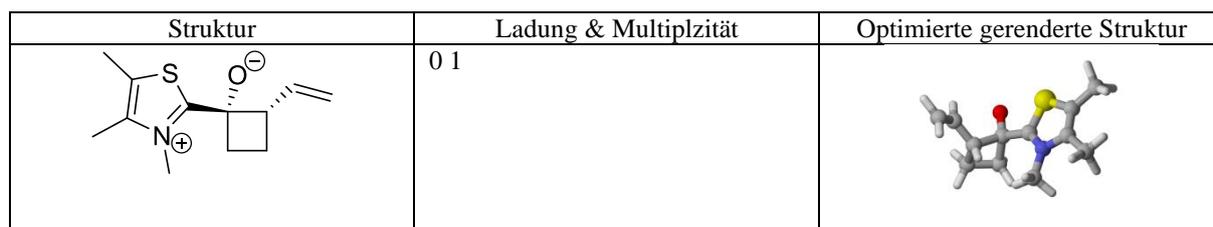
H	-2.5623620000	2.7821490000	-0.7408470000
H	-4.0220440000	1.8644190000	-0.3584290000
C	-3.0006560000	2.0658950000	-0.0428920000
H	-3.0361310000	2.5338360000	0.9438200000
H	0.0364840000	2.5877860000	-0.5810850000
H	-4.7375330000	-0.1478510000	-0.5418090000
C	-2.2097420000	0.7989920000	-0.0094990000
C	-0.1093020000	2.1295840000	0.3981110000
H	-4.0762660000	-1.5802060000	-1.3324970000
H	0.8459960000	1.8866210000	0.8743420000
C	-4.0380910000	-0.9743540000	-0.4250220000
H	-0.7061980000	2.7814800000	1.0337030000
N	-0.8296430000	0.8545650000	0.2261450000
C	-2.6522540000	-0.4686130000	-0.1767410000
H	-4.3820660000	-1.5912130000	0.4079250000
O	1.6670700000	0.2269940000	1.5446340000
C	-0.2053620000	-0.3147400000	0.2392960000
S	-1.3185120000	-1.5801390000	-0.0383450000
C	1.2861900000	-0.4940720000	0.5243040000
H	3.9001570000	1.1588770000	0.6241980000
H	2.0029210000	-2.3712240000	1.4854020000
C	3.5827450000	1.6373810000	-0.2945510000
C	1.8026530000	-1.9655780000	0.4940240000
H	1.1719350000	-2.6531670000	-0.0808180000
C	2.7397160000	1.0305410000	-1.1319340000
C	2.1474650000	-0.3053120000	-0.8838410000
H	3.7921660000	-1.1118150000	0.2863520000
H	1.5499550000	-0.6421810000	-1.7372010000
C	2.9929370000	-1.4809680000	-0.3551870000
H	3.4045850000	-2.1633850000	-1.1004120000
H	3.9531720000	2.6358460000	-0.5001850000
H	2.4145610000	1.5618120000	-2.0254230000

Zero-point correction=	0.268032 (Hartree/Particle)
Thermal correction to Energy=	0.283986
Thermal correction to Enthalpy=	0.284930
Thermal correction to Gibbs Free Energy=	0.224914
Sum of electronic and zero-point Energies=	-995.192414
Sum of electronic and thermal Energies=	-995.176459
Sum of electronic and thermal Enthalpies=	-995.175515
Sum of electronic and thermal Free Energies=	-995.235531

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.204	60.470	126.314

#M062X/6-311+G\*\*

(22-anti-anti)



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XYZ file generated by gabedit : coordinates in Angstrom

H	3.6846240000	1.4053370000	1.4382490000
H	1.4562510000	2.5722700000	1.3040900000
C	3.1783520000	1.4556030000	0.4730490000
H	3.9090900000	1.6685120000	-0.3070250000
H	0.5679340000	0.9376670000	2.1306660000
C	1.9485180000	2.3807390000	0.3458890000
H	2.0790180000	3.3189280000	-0.1914800000
H	1.9205930000	-0.2678950000	0.9788060000
H	-1.0839660000	1.1594650000	2.7362080000
C	-0.4454800000	0.5560000000	2.0916190000
H	-0.4553040000	-0.4807930000	2.4304730000
C	2.3124110000	0.2283740000	0.0844590000
H	2.8730110000	-2.4589780000	0.3975370000
C	2.8544350000	-0.7687500000	-0.8707540000
C	1.2905220000	1.2837110000	-0.5698510000
C	3.0766570000	-2.0503840000	-0.5885940000
N	-0.9377910000	0.6287040000	0.7157860000
C	-0.1810520000	0.9405370000	-0.3342400000
O	1.4322090000	1.4792010000	-1.8647750000
H	-3.3917520000	0.8226940000	2.1759500000
H	-2.8675820000	-0.8651860000	2.0924760000
C	-3.2276530000	-0.0206970000	1.4999610000
C	-2.2729870000	0.3311960000	0.4048040000
S	-1.0586040000	0.8859490000	-1.7852060000
H	-4.1910220000	-0.2952780000	1.0749910000
C	-2.5058010000	0.4289600000	-0.9262570000
C	-3.7938750000	0.2133480000	-1.6593730000
H	-4.2889410000	1.1647590000	-1.8676990000
H	-4.4780750000	-0.4087000000	-1.0823860000
H	-3.6146150000	-0.2848830000	-2.6133450000
H	3.0464090000	-0.3690510000	-1.8637660000
H	3.4745660000	-2.7341610000	-1.3297870000

Zero-point correction=  
(Hartree/Particle)

0.267572

Thermal correction to Energy=

0.283928

Thermal correction to Enthalpy=

0.284872

Thermal correction to Gibbs Free Energy=

0.223395

Sum of electronic and zero-point Energies=

-995.187461

Sum of electronic and thermal Energies=

-995.171105

Sum of electronic and thermal Enthalpies=

-995.170161

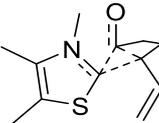
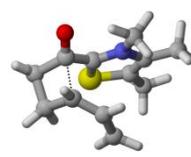
Sum of electronic and thermal Free Energies=

-995.231638

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.167	60.717	129.388

#M062X/6-311+G\*\*

(23-syn-syn)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	2.9793500000	-2.5002040000	0.3963020000
H	-0.5871590000	-2.0841880000	2.0532820000
H	3.2559560000	-2.2607490000	-1.3335250000
C	3.1450230000	-1.7459000000	-0.3770590000
C	-0.4708430000	-1.0956780000	2.4836160000
H	-1.8964630000	-2.0803480000	0.3172000000
H	4.0850510000	-1.2390190000	-0.1627080000
H	-3.5817220000	-1.6371930000	0.5507390000
C	-2.6101330000	-1.2601440000	0.2258180000
S	0.4307650000	-1.2856700000	-0.9427390000
C	2.0137140000	-0.7699840000	-0.4192820000
C	-1.1942460000	-0.0448490000	2.0639910000
H	-2.2236490000	-1.2309010000	-2.0026280000
C	-2.1319450000	-0.0091270000	0.9473420000
H	3.9879680000	0.7700210000	0.5909110000
C	-2.5818140000	-0.6159290000	-1.1699400000
C	1.9735400000	0.5291510000	-0.0587290000
C	-0.2450610000	0.2610690000	-0.6486920000
H	-2.9149240000	0.7388990000	1.0627760000
H	-3.5476970000	-0.1932570000	-1.4453430000
H	2.8308620000	1.7985970000	1.4382690000
C	3.0897880000	1.3708930000	0.4670690000
C	-1.6914160000	0.5972730000	-0.8029490000
N	0.7016930000	1.0967650000	-0.2114670000
H	3.3211250000	2.1934240000	-0.2139090000
O	-2.0047380000	1.7743180000	-1.1412210000
H	0.4577920000	2.5110180000	1.3122650000
C	0.4176560000	2.4716680000	0.2220090000
H	-0.5749970000	2.7317860000	-0.1441890000
H	1.1667630000	3.1404970000	-0.1998490000
H	0.2349330000	-0.9958290000	3.2994880000
H	-1.0449520000	0.9056210000	2.5756070000

Zero-point correction=  
(Hartree/Particle)

0.267001

Thermal correction to Energy=

0.282658

Thermal correction to Enthalpy=

0.283603

Thermal correction to Gibbs Free Energy=

0.225087

Sum of electronic and zero-point Energies=

-995.195899

Sum of electronic and thermal Energies=

-995.180241

Sum of electronic and thermal Enthalpies=

-995.179297

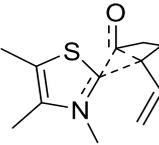
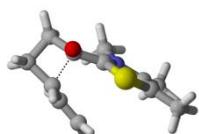
Sum of electronic and thermal Free Energies=

-995.237813

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.371	59.613	123.157

#M062X/6-311+G\*\*

(23-syn-anti)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	0.5074220000	2.8827410000	1.0049480000
H	0.6466300000	1.3520160000	1.9114970000
H	-3.0028040000	2.0693340000	1.5854140000
C	-0.0274270000	2.0014380000	1.3533300000
H	-0.8412000000	2.3169820000	1.9994390000
H	2.4317880000	1.9433830000	0.6141680000
H	3.2797750000	2.3985770000	-0.8947380000
H	-2.3637820000	0.5276090000	2.1874350000
C	-2.8126930000	1.0251290000	1.3238160000
C	2.7331660000	1.6074270000	-0.3790500000
N	-0.5799030000	1.2883870000	0.2032290000
H	-3.7726990000	0.5523420000	1.1282030000
C	-1.9306100000	0.8951890000	0.1247080000
H	3.9752250000	0.0184510000	0.6061320000
C	0.1323470000	1.0496320000	-0.9015920000
C	1.5783410000	1.0507860000	-1.2460210000
C	3.3907520000	0.2219840000	-0.2946990000
C	1.4458900000	-0.9229600000	0.8841940000
C	2.0565490000	-0.5336030000	-0.3851920000
C	-2.2438610000	0.3948530000	-1.0884290000
C	0.3269020000	-1.6480770000	1.0302510000
H	4.0018570000	0.0334120000	-1.1748870000
O	1.7880120000	0.9650640000	-2.4972630000
H	-3.4858570000	-1.2060400000	-1.7926690000
S	-0.8506220000	0.3959160000	-2.1458920000
C	-3.5520550000	-0.1358000000	-1.5835620000
H	-0.1996970000	-2.0437860000	0.1660430000
H	-4.3442820000	0.0203050000	-0.8524890000
H	1.9259390000	-1.2493230000	-1.1944880000
H	-3.8467200000	0.3669210000	-2.5072810000
H	1.9387740000	-0.5580290000	1.7880060000
H	-0.0689950000	-1.8904810000	2.0094730000

Zero-point correction=  
(Hartree/Particle)

0.266861

Thermal correction to Energy=

0.282636

Thermal correction to Enthalpy=

0.283580

Thermal correction to Gibbs Free Energy=

0.224148

Sum of electronic and zero-point Energies=

-995.182226

Sum of electronic and thermal Energies=

-995.166450

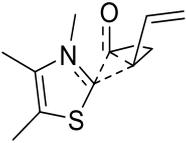
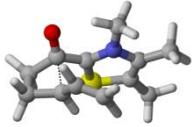
Sum of electronic and thermal Enthalpies=

-995.165506

Sum of electronic and thermal Free Energies=

-995.224939

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.357	59.652	125.087

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.386200000	-1.654323000	1.458448000
C	-3.049889000	-1.029425000	0.628650000
H	-3.900784000	-0.480591000	0.223487000
H	-1.177241000	-0.480986000	1.645842000
H	-1.670148000	-2.547799000	-0.137004000
H	-0.589525000	1.728230000	2.552124000
C	-1.908807000	-0.062020000	0.953587000
C	-2.288726000	-1.725846000	-0.509844000
H	-2.871900000	-2.063346000	-1.366396000
C	-2.098843000	1.371481000	1.112741000
C	-1.343074000	2.153157000	1.894802000
C	-1.507402000	-0.430545000	-0.836367000
S	0.861429000	-1.726266000	0.043075000
O	-2.028475000	0.373478000	-1.671089000
C	-0.046486000	-0.398079000	-0.582022000
H	3.358798000	-1.586687000	1.900226000
C	2.286102000	-0.731538000	0.250533000
N	0.736126000	0.685465000	-0.680109000
H	-0.720660000	1.851039000	-1.597079000
H	0.476233000	2.767342000	-0.620112000
C	3.522382000	-1.316654000	0.854354000
C	0.327982000	1.949342000	-1.322006000
C	2.040917000	0.520166000	-0.186283000
H	3.828308000	-2.217538000	0.318038000
H	4.347589000	-0.606984000	0.812274000
H	2.575048000	2.478566000	0.490923000
H	0.938864000	2.100775000	-2.214435000
C	2.962594000	1.695558000	-0.166068000
H	3.943416000	1.399819000	0.199378000
H	3.084414000	2.123578000	-1.163070000
H	-2.850492000	1.820773000	0.466239000
H	-1.474170000	3.228730000	1.918931000

Zero-point correction=  
(Hartree/Particle)

0.266744

Thermal correction to Energy=

0.282627

Thermal correction to Enthalpy=

0.283571

Thermal correction to Gibbs Free Energy=

0.223746

Sum of electronic and zero-point Energies=

-995.191307

Sum of electronic and thermal Energies=

-995.175424

Sum of electronic and thermal Enthalpies=

-995.174480

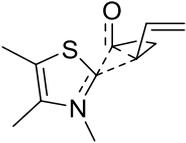
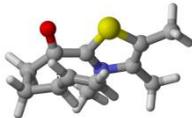
Sum of electronic and thermal Free Energies=

-995.234304

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.351	59.664	125.912

#M062X/6-311+G\*\*

(23-anti-anti)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	3.6200880000	1.3391690000	1.2750820000
H	3.9702350000	0.0023830000	0.1563840000
C	3.1991380000	0.6909470000	0.5031320000
H	1.2882510000	0.4552670000	1.5882380000
C	1.9441930000	-0.0906510000	0.9056650000
H	2.0890300000	2.3402600000	-0.4156640000
C	1.9635470000	-1.5247070000	1.1518030000
C	2.5241910000	1.3804990000	-0.6934110000
H	0.2822820000	-1.6382730000	2.4310570000
H	0.4287780000	2.5105790000	1.0686740000
C	1.0510610000	-2.1761520000	1.8821130000
H	3.1219260000	1.4969380000	-1.5972810000
C	-0.3573360000	2.5316370000	0.3122840000
C	1.5197820000	0.2108650000	-0.8555680000
H	0.0100850000	3.0362250000	-0.5799720000
H	-1.2097990000	3.0794540000	0.7019100000
O	1.8513360000	-0.7409000000	-1.6370680000
H	-2.7326780000	1.8604160000	1.8827060000
N	-0.7722400000	1.1729090000	-0.0250280000
C	0.0521860000	0.2975350000	-0.6288780000
C	-2.0671300000	0.6785130000	0.2118860000
C	-3.0826020000	1.5337510000	0.9004880000
S	-0.7528000000	-1.1639440000	-0.9954930000
H	-3.3311640000	2.4206500000	0.3115740000
H	-3.9999730000	0.9684470000	1.0480300000
C	-2.2248730000	-0.5787940000	-0.2575560000
H	-4.2752010000	-0.9628630000	0.2582530000
C	-3.4282480000	-1.4665410000	-0.2058220000
H	-3.7284530000	-1.7723120000	-1.2105230000
H	-3.2158100000	-2.3714920000	0.3682950000
H	2.7052560000	-2.0899090000	0.5932720000
H	1.0534920000	-3.2564050000	1.9627820000

Zero-point correction=  
(Hartree/Particle)

0.266437

Thermal correction to Energy=

0.281553

Thermal correction to Enthalpy=

0.282497

Thermal correction to Gibbs Free Energy=

0.225117

Sum of electronic and zero-point Energies=

-995.183966

Sum of electronic and thermal Energies=

-995.168850

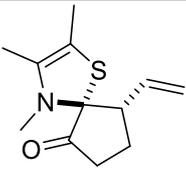
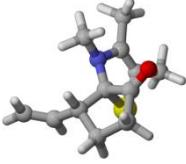
Sum of electronic and thermal Enthalpies=

-995.167906

Sum of electronic and thermal Free Energies=

-995.225286

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	176.677	57.874	120.767

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	3.2582700000	-1.8059400000	-1.4399190000
H	3.0888090000	-0.5135960000	-2.6312520000
H	4.0639420000	-0.2540060000	-1.1835400000
C	3.1552320000	-0.7239300000	-1.5590370000
C	1.9486240000	-0.2191070000	-0.8406580000
H	3.8998130000	1.1067160000	0.4148100000
S	0.3496150000	-0.7948810000	-1.3959530000
C	1.8244560000	0.6752680000	0.1471660000
C	2.9377150000	1.4082750000	0.8223810000
H	-1.5253580000	-3.0546180000	0.5072380000
H	2.9428860000	1.2046240000	1.8964330000
O	0.3881160000	-1.5279170000	1.9477110000
C	-0.4375850000	-1.2853730000	1.1115630000
H	-2.3799610000	-1.5514290000	-1.1704310000
H	2.8309240000	2.4877370000	0.6807400000
C	-0.3965930000	-0.0876780000	0.1418720000
C	-1.7357970000	-2.0434420000	0.8571910000
N	0.4940150000	0.9840550000	0.5144400000
C	-2.5145500000	-1.1791550000	-0.1510930000
H	-2.2519430000	-2.1288610000	1.8169640000
H	0.2541120000	0.9408300000	2.6369870000
C	-1.8876900000	0.2306310000	-0.0334010000
C	0.2054930000	1.6307810000	1.7855790000
H	-3.5851820000	-1.1497600000	0.0500630000
C	-2.2258480000	1.1698210000	-1.1454300000
H	0.9117770000	2.4429420000	1.9466930000
H	-2.2346370000	0.6653150000	0.9132020000
C	-2.9274910000	2.2852920000	-0.9814160000
H	-0.7882110000	2.0792340000	1.7386510000
H	-3.2885790000	2.5884010000	-0.0030230000
H	-1.8659830000	0.8931550000	-2.1331440000
H	-3.1633370000	2.9339970000	-1.8163020000

Zero-point correction=  
(Hartree/Particle)

0.269638

Thermal correction to Energy=

0.285685

Thermal correction to Enthalpy=

0.286629

Thermal correction to Gibbs Free Energy=

0.226697

Sum of electronic and zero-point Energies=

-995.260508

Sum of electronic and thermal Energies=

-995.244460

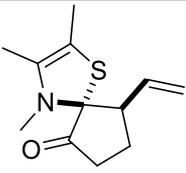
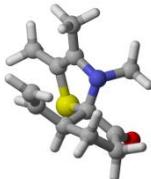
Sum of electronic and thermal Enthalpies=

-995.243516

Sum of electronic and thermal Free Energies=

-995.303449

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	179.270	60.088	126.138

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.7363960000	0.0403810000	-0.6709310000
H	-1.3321750000	0.8620750000	-1.8372160000
H	-2.7656210000	2.2600470000	-0.3906070000
C	-2.9998400000	0.1320050000	0.1327480000
O	-2.2056270000	-2.1518780000	-0.1147820000
H	-3.5300950000	-0.0178210000	1.0750720000
C	-1.9756420000	-0.9786760000	-0.0625350000
C	-2.1987350000	1.4371920000	0.0460100000
C	-0.9832330000	1.0599550000	-0.8135470000
S	0.5553750000	-1.2715750000	-1.3226110000
C	-0.5876380000	-0.3249750000	-0.2366570000
C	0.1280980000	2.0605490000	-0.8986690000
H	-1.8590270000	1.7372580000	1.0389330000
C	0.1857000000	3.2065360000	-0.2283410000
H	3.3347310000	-0.0495030000	-1.8690970000
N	0.0874850000	-0.1588730000	1.0495350000
H	-1.2256420000	-1.1869840000	2.3460860000
C	1.9054330000	-0.5976490000	-0.3708960000
H	-0.5913810000	3.5098400000	0.4642850000
H	0.0431800000	-2.2180270000	1.6359240000
H	3.5258710000	-1.6846890000	-1.2394460000
C	3.2763550000	-0.6570680000	-0.9615590000
C	-0.1806630000	-1.2205290000	2.0331120000
C	1.4983450000	-0.0549010000	0.7824150000
H	4.0282070000	-0.3033170000	-0.2569380000
H	0.4340690000	-1.0372820000	2.9135120000
C	2.3179780000	0.6777330000	1.7939330000
H	1.9916120000	1.7218080000	1.8251700000
H	3.3798280000	0.6459520000	1.5547770000
H	2.1853960000	0.2604010000	2.7952640000
H	0.9281540000	1.8040840000	-1.5896180000
H	1.0189520000	3.8870740000	-0.3579540000

Zero-point correction=  
(Hartree/Particle)

0.269776

Thermal correction to Energy=

0.285481

Thermal correction to Enthalpy=

0.286425

Thermal correction to Gibbs Free Energy=

0.227751

Sum of electronic and zero-point Energies=

-995.257230

Sum of electronic and thermal Energies=

-995.241525

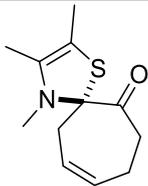
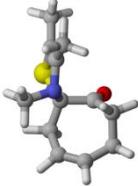
Sum of electronic and thermal Enthalpies=

-995.240581

Sum of electronic and thermal Free Energies=

-995.299254

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	179.142	59.750	123.490

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.6357330000	-1.0887120000	-1.8252610000
H	-0.9260910000	0.3799460000	-2.4616200000
S	1.2714680000	-1.0283080000	-1.2815900000
C	-1.3387740000	-0.0682430000	-1.5565610000
H	4.1943090000	-0.8112580000	-0.6632450000
H	3.5504440000	-1.7862830000	0.6562500000
H	0.9369850000	1.9586110000	-1.7931510000
H	-2.8902460000	1.4643770000	-1.8409860000
C	-0.2065240000	-0.2008450000	-0.5251130000
C	3.6102730000	-0.7698050000	0.2602060000
C	2.2445630000	-0.2324640000	-0.0198470000
C	-2.5503090000	0.7256140000	-1.1203400000
O	-0.6106360000	-2.2958310000	0.5948250000
C	-0.7417780000	-1.1013510000	0.6207910000
C	0.3264870000	2.1807170000	-0.9075820000
H	-0.6834230000	2.4563840000	-1.2108060000
N	0.2797650000	1.0516170000	0.0280260000
H	4.1478240000	-0.1459780000	0.9736080000
C	1.5921770000	0.7821300000	0.5651400000
C	-3.2632030000	0.6106450000	0.0001010000
H	-3.3630300000	-1.3534290000	0.8505750000
H	0.7601110000	3.0371220000	-0.3917930000
H	-4.1216180000	1.2695800000	0.0965470000
C	-3.0462960000	-0.3457830000	1.1458970000
C	-1.5972420000	-0.4295750000	1.6693450000
C	2.0652450000	1.6680860000	1.6736040000
H	-1.5740640000	-1.0642690000	2.5561750000
H	-1.2272260000	0.5680920000	1.9013800000
H	-3.6908320000	-0.0508490000	1.9756460000
H	3.0652630000	1.3957020000	2.0068410000
H	1.3834960000	1.5984820000	2.5254580000
H	2.0893650000	2.7160000000	1.3612010000

Zero-point correction=

0.271406

(Hartree/Particle)

Thermal correction to Energy=

0.286727

Thermal correction to Enthalpy=

0.287671

Thermal correction to Gibbs Free Energy=

0.229836

Sum of electronic and zero-point Energies=

-995.256537

Sum of electronic and thermal Energies=

-995.241216

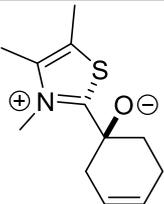
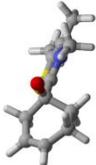
Sum of electronic and thermal Enthalpies=

-995.240272

Sum of electronic and thermal Free Energies=

-995.298107

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	179.924	58.764	121.724

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

```

H      -3.8170630000      1.0381470000      1.9124480000
H      -1.7106910000      -0.2605260000      1.8315050000
H      -5.1413140000      -0.3691870000      0.3561930000
C      -3.3587320000      0.8302710000      0.9408070000
H      -1.3521130000      1.4416010000      1.4642080000
C      -1.8680190000      0.5456100000      1.1036230000
C      -4.0598030000      -0.3160210000      0.2680210000
H      -3.4724730000      1.7260820000      0.3203450000
C      -3.4179860000      -1.2311040000      -0.4534230000
H      -1.4985280000      -2.0568200000      -0.0865980000
H      0.8075650000      2.8147720000      0.7351920000
H      -3.9808330000      -2.0288730000      -0.9301570000
C      -1.3120070000      0.1530440000      -0.3047360000
C      -1.9283040000      -1.2276210000      -0.6691460000
S      1.0207370000      -1.5593070000      0.0885950000
C      0.2279140000      -0.0550800000      -0.0995000000
N      1.1253710000      0.9225880000      -0.1177590000
H      4.4997780000      1.1027920000      0.2520260000
C      2.5913660000      -0.8150500000      0.1441530000
C      0.7486250000      2.3427910000      -0.2470180000
C      3.8248880000      -1.6490710000      0.2913320000
C      2.4628060000      0.5254120000      0.0193680000
H      3.3422370000      2.3445460000      0.7350680000
H      -0.2712610000      2.3444370000      -0.6562470000
O      -1.5186790000      1.0741610000      -1.2338610000
C      3.5427070000      1.5573350000      0.0054740000
H      -1.7000980000      -1.4092450000      -1.7236980000
H      1.4449780000      2.8226640000      -0.9324070000
H      3.6317010000      2.0237420000      -0.9785990000
H      3.8062240000      -2.2146370000      1.2251130000
H      4.7172480000      -1.0246560000      0.2917460000
H      3.9139650000      -2.3604290000      -0.5321880000

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Zero-point correction=  
(Hartree/Particle)

0.270074

Thermal correction to Energy=

0.285258

Thermal correction to Enthalpy=

0.286202

Thermal correction to Gibbs Free Energy=

0.228463

Sum of electronic and zero-point Energies=

-995.224121

Sum of electronic and thermal Energies=

-995.208937

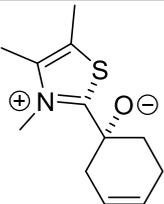
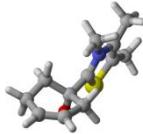
Sum of electronic and thermal Enthalpies=

-995.207993

Sum of electronic and thermal Free Energies=

-995.265733

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	179.002	58.665	121.523

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.9249110000	0.7010370000	2.0838400000
H	0.9864990000	2.9542050000	0.6597360000
H	-0.5665800000	2.3286720000	0.0711120000
H	-1.4423500000	1.2265190000	1.5828960000
C	-3.3813670000	0.4251940000	1.1838670000
H	-5.1339840000	0.3271980000	0.0518380000
C	0.5041750000	2.3391020000	-0.0992880000
C	-4.0524760000	0.2247210000	0.0517300000
H	0.7085480000	2.7485620000	-1.0895150000
C	-1.8922970000	0.2586890000	1.3187830000
H	-1.8269570000	1.3033270000	-1.2637690000
H	-1.6688970000	-0.4261580000	2.1425010000
H	-3.9007550000	0.2706670000	-2.0865910000
N	1.0176360000	0.9715070000	-0.0158970000
C	-3.3862890000	-0.1806800000	-1.2332050000
C	-1.9115980000	0.2097930000	-1.2287310000
C	3.3672120000	1.8363640000	-0.0926090000
C	-1.2712910000	-0.4075990000	0.0499690000
C	0.2441980000	-0.1092760000	0.0341520000
C	2.3954070000	0.7015100000	-0.0290320000
H	-3.4480850000	-1.2688110000	-1.3408510000
H	-1.4014560000	-0.2113710000	-2.0994460000
O	-1.3619880000	-1.7357910000	0.0659880000
C	2.6369950000	-0.6307000000	0.0205990000
H	4.7809430000	-0.6344380000	0.1690600000
S	1.1462410000	-1.5428540000	0.0715920000
C	3.9588420000	-1.3341350000	0.0220590000
H	4.0017980000	-2.0725910000	0.8248180000
H	4.1214940000	-1.8589230000	-0.9220740000
H	3.1622940000	2.4883180000	-0.9450830000
H	4.3786670000	1.4519310000	-0.2051970000
H	3.3372580000	2.4454040000	0.8148680000

Zero-point correction=  
(Hartree/Particle)

0.269951

Thermal correction to Energy=

0.285556

Thermal correction to Enthalpy=

0.286500

Thermal correction to Gibbs Free Energy=

0.226117

Sum of electronic and zero-point Energies=

-995.220753

Sum of electronic and thermal Energies=

-995.205148

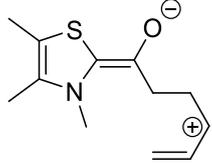
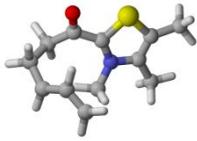
Sum of electronic and thermal Enthalpies=

-995.204204

Sum of electronic and thermal Free Energies=

-995.264587

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.189	58.920	127.088

structure	Ladung & Multiplizität	optimized structure
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.5838650000	-1.3954760000	-0.0845760000
H	-4.1441760000	-0.6440190000	1.4233730000
O	-1.1150880000	-2.4083240000	-0.3867880000
C	-3.3880100000	-0.5960040000	0.6381370000
H	-2.2291150000	-1.9738520000	1.8661160000
C	-0.9818810000	-1.4069450000	0.3147450000
C	-3.3297180000	0.7261970000	0.0016410000
C	-2.0076730000	-1.0479330000	1.3310950000
H	-3.6494330000	1.6021080000	0.5603820000
C	-2.6594290000	0.8824360000	-1.2043310000
S	1.5857920000	-1.5139080000	-0.5347170000
H	-1.6762050000	-0.3038380000	2.0535060000
C	0.2603930000	-0.6449340000	0.1526260000
C	-2.2106400000	2.0571810000	-1.7717530000
H	-2.4713540000	3.0189570000	-1.3398970000
H	4.2384080000	-0.6415490000	-1.5671030000
H	4.6102410000	-1.0639710000	0.1060670000
C	2.6694810000	-0.1985070000	-0.1826210000
N	0.6474380000	0.5853080000	0.5762590000
H	-0.4628800000	2.1652520000	-0.2214970000
C	4.1190920000	-0.3234120000	-0.5293920000
H	-1.2437780000	1.3416410000	1.0951900000
C	-0.2689720000	1.6926740000	0.7614060000
C	2.0138950000	0.8338790000	0.3971050000
H	4.6372280000	0.6265790000	-0.4087170000
H	0.1480400000	2.4003730000	1.4734830000
C	2.5794600000	2.1521210000	0.8161620000
H	2.1145810000	2.9737680000	0.2663310000
H	3.6497650000	2.1784040000	0.6259810000
H	2.4229290000	2.3253410000	1.8836790000
H	-2.3958160000	-0.0396160000	-1.7265630000
H	-1.7245990000	2.0613530000	-2.7387260000

Zero-point correction=  
(Hartree/Particle)

0.266990

Thermal correction to Energy=

0.283326

Thermal correction to Enthalpy=

0.284270

Thermal correction to Gibbs Free Energy=

0.223584

Sum of electronic and zero-point Energies=

-995.166096

Sum of electronic and thermal Energies=

-995.149760

Sum of electronic and thermal Enthalpies=

-995.148816

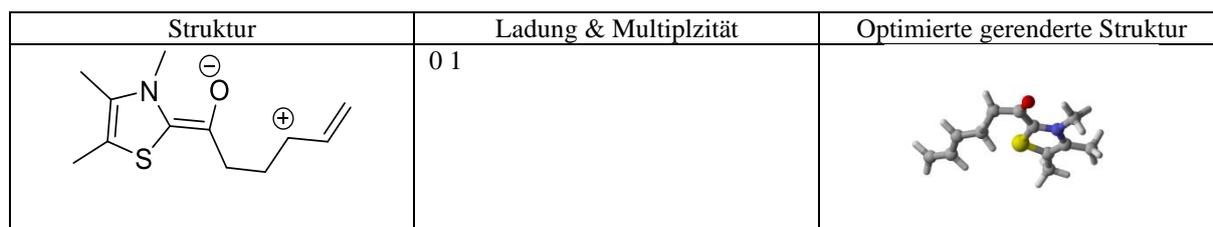
Sum of electronic and thermal Free Energies=

-995.209502

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.790	61.800	127.726

#M062X/6-311+G\*\*

(24ion-b)



32

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.7174050000	0.3801150000	-1.3929570000
H	-2.1867310000	2.0990500000	-1.3235100000
C	-1.6714180000	1.2939260000	-0.8037960000
S	0.2018850000	-1.0397410000	-0.4082990000
H	-2.5712630000	2.0598080000	1.0090930000
C	2.1770310000	-3.0067930000	-0.1180740000
C	-0.3144000000	1.7150420000	-0.4133570000
C	1.8417020000	-1.5508560000	-0.0941120000
C	-2.4901020000	1.0485000000	0.6013340000
C	0.6347440000	0.6305340000	-0.2470730000
H	-4.5350250000	0.9348160000	-0.1624180000
O	-0.0612540000	2.8849500000	-0.0747870000
C	-3.7426830000	0.3781820000	0.3331400000
H	-1.8523240000	0.4469340000	1.2542040000
C	2.6342310000	-0.4770870000	0.1353320000
H	4.6642730000	-0.0018440000	-0.3735890000
N	1.9576430000	0.7353570000	0.0645140000
H	1.9700090000	2.8169100000	0.0729560000
C	4.0995510000	-0.4781910000	0.4315880000
C	2.6516830000	2.0049000000	0.3039060000
C	-3.9048950000	-1.0110700000	0.4929580000
H	-5.7932730000	-1.2909050000	-0.4598640000
H	4.4635160000	-1.4968350000	0.5420350000
H	4.3134210000	0.0613940000	1.3565840000
H	3.5412170000	2.0500880000	-0.3251490000
H	-3.0950870000	-1.5304930000	1.0080390000
H	2.9445790000	2.0702920000	1.3538750000
C	-4.9716360000	-1.7500080000	0.0788100000
H	-5.0406030000	-2.8087700000	0.2897300000
H	3.2197140000	-3.1716600000	0.1497140000
H	2.0124290000	-3.4302220000	-1.1119480000
H	1.5560870000	-3.5623810000	0.5887540000

Zero-point correction=  
(Hartree/Particle)

0.265921

Thermal correction to Energy=

0.283286

Thermal correction to Enthalpy=

0.284230

Thermal correction to Gibbs Free Energy=

0.218780

Sum of electronic and zero-point Energies=

-995.164091

Sum of electronic and thermal Energies=

-995.146726

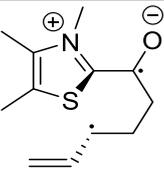
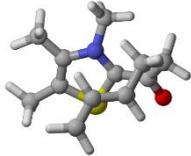
Sum of electronic and thermal Enthalpies=

-995.145782

Sum of electronic and thermal Free Energies=

-995.211232

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.764	62.753	137.750

structure	Ladung & Multiplizität	optimized structure
	0 1 Guess=(mix,always)	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	3.3758200000	-0.6725610000	1.7231790000
H	1.7804720000	0.0144930000	1.9641400000
O	2.0547010000	0.7269230000	-2.1408840000
C	2.4526670000	-0.3908990000	1.2029310000
H	3.6955470000	0.3635990000	-0.4107140000
C	1.7291760000	0.7757430000	-0.9500720000
C	1.8080520000	-1.5877750000	0.5733580000
C	2.8006970000	0.6679640000	0.1357410000
H	2.3032200000	-2.0245930000	-0.2914320000
C	0.5906500000	-2.1143880000	0.9780910000
S	-0.7996650000	0.1387800000	-1.7622170000
H	3.0338570000	1.6341440000	0.5939540000
C	0.3396460000	0.7646990000	-0.6041260000
C	-0.0683490000	-3.1485020000	0.3508370000
H	0.3604060000	-3.6349200000	-0.5173250000
H	-3.2965700000	-1.5782620000	-1.0270020000
H	-3.7685940000	-0.0597220000	-1.7938210000
C	-2.0501520000	0.0891160000	-0.5281540000
N	-0.2650770000	0.9850810000	0.6189290000
H	0.0229170000	1.7564270000	2.5519360000
C	-3.3800600000	-0.4988500000	-0.8718210000
H	1.2296760000	2.2470720000	1.3577210000
C	0.1736720000	2.0519420000	1.5128610000
C	-1.6066080000	0.5762380000	0.6468200000
H	-4.1100450000	-0.3213320000	-0.0827180000
H	-0.3831240000	2.9736750000	1.3131700000
C	-2.3625070000	0.7022560000	1.9311290000
H	-1.8537000000	0.1594070000	2.7331940000
H	-3.3635970000	0.2896900000	1.8269100000
H	-2.4573810000	1.7462950000	2.2415360000
H	0.1100140000	-1.6479810000	1.8373780000
H	-1.0276350000	-3.5021250000	0.7043660000

Zero-point correction= 0.265545  
(Hartree/Particle)

Thermal correction to Energy= 0.282682

Thermal correction to Enthalpy= 0.283626

Thermal correction to Gibbs Free Energy= 0.220652

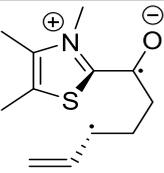
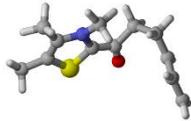
Sum of electronic and zero-point Energies= -995.198433

Sum of electronic and thermal Energies= -995.181297

Sum of electronic and thermal Enthalpies= -995.180353

Sum of electronic and thermal Free Energies= -995.243327

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.386	62.788	132.540

structure	Ladung & Multiplizität	optimized structure
	0 3	

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XYZ file generated by gabedit : coordinates in Angstrom

H	3.3636320000	1.7016400000	1.7682050000
H	2.2404140000	0.3627950000	1.5825220000
O	1.2398240000	1.8194560000	-1.7648270000
C	2.7208480000	1.1842270000	1.0433310000
H	2.2030800000	3.0599780000	0.1193440000
C	0.8238110000	1.6800290000	-0.6049050000
C	3.5503130000	0.6209380000	-0.0648960000
C	1.6748120000	2.2020180000	0.5418240000
H	3.9848720000	1.3242060000	-0.7700840000
C	3.7670730000	-0.7320570000	-0.2550000000
S	-1.4197730000	0.8379660000	-1.8551340000
H	1.0681370000	2.5770060000	1.3695130000
C	-0.4630630000	1.0857960000	-0.4206480000
C	4.5260030000	-1.2691920000	-1.2748980000
H	5.0001100000	-0.6284770000	-2.0085780000
H	-3.8866040000	-0.7934540000	-2.3452230000
H	-4.5051710000	0.8312840000	-2.0450690000
C	-2.7791650000	0.3068970000	-0.8832770000
N	-1.1771960000	0.7447560000	0.7168860000
H	0.0131590000	-0.6527420000	1.7500440000
C	-4.0612950000	-0.0459280000	-1.5675990000
H	0.2102880000	1.0334580000	2.2746030000
C	-0.5064630000	0.2946690000	1.9317600000
C	-2.4802850000	0.3047960000	0.4312360000
H	-4.7875320000	-0.4567900000	-0.8674450000
H	-1.2429760000	0.1555960000	2.7188240000
C	-3.3877830000	-0.0843770000	1.5564060000
H	-3.0618570000	-1.0081010000	2.0416640000
H	-4.3972410000	-0.2425790000	1.1838490000
H	-3.4309440000	0.7028030000	2.3133600000
H	3.3015850000	-1.4191420000	0.4500930000
H	4.6563590000	-2.3374870000	-1.3796580000

Zero-point correction= 0.266041  
(Hartree/Particle)

Thermal correction to Energy= 0.283139

Thermal correction to Enthalpy= 0.284084

Thermal correction to Gibbs Free Energy= 0.218945

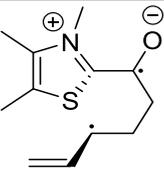
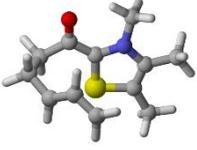
Sum of electronic and zero-point Energies= -995.193852

Sum of electronic and thermal Energies= -995.176754

Sum of electronic and thermal Enthalpies= -995.175809

Sum of electronic and thermal Free Energies= -995.240949

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.673	62.583	137.097

structure	Ladung & Multiplizität	optimized structure
	0 1	

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XYZ file generated by gabedit : coordinates in Angstrom

H	-1.9934010000	-0.2478380000	-2.0627870000
H	-2.9667560000	1.2199790000	-1.9011950000
C	-2.3944840000	0.4732390000	-1.3457780000
S	0.3915200000	-0.9024970000	-1.2375090000
H	-4.1694300000	-0.6814160000	-0.8842940000
C	2.9178960000	-2.0165620000	-0.7694120000
C	-1.3123210000	1.2179690000	-0.5820850000
C	1.9985980000	-0.8609910000	-0.5414140000
C	-3.3314060000	-0.2409080000	-0.3380360000
C	-0.0087290000	0.6427550000	-0.5243460000
H	-2.4918870000	-2.2738870000	0.0063360000
O	-1.6291200000	2.2567740000	0.0258000000
C	-2.6010360000	-1.2846170000	0.4443060000
H	-3.7314110000	0.5234300000	0.3340920000
C	2.1834900000	0.2729440000	0.1681790000
H	3.7904940000	1.6412050000	0.5656550000
N	1.0756790000	1.1159020000	0.1869110000
H	0.1766370000	2.8991850000	0.7642420000
C	3.4133740000	0.6777270000	0.9165690000
C	1.1755970000	2.4814830000	0.7010030000
C	-1.9332540000	-1.0085950000	1.6315670000
H	-0.9594140000	-2.8987440000	1.9024590000
H	4.1992690000	-0.0622100000	0.7843630000
H	3.2076810000	0.7671920000	1.9862430000
H	1.7895820000	3.0901500000	0.0301340000
H	-2.0504460000	-0.0078130000	2.0449450000
H	1.6334300000	2.4635310000	1.6897680000
C	-1.1162150000	-1.8984940000	2.2905880000
H	-0.6144100000	-1.6318140000	3.2108750000
H	3.8932270000	-1.8385720000	-0.3180870000
H	3.0686740000	-2.1907750000	-1.8378010000
H	2.5079890000	-2.9328570000	-0.3364260000

Zero-point correction= 0.266208  
(Hartree/Particle)

Thermal correction to Energy= 0.283295

Thermal correction to Enthalpy= 0.284239

Thermal correction to Gibbs Free Energy= 0.219864

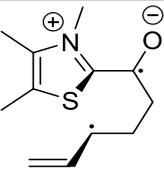
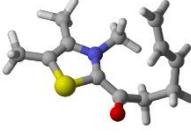
Sum of electronic and zero-point Energies= -995.206202

Sum of electronic and thermal Energies= -995.189115

Sum of electronic and thermal Enthalpies= -995.188171

Sum of electronic and thermal Free Energies= -995.252546

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.770	62.539	135.489

structure	Ladung & Multiplizität	optimized structure
	0 1	

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XYZ file generated by gabedit : coordinates in Angstrom

H	3.5828340000	-1.3870520000	0.1119630000
H	4.1593920000	-0.6424100000	-1.3931410000
O	1.1141550000	-2.4108770000	0.3852900000
C	3.3938440000	-0.5914880000	-0.6170650000
H	2.2521870000	-1.9766840000	-1.8541500000
C	0.9878650000	-1.4090420000	-0.3171570000
C	3.3247590000	0.7338850000	0.0126000000
C	2.0222840000	-1.0500390000	-1.3239700000
H	3.6465720000	1.6083260000	-0.5475070000
C	2.6375580000	0.8940210000	1.2080270000
S	-1.5782390000	-1.5169300000	0.5297930000
H	1.6952280000	-0.3087720000	-2.0514770000
C	-0.2563970000	-0.6470630000	-0.1610470000
C	2.1791030000	2.0706200000	1.7647810000
H	2.4473460000	3.0310440000	1.3345170000
H	-4.2297150000	-0.6782870000	1.5622000000
H	-4.6112250000	-1.0460390000	-0.1217220000
C	-2.6638120000	-0.2021540000	0.1846640000
N	-0.6458580000	0.5822710000	-0.5844360000
H	0.4658320000	2.1674870000	0.2010220000
C	-4.1126920000	-0.3286450000	0.5344650000
H	1.2407140000	1.3372940000	-1.1162750000
C	0.2678170000	1.6898600000	-0.7793910000
C	-2.0113740000	0.8308060000	-0.3978630000
H	-4.6250910000	0.6281150000	0.4459310000
H	-0.1530930000	2.3937350000	-1.4931980000
C	-2.5801440000	2.1486700000	-0.8137970000
H	-2.1057500000	2.9713590000	-0.2735770000
H	-3.6476950000	2.1777150000	-0.6089060000
H	-2.4379670000	2.3179720000	-1.8841280000
H	2.3682800000	-0.0262730000	1.7305880000
H	1.6788640000	2.0778900000	2.7244260000

Zero-point correction= 0.266539  
(Hartree/Particle)

Thermal correction to Energy= 0.282887

Thermal correction to Enthalpy= 0.283831

Thermal correction to Gibbs Free Energy= 0.222955

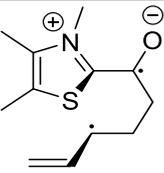
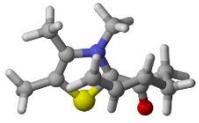
Sum of electronic and zero-point Energies= -995.166446

Sum of electronic and thermal Energies= -995.150098

Sum of electronic and thermal Enthalpies= -995.149154

Sum of electronic and thermal Free Energies= -995.210030

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.514	61.830	128.124

structure	Ladung & Multiplizität	optimized structure
	0 3	

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XYZ file generated by gabedit : coordinates in Angstrom

H	3.1791490000	-0.4177620000	1.2939090000
H	4.2039530000	0.5787000000	0.2592770000
O	1.6595090000	-2.4786420000	0.1170860000
C	3.1733100000	0.2611740000	0.4363150000
H	3.4568780000	-1.2740240000	-1.0702370000
C	1.4661670000	-1.3708530000	-0.4138800000
C	2.3143440000	1.4539830000	0.7115810000
C	2.6873540000	-0.5493050000	-0.7985240000
H	2.5813790000	2.3915090000	0.2272110000
C	1.1501170000	1.4189620000	1.4664180000
S	-1.0501050000	-1.7471590000	0.4998210000
H	2.5395040000	0.1219910000	-1.6430490000
C	0.1251490000	-0.8806040000	-0.4540600000
C	0.2832970000	2.4820200000	1.6070690000
H	0.4947570000	3.4374710000	1.1385010000
H	-3.4936830000	-0.6282780000	1.9651310000
H	-4.0784510000	-1.5227140000	0.5613410000
C	-2.2363140000	-0.4825440000	0.2330910000
N	-0.4417900000	0.2504840000	-0.9971850000
H	-0.5259850000	1.6575460000	-2.5279470000
C	-3.5807400000	-0.6017670000	0.8759390000
H	0.9452350000	1.7452650000	-1.5376580000
C	0.2184910000	1.0702680000	-1.9967810000
C	-1.7485040000	0.4899740000	-0.5672030000
H	-4.2256380000	0.2339640000	0.6072090000
H	0.7212790000	0.4240060000	-2.7170280000
C	-2.4473630000	1.7413710000	-0.9956240000
H	-1.8315300000	2.6178130000	-0.7771540000
H	-3.3857110000	1.8482430000	-0.4560810000
H	-2.6769470000	1.7374130000	-2.0646470000
H	0.8972680000	0.4804530000	1.9572210000
H	-0.6151590000	2.4026210000	2.2044130000

Zero-point correction= 0.266156  
(Hartree/Particle)

Thermal correction to Energy= 0.282932

Thermal correction to Enthalpy= 0.283876

Thermal correction to Gibbs Free Energy= 0.221043

Sum of electronic and zero-point Energies= -995.200989

Sum of electronic and thermal Energies= -995.184213

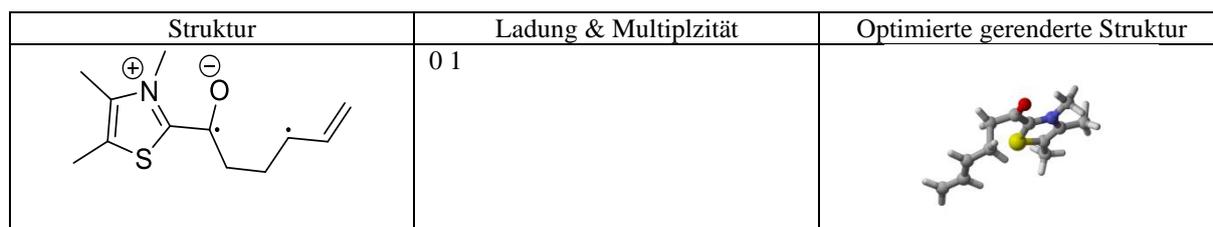
Sum of electronic and thermal Enthalpies= -995.183268

Sum of electronic and thermal Free Energies= -995.246101

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.542	62.431	132.243

#UM062X/6-311+G\*\*

(24rad-d)



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XYZ file generated by gabedit : coordinates in Angstrom

H	1.7174050000	-0.3801150000	-1.3929570000
H	2.1867310000	-2.0990500000	-1.3235100000
C	1.6714180000	-1.2939260000	-0.8037960000
S	-0.2018850000	1.0397410000	-0.4082990000
H	2.5712630000	-2.0598080000	1.0090930000
C	-2.1770310000	3.0067930000	-0.1180740000
C	0.3144000000	-1.7150420000	-0.4133570000
C	-1.8417020000	1.5508560000	-0.0941120000
C	2.4901020000	-1.0485000000	0.6013340000
C	-0.6347440000	-0.6305340000	-0.2470730000
H	4.5350250000	-0.9348160000	-0.1624180000
O	0.0612540000	-2.8849500000	-0.0747870000
C	3.7426830000	-0.3781820000	0.3331400000
H	1.8523240000	-0.4469340000	1.2542040000
C	-2.6342310000	0.4770870000	0.1353320000
H	-4.6642730000	0.0018440000	-0.3735890000
N	-1.9576430000	-0.7353570000	0.0645140000
H	-1.9700090000	-2.8169100000	0.0729560000
C	-4.0995510000	0.4781910000	0.4315880000
C	-2.6516830000	-2.0049000000	0.3039060000
C	3.9048950000	1.0110700000	0.4929580000
H	5.7932730000	1.2909050000	-0.4598640000
H	-4.4635160000	1.4968350000	0.5420350000
H	-4.3134210000	-0.0613940000	1.3565840000
H	-3.5412170000	-2.0500880000	-0.3251490000
H	3.0950870000	1.5304930000	1.0080390000
H	-2.9445790000	-2.0702920000	1.3538750000
C	4.9716360000	1.7500080000	0.0788100000
H	5.0406030000	2.8087700000	0.2897300000
H	-3.2197140000	3.1716600000	0.1497140000
H	-2.0124290000	3.4302220000	-1.1119480000
H	-1.5560870000	3.5623810000	0.5887540000

Zero-point correction=  
(Hartree/Particle)

0.265916

Thermal correction to Energy=

0.283283

Thermal correction to Enthalpy=

0.284228

Thermal correction to Gibbs Free Energy=

0.218747

Sum of electronic and zero-point Energies=

-995.164096

Sum of electronic and thermal Energies=

-995.146729

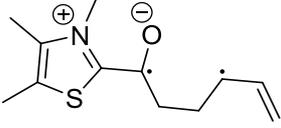
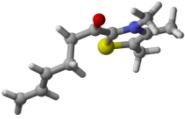
Sum of electronic and thermal Enthalpies=

-995.145784

Sum of electronic and thermal Free Energies=

-995.211265

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.763	62.755	137.816

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3	

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XYZ file generated by gabedit : coordinates in Angstrom

H	1.7010940000	-0.1827420000	-1.4072540000
H	2.2189080000	-1.8687400000	-1.3020960000
C	1.7100750000	-1.0672150000	-0.7628530000
S	-0.4215250000	1.1230420000	-0.5095480000
H	2.4701950000	-1.6552550000	1.1549220000
C	-2.5318330000	2.9277000000	-0.1295790000
C	0.3114480000	-1.5727410000	-0.4500310000
C	-2.0857120000	1.5018640000	-0.1034030000
C	2.4782380000	-0.7495410000	0.5379450000
C	-0.7078470000	-0.5881730000	-0.2784320000
H	4.5562560000	-1.0489400000	-0.1667340000
O	0.1208670000	-2.7927060000	-0.3100870000
C	3.8803990000	-0.3151830000	0.2674470000
H	1.9489590000	0.0300020000	1.0949080000
C	-2.7786300000	0.3762970000	0.1738010000
H	-4.7939950000	-0.2556140000	-0.2075210000
N	-2.0288410000	-0.7918660000	0.0683290000
H	-1.9088510000	-2.8671230000	0.1332140000
C	-4.2218720000	0.2797190000	0.5545020000
C	-2.5637510000	-2.0834400000	0.4975630000
C	4.3544670000	0.9640690000	0.5007840000
H	6.3718730000	0.7122870000	-0.1917290000
H	-4.6523760000	1.2722690000	0.6645410000
H	-4.3443800000	-0.2505550000	1.5014860000
H	-3.5667770000	-2.2111000000	0.0918580000
H	3.6568420000	1.6821070000	0.9289250000
H	-2.6055020000	-2.1302410000	1.5899950000
C	5.6402100000	1.3897360000	0.2326910000
H	5.9540380000	2.4036040000	0.4391950000
H	-3.5728470000	3.0195560000	0.1775730000
H	-2.4387170000	3.3494710000	-1.1337440000
H	-1.9265130000	3.5385080000	0.5450100000

Zero-point correction=  
(Hartree/Particle)

0.266559

Thermal correction to Energy=

0.283760

Thermal correction to Enthalpy=

0.284704

Thermal correction to Gibbs Free Energy=

0.219445

Sum of electronic and zero-point Energies=

-995.203616

Sum of electronic and thermal Energies=

-995.186416

Sum of electronic and thermal Enthalpies=

-995.185472

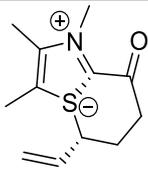
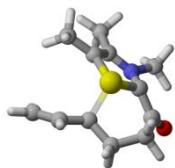
Sum of electronic and thermal Free Energies=

-995.250731

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.062	62.470	137.349

#M062X/6-311+G\*\*

(48ion-a)

structure	Ladung & Multiplizität	optimized structure
	0 1	

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XYZ file generated by gabedit : coordinates in Angstrom

H	1.4428730000	-2.1629090000	-1.6375100000
H	1.6520880000	-3.4264390000	-0.4157840000
H	3.2685850000	-1.4109880000	-0.2663510000
C	1.3544940000	-2.3905950000	-0.5707590000
H	3.5806800000	0.9540320000	-0.3319890000
C	2.2988760000	-1.4479790000	0.2368070000
C	-0.0836790000	-2.2226130000	-0.1118580000
O	-0.6270030000	-3.0576450000	0.6180650000
H	2.4614650000	-1.8935980000	1.2208190000
S	0.4715750000	0.2541220000	-0.9929140000
C	2.7914060000	1.0553870000	0.4110420000
C	-0.6601300000	-0.9866340000	-0.5075870000
C	1.7813920000	-0.0223920000	0.4436730000
H	0.4652960000	3.0548480000	-1.5403660000
H	3.4921230000	2.9279240000	1.0898230000
C	2.7524370000	2.1419710000	1.1822430000
H	-3.5626880000	-1.1271480000	-0.5432240000
H	1.1215980000	0.0577950000	1.3104010000
C	-0.6164740000	1.5291520000	-0.5019920000
N	-1.7368480000	-0.3678260000	0.1930780000
C	-0.3094140000	2.9731350000	-0.7753920000
C	-2.9694880000	-1.1256620000	0.3786690000
H	0.0549290000	3.5046460000	0.1075170000
C	-1.7103470000	0.9805650000	0.1212230000
H	1.9824270000	2.2664600000	1.9376370000
H	-2.6991540000	-2.1454020000	0.6421070000
H	-1.1915740000	3.4966590000	-1.1518560000
H	-3.5502020000	-0.6852720000	1.1883450000
H	-3.7760350000	1.5491460000	0.0830890000
C	-2.8636640000	1.7827320000	0.6379540000
H	-2.6607190000	2.8474480000	0.5421980000
H	-3.0453800000	1.5603750000	1.6915600000

Zero-point correction=  
(Hartree/Particle)

0.268793

Thermal correction to Energy=

0.285033

Thermal correction to Enthalpy=

0.285977

Thermal correction to Gibbs Free Energy=

0.225720

Sum of electronic and zero-point Energies=

-995.191854

Sum of electronic and thermal Energies=

-995.175614

Sum of electronic and thermal Enthalpies=

-995.174670

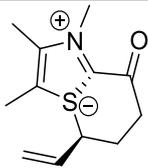
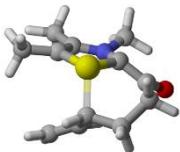
Sum of electronic and thermal Free Energies=

-995.234927

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.861	60.791	126.821

#M062X/6-311+G\*\*

(48ion-b)

structure	Ladung & Multiplizität	optimized structure
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	-2.6385450000	0.1473130000	-1.7810950000
H	-3.7459370000	0.6871470000	-0.5096400000
C	-2.7545280000	0.2795350000	-0.7011670000
S	-0.1503630000	-0.6677590000	-1.1895200000
H	-3.2074070000	-1.8379780000	-0.5479380000
C	2.3967190000	-1.8296420000	-1.0305240000
C	-1.7154560000	1.2528250000	-0.1705080000
C	1.5348570000	-0.6435400000	-0.7300650000
C	-2.6191820000	-1.1059470000	0.0077370000
C	-0.3994380000	0.9577760000	-0.6034800000
H	-1.0853400000	-2.6878270000	-0.0704360000
O	-2.0152980000	2.1339400000	0.6439270000
C	-1.1853330000	-1.6323430000	0.1894210000
H	-3.0671170000	-1.0148990000	0.9999380000
C	1.8053060000	0.5106710000	-0.0387930000
H	3.5276890000	1.7857330000	0.0308130000
N	0.7698470000	1.3699340000	0.1003170000
H	-0.0069750000	3.2057150000	0.6564980000
C	3.1489730000	0.8784460000	0.5077990000
C	0.9513220000	2.7969110000	0.3444560000
C	-0.5686000000	-1.3180920000	1.4979610000
H	0.5037470000	-3.1194290000	1.7554320000
H	3.8659860000	0.0772450000	0.3465110000
H	3.0809320000	1.0653100000	1.5817930000
H	1.2906400000	3.3041270000	-0.5663310000
H	-0.7992810000	-0.3365440000	1.9101370000
H	1.6805090000	2.9433670000	1.1403420000
C	0.2628010000	-2.1341430000	2.1439350000
H	0.7094240000	-1.8517230000	3.0894270000
H	3.4531650000	-1.5649560000	-0.9742400000
H	2.2107350000	-2.1943150000	-2.0443700000
H	2.2223880000	-2.6599370000	-0.3388090000

Zero-point correction= 0.268090  
(Hartree/Particle)

Thermal correction to Energy= 0.284486

Thermal correction to Enthalpy= 0.285430

Thermal correction to Gibbs Free Energy= 0.224380

Sum of electronic and zero-point Energies= -995.193911

Sum of electronic and thermal Energies= -995.177515

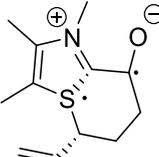
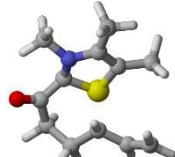
Sum of electronic and thermal Enthalpies= -995.176571

Sum of electronic and thermal Free Energies= -995.237621

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.517	60.950	128.489

#UM062X/6-311+G\*\*

(48rad-a)

structure	Ladung & Multiplizität	optimized structure
	0 1	

32

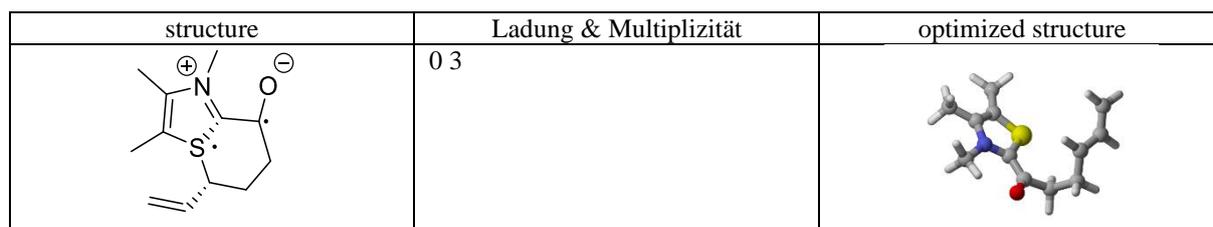
XYZ file generated by gabedit : coordinates in Angstrom

H	-3.7770520000	1.5462790000	0.0832640000
H	-3.5624010000	-1.1292490000	-0.5423130000
H	-3.5489400000	-0.6877700000	1.1893510000
C	-2.9685350000	-1.1275880000	0.3791340000
C	-2.8648010000	1.7807960000	0.6379330000
N	-1.7365250000	-0.3689160000	0.1928570000
H	-2.6973390000	-2.1471820000	0.6422370000
H	-2.6627890000	2.8456590000	0.5418260000
C	-1.7108760000	0.9795030000	0.1212190000
H	-3.0461500000	1.5585890000	1.6916300000
O	-0.6247760000	-3.0581580000	0.6176790000
C	-0.6594340000	-0.9870160000	-0.5077750000
H	-1.1941150000	3.4956720000	-1.1522250000
C	-0.6172520000	1.5288100000	-0.5018080000
H	0.4628920000	3.0548180000	-1.5413900000
C	-0.0821350000	-2.2227140000	-0.1122780000
S	0.4715910000	0.2545350000	-0.9927390000
C	-0.3113960000	2.9729170000	-0.7760050000
H	1.6544730000	-3.4252430000	-0.4167890000
C	1.3561200000	-2.3895400000	-0.5712250000
H	1.4445450000	-2.1611780000	-1.6378210000
H	0.0530500000	3.5050300000	0.1064800000
H	2.4618810000	-1.8926310000	1.2210770000
C	2.2996350000	-1.4467060000	0.2371440000
C	1.7813310000	-0.0214610000	0.4441300000
H	3.2695980000	-1.4091020000	-0.2654770000
H	1.1212150000	0.0582030000	1.3106530000
C	2.7905700000	1.0569670000	0.4117460000
C	2.7501570000	2.1440890000	1.1821320000
H	1.9794250000	2.2685850000	1.9367840000
H	3.5805240000	0.9557490000	-0.3305920000
H	3.4893020000	2.9305360000	1.0896090000

Zero-point correction= 0.268711  
(Hartree/Particle)

Thermal correction to Energy= 0.284978  
 Thermal correction to Enthalpy= 0.285922  
 Thermal correction to Gibbs Free Energy= 0.225535  
 Sum of electronic and zero-point Energies= -995.191936  
 Sum of electronic and thermal Energies= -995.175669  
 Sum of electronic and thermal Enthalpies= -995.174725  
 Sum of electronic and thermal Free Energies= -995.235112

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.826	60.851	127.095



32

XYZ file generated by gabedit : coordinates in Angstrom

H	-4.3641610000	-0.6255900000	0.5053040000
H	-2.7987310000	-2.5775370000	0.0318610000
H	-2.6350770000	-2.0327190000	1.7200550000
C	-2.1089950000	-2.1663860000	0.7754670000
C	-3.7629830000	0.1937200000	0.9060010000
N	-1.5927590000	-0.8752250000	0.3211780000
H	-1.2728460000	-2.8439570000	0.9096310000
H	-4.3019420000	1.1230160000	0.7372930000
C	-2.4171850000	0.2457490000	0.2556880000
H	-3.6703020000	0.0454300000	1.9849830000
O	0.6633200000	-2.7649310000	0.2078730000
C	-0.3808480000	-0.7250480000	-0.3253170000
H	-3.4137050000	2.7713950000	-0.2420980000
C	-1.8710620000	1.2908760000	-0.4022670000
H	-2.4718010000	2.8596880000	-1.7327680000
C	0.6844450000	-1.6722260000	-0.3866540000
S	-0.2672950000	0.8916150000	-0.9843910000
C	-2.4139910000	2.6590810000	-0.6599680000
H	2.1818540000	-2.1763980000	-1.7858450000
C	1.9295810000	-1.3037810000	-1.1779230000
H	1.7691980000	-0.4583530000	-1.8512450000
H	-1.7739450000	3.4237320000	-0.2123630000
H	3.2762840000	-1.8910760000	0.3809440000
C	3.1054900000	-0.9953920000	-0.2257310000
C	2.8242600000	0.1777710000	0.6551300000
H	4.0083620000	-0.8133260000	-0.8149900000
H	2.0480830000	0.0592920000	1.4081870000
C	3.4538060000	1.4069340000	0.5464620000
C	3.1622180000	2.5068660000	1.3259020000
H	2.3957310000	2.4545640000	2.0905000000
H	4.2293050000	1.5079240000	-0.2111030000
H	3.6847550000	3.4451220000	1.1999380000

Zero-point correction= 0.265269  
(Hartree/Particle)

Thermal correction to Energy= 0.282870

Thermal correction to Enthalpy= 0.283814

Thermal correction to Gibbs Free Energy= 0.216195

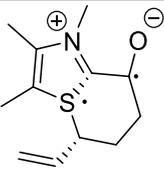
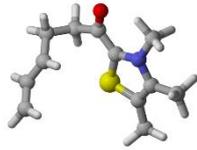
Sum of electronic and zero-point Energies= -995.205843

Sum of electronic and thermal Energies= -995.188243

Sum of electronic and thermal Enthalpies= -995.187299

Sum of electronic and thermal Free Energies= -995.254917

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.503	62.872	142.315

structure	Ladung & Multiplizität	optimized structure
	0 3 Guess=(mix,always)	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	4.3641610000	0.6255900000	0.5053040000
H	2.7987310000	2.5775370000	0.0318610000
H	2.6350770000	2.0327190000	1.7200550000
C	2.1089950000	2.1663860000	0.7754670000
C	3.7629830000	-0.1937200000	0.9060010000
N	1.5927590000	0.8752250000	0.3211780000
H	1.2728460000	2.8439570000	0.9096310000
H	4.3019420000	-1.1230160000	0.7372930000
C	2.4171850000	-0.2457490000	0.2556880000
H	3.6703020000	-0.0454300000	1.9849830000
O	-0.6633200000	2.7649310000	0.2078730000
C	0.3808480000	0.7250480000	-0.3253170000
H	3.4137050000	-2.7713950000	-0.2420980000
C	1.8710620000	-1.2908760000	-0.4022670000
H	2.4718010000	-2.8596880000	-1.7327680000
C	-0.6844450000	1.6722260000	-0.3866540000
S	0.2672950000	-0.8916150000	-0.9843910000
C	2.4139910000	-2.6590810000	-0.6599680000
H	-2.1818540000	2.1763980000	-1.7858450000
C	-1.9295810000	1.3037810000	-1.1779230000
H	-1.7691980000	0.4583530000	-1.8512450000
H	1.7739450000	-3.4237320000	-0.2123630000
H	-3.2762840000	1.8910760000	0.3809440000
C	-3.1054900000	0.9953920000	-0.2257310000
C	-2.8242600000	-0.1777710000	0.6551300000
H	-4.0083620000	0.8133260000	-0.8149900000
H	-2.0480830000	-0.0592920000	1.4081870000
C	-3.4538060000	-1.4069340000	0.5464620000
C	-3.1622180000	-2.5068660000	1.3259020000
H	-2.3957310000	-2.4545640000	2.0905000000
H	-4.2293050000	-1.5079240000	-0.2111030000
H	-3.6847550000	-3.4451220000	1.1999380000

Zero-point correction= 0.265269  
(Hartree/Particle)

Thermal correction to Energy= 0.282870

Thermal correction to Enthalpy= 0.283814

Thermal correction to Gibbs Free Energy= 0.216195

Sum of electronic and zero-point Energies= -995.205843

Sum of electronic and thermal Energies= -995.188243

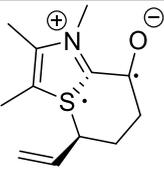
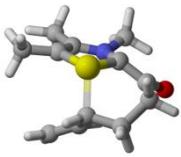
Sum of electronic and thermal Enthalpies= -995.187299

Sum of electronic and thermal Free Energies= -995.254917

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.503	62.872	142.315

#UM062X/6-311+G\*\*

(48rad-b)

structure	Ladung & Multiplizität	optimized structure
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	-2.6385450000	0.1473130000	-1.7810950000
H	-3.7459370000	0.6871470000	-0.5096400000
C	-2.7545280000	0.2795350000	-0.7011670000
S	-0.1503630000	-0.6677590000	-1.1895200000
H	-3.2074070000	-1.8379780000	-0.5479380000
C	2.3967190000	-1.8296420000	-1.0305240000
C	-1.7154560000	1.2528250000	-0.1705080000
C	1.5348570000	-0.6435400000	-0.7300650000
C	-2.6191820000	-1.1059470000	0.0077370000
C	-0.3994380000	0.9577760000	-0.6034800000
H	-1.0853400000	-2.6878270000	-0.0704360000
O	-2.0152980000	2.1339400000	0.6439270000
C	-1.1853330000	-1.6323430000	0.1894210000
H	-3.0671170000	-1.0148990000	0.9999380000
C	1.8053060000	0.5106710000	-0.0387930000
H	3.5276890000	1.7857330000	0.0308130000
N	0.7698470000	1.3699340000	0.1003170000
H	-0.0069750000	3.2057150000	0.6564980000
C	3.1489730000	0.8784460000	0.5077990000
C	0.9513220000	2.7969110000	0.3444560000
C	-0.5686000000	-1.3180920000	1.4979610000
H	0.5037470000	-3.1194290000	1.7554320000
H	3.8659860000	0.0772450000	0.3465110000
H	3.0809320000	1.0653100000	1.5817930000
H	1.2906400000	3.3041270000	-0.5663310000
H	-0.7992810000	-0.3365440000	1.9101370000
H	1.6805090000	2.9433670000	1.1403420000
C	0.2628010000	-2.1341430000	2.1439350000
H	0.7094240000	-1.8517230000	3.0894270000
H	3.4531650000	-1.5649560000	-0.9742400000
H	2.2107350000	-2.1943150000	-2.0443700000
H	2.2223880000	-2.6599370000	-0.3388090000

Zero-point correction=  
(Hartree/Particle)

0.268090

Thermal correction to Energy=

0.284486

Thermal correction to Enthalpy=

0.285430

Thermal correction to Gibbs Free Energy=

0.224380

Sum of electronic and zero-point Energies=

-995.193911

Sum of electronic and thermal Energies=

-995.177515

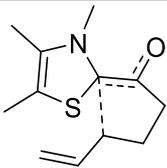
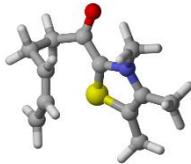
Sum of electronic and thermal Enthalpies=

-995.176571

Sum of electronic and thermal Free Energies=

-995.237621

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.517	60.950	128.489

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 Guess=(mix,always)	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	3.1773700000	-2.0701990000	-1.7189380000
H	-2.0231360000	-2.7980460000	0.0725500000
H	3.9846530000	-1.5776750000	-0.2310060000
C	3.0198680000	-1.8550330000	-0.6571350000
C	-1.4007450000	-2.6399480000	0.9455520000
H	-3.6865990000	-1.1281860000	0.1168480000
H	2.6987200000	-2.7861520000	-0.1778020000
H	-3.8655770000	0.5748900000	0.5071690000
C	-3.1374160000	-0.1847830000	0.2102530000
S	0.3751790000	-1.0013510000	-1.0731770000
C	2.0091400000	-0.7707980000	-0.4589410000
C	-1.4038160000	-1.4552340000	1.6420150000
H	-2.1701660000	-0.6536510000	-1.6959570000
C	-2.0699090000	-0.2779500000	1.2882010000
H	4.1686040000	0.2715210000	0.7558530000
C	-2.5285650000	0.2252270000	-1.1502690000
C	2.1190000000	0.4287940000	0.1671470000
C	-0.1295310000	0.5449340000	-0.4370720000
H	-2.0093820000	0.5560320000	1.9789180000
H	-3.2476050000	0.7441350000	-1.7864460000
H	3.1718030000	1.1745020000	1.8953820000
C	3.3439040000	0.9777220000	0.8332430000
C	-1.3785910000	1.1776970000	-0.8326720000
N	0.9512910000	1.1900020000	0.1400370000
H	3.6631960000	1.9156920000	0.3686010000
O	-1.5420970000	2.3994490000	-0.8301540000
H	1.6770300000	2.9586940000	1.0056670000
C	0.7663750000	2.3624990000	0.9991290000
H	0.5283750000	2.0498680000	2.0228840000
H	-0.0485990000	2.9583500000	0.5995100000
H	-0.8359610000	-3.4935520000	1.2988620000
H	-0.7661320000	-1.3989840000	2.5230120000

Zero-point correction= 0.263783  
(Hartree/Particle)

Thermal correction to Energy= 0.280091

Thermal correction to Enthalpy= 0.281035

Thermal correction to Gibbs Free Energy= 0.220627

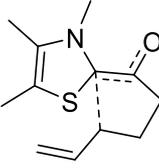
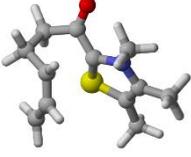
Sum of electronic and zero-point Energies= -995.509991

Sum of electronic and thermal Energies= -995.493684

Sum of electronic and thermal Enthalpies= -995.492740

Sum of electronic and thermal Free Energies= -995.553147

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	175.759	60.888	127.138

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 Guess=(mix,always)	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.1978100000	1.9394630000	-1.8527650000
H	1.9258900000	2.8974890000	0.1438840000
H	-4.0268380000	1.4681160000	-0.3580990000
C	-3.0561890000	1.7666790000	-0.7739260000
C	1.2889490000	2.7141230000	1.0090810000
H	3.5607530000	1.2581740000	0.1756830000
H	-2.7801710000	2.7328900000	-0.3204580000
H	3.8472460000	-0.4198120000	0.6429690000
C	3.0799410000	0.2713000000	0.2623320000
S	-0.3570560000	0.9854060000	-1.1264620000
C	-2.0080370000	0.7211380000	-0.5104410000
C	1.2654620000	1.5033580000	1.6646710000
H	2.2770250000	0.6063840000	-1.7683510000
C	1.9183710000	0.3099750000	1.2664740000
H	-4.1612630000	-0.3481820000	0.7247220000
C	2.6064310000	-0.2339640000	-1.1354680000
C	-2.0845770000	-0.4599710000	0.1740710000
C	0.2151290000	-0.5158300000	-0.3625410000
H	1.8746430000	-0.5264140000	1.9662200000
H	3.3894110000	-0.7784680000	-1.6773290000
H	-3.1537090000	-1.1771280000	1.9247130000
C	-3.3102300000	-1.0267360000	0.8457010000
C	1.4327550000	-1.1870380000	-0.8596270000
N	-0.8808240000	-1.1916870000	0.1936200000
H	-3.5939900000	-1.9983710000	0.4117460000
O	1.5488520000	-2.4201030000	-0.9189430000
H	-1.5709130000	-2.9597820000	1.1224640000
C	-0.6718350000	-2.3352240000	1.1047170000
H	-0.4512900000	-1.9824230000	2.1265250000
H	0.1626850000	-2.9310520000	0.7281480000
H	0.7217750000	3.5660250000	1.3820770000
H	0.6073860000	1.4223870000	2.5371790000

Zero-point correction= 0.256682  
(Hartree/Particle)

Thermal correction to Energy= 0.273145

Thermal correction to Enthalpy= 0.274089

Thermal correction to Gibbs Free Energy= 0.213706

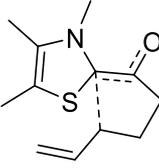
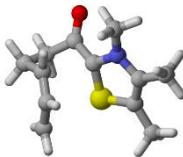
Sum of electronic and zero-point Energies= -995.239992

Sum of electronic and thermal Energies= -995.223528

Sum of electronic and thermal Enthalpies= -995.222584

Sum of electronic and thermal Free Energies= -995.282967

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.401	62.263	127.086

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

32

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.1978100000	1.9394630000	-1.8527650000
H	1.9258900000	2.8974890000	0.1438840000
H	-4.0268380000	1.4681160000	-0.3580990000
C	-3.0561890000	1.7666790000	-0.7739260000
C	1.2889490000	2.7141230000	1.0090810000
H	3.5607530000	1.2581740000	0.1756830000
H	-2.7801710000	2.7328900000	-0.3204580000
H	3.8472460000	-0.4198120000	0.6429690000
C	3.0799410000	0.2713000000	0.2623320000
S	-0.3570560000	0.9854060000	-1.1264620000
C	-2.0080370000	0.7211380000	-0.5104410000
C	1.2654620000	1.5033580000	1.6646710000
H	2.2770250000	0.6063840000	-1.7683510000
C	1.9183710000	0.3099750000	1.2664740000
H	-4.1612630000	-0.3481820000	0.7247220000
C	2.6064310000	-0.2339640000	-1.1354680000
C	-2.0845770000	-0.4599710000	0.1740710000
C	0.2151290000	-0.5158300000	-0.3625410000
H	1.8746430000	-0.5264140000	1.9662200000
H	3.3894110000	-0.7784680000	-1.6773290000
H	-3.1537090000	-1.1771280000	1.9247130000
C	-3.3102300000	-1.0267360000	0.8457010000
C	1.4327550000	-1.1870380000	-0.8596270000
N	-0.8808240000	-1.1916870000	0.1936200000
H	-3.5939900000	-1.9983710000	0.4117460000
O	1.5488520000	-2.4201030000	-0.9189430000
H	-1.5709130000	-2.9597820000	1.1224640000
C	-0.6718350000	-2.3352240000	1.1047170000
H	-0.4512900000	-1.9824230000	2.1265250000
H	0.1626850000	-2.9310520000	0.7281480000
H	0.7217750000	3.5660250000	1.3820770000
H	0.6073860000	1.4223870000	2.5371790000

Zero-point correction= 0.256682  
(Hartree/Particle)

Thermal correction to Energy= 0.273145

Thermal correction to Enthalpy= 0.274089

Thermal correction to Gibbs Free Energy= 0.213706

Sum of electronic and zero-point Energies= -995.239992

Sum of electronic and thermal Energies= -995.223528

Sum of electronic and thermal Enthalpies= -995.222584

Sum of electronic and thermal Free Energies= -995.282967

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.401	62.263	127.086

## BOMD

BOMD-Simulationen wurden mit folgenden Simulationsparametern durchgeführt:

### General parameters:

Max. points for each Traj. = 800  
Total Number of Trajectories = 1  
Random Number Generator Seed = 167924  
Trajectory Step Size = 0.250 sqrt(amu)\*bohr

### Sampling parameters:

Vib Energy Sampling Option = Thermal sampling  
TS Sampling direction = Forward  
Vib Sampling Temperature = 298.0 K  
Rot Energy Sampling Option = Thermal distribution (symmetric top)  
Rot Sampling Temperature = 298.0 K  
Start point scaling criteria = 1.000D-05 Hartree

### Integration parameters:

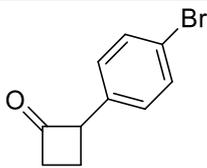
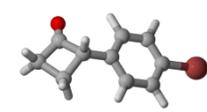
Correction Scheme = Fifth order polynomial fit  
Project trans/rot in grad. = True  
Project in prediction step = True  
Project in correction step = True  
Integration Scheme = Bulirsch-Stoer method  
Integration Step Size = 2.000D-01 femtosec  
Truncation Error Criteria = 1.000D-08 bohr  
Energy Error Criteria = 1.000D-04 Hartree  
Hessian evaluation = Update for 7 steps.  
Hessian update method = Bofill update  
Back integrate previous updated step with new Hessian.

Simulationen wurden von Übergangszustandsstrukturen ausgehend gestartet 46-syn-syn, 23-syn-syn, 42-syn-syn und 42-syn-anti. Von jeder Struktur wurden 100 Simulationen gestartet, jeweils mit den folgenden Seed-Nummern:

7370068	6299312	7192312	4859637	5272047
4050500	9479256	2614460	4834105	3827072
807960	7084842	5258232	4380682	3601921
2332816	3117024	7644650	2516812	887554
4114769	2836096	5265698	1863048	5663112
6710949	7100857	2897459	638796	869890
1267775	6783533	9308913	1242377	4284499
5568158	1207708	9571789	2312522	5796427
2915836	7310712	9743753	8441627	167924
9395582	1277251	7837325	7314046	4283381
6534229	7516040	1181527	8958929	8125237
9424842	3735889	6529055	7277067	7097160
5825786	2177873	5165534	5447562	8107813
6414839	4443623	9942952	9607121	1135809
202549	4622852	8277718	2092144	8011762
2383442	5200063	6737714	1546739	4822923
5632513	565649	8569721	4205535	9660756
2522099	9763918	8711497	1143751	1295763
1690304	2099832	7898281	9564717	9881887
8429346	8127251	5082092	1814670	9253905

## Substituenten:

#M062X/6-311+G**	(32f)
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Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

21

XYZ file generated by gabedit : coordinates in Angstrom

H	-2.9561270000	-1.7656050000	-1.0033000000
H	-0.8743620000	-2.3207810000	0.1168590000
H	1.5756290000	-2.1764020000	-0.1742900000
H	-4.9173270000	-0.3116180000	-1.5153560000
H	-3.7929910000	-2.2236630000	0.5003170000
C	-3.4680870000	-1.3889500000	-0.1171830000
C	-0.3858400000	-1.3537030000	0.1701300000
C	-4.5480240000	-0.3375640000	-0.4907840000
C	0.9932550000	-1.2820380000	0.0055590000
H	-5.3937830000	-0.3271970000	0.2006500000
C	-2.6284910000	-0.2876150000	0.5922410000
C	-1.1413220000	-0.2059330000	0.4036280000
C	-3.5303020000	0.7357360000	-0.1182750000
C	1.6149570000	-0.0432040000	0.0714740000
Br	3.4982840000	0.0668320000	-0.1559740000
H	-2.8828150000	-0.2575360000	1.6594830000
O	-3.4132740000	1.8941740000	-0.3753430000
C	-0.4920530000	1.0283630000	0.4672590000
C	0.8847790000	1.1158960000	0.2995150000
H	-1.0703640000	1.9297080000	0.6332110000
H	1.3851510000	2.0746460000	0.3429050000

Zero-point correction=  
(Hartree/Particle)

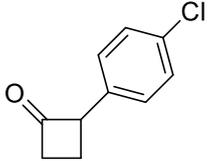
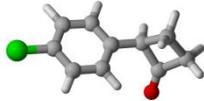
0.163120

Thermal correction to Energy=	0.173704
Thermal correction to Enthalpy=	0.174648
Thermal correction to Gibbs Free Energy=	0.124557
Sum of electronic and zero-point Energies=	-3035.612052
Sum of electronic and thermal Energies=	-3035.601469
Sum of electronic and thermal Enthalpies=	-3035.600525
Sum of electronic and thermal Free Energies=	-3035.650615

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	109.001	39.603	105.425

#M062X/6-311+G\*\*

(32e)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

21

XYZ file generated by gabedit : coordinates in Angstrom

Cl	-4.0352780000	-0.2953130000	0.1437650000
C	-2.3154760000	-0.0242140000	0.0284220000
H	-2.5478180000	1.9128340000	-0.8611820000
H	-1.8256370000	-1.9305150000	0.8810600000
C	-1.8478540000	1.1642220000	-0.5127360000
C	-1.4387590000	-1.0049370000	0.4741050000
C	-0.4758530000	1.3691540000	-0.6015660000
C	-0.0715360000	-0.7830400000	0.3789020000
H	-0.1051750000	2.2959040000	-1.0266050000
H	0.6124100000	-1.5573790000	0.7094730000
C	0.4285650000	0.4069400000	-0.1543350000
O	2.7604040000	-1.5360450000	-1.0962260000
C	1.9048290000	0.6521420000	-0.2173340000
H	2.1364220000	1.4483640000	-0.9327030000
H	2.2481200000	0.4032150000	1.9393780000
C	2.8670780000	-0.5176110000	-0.4857850000
C	2.7330170000	0.8824010000	1.0881280000
H	2.9662120000	1.9166860000	1.3322550000
C	3.8860010000	0.0114110000	0.5189370000
H	4.3592900000	-0.7278720000	1.1639070000
H	4.6525920000	0.6086360000	0.0197910000

Zero-point correction=  
(Hartree/Particle)

0.163885

Thermal correction to Energy=

0.174307

Thermal correction to Enthalpy=

0.175251

Thermal correction to Gibbs Free Energy=

0.125374

Sum of electronic and zero-point Energies=

-921.638524

Sum of electronic and thermal Energies=

-921.628102

Sum of electronic and thermal Enthalpies=

-921.627158

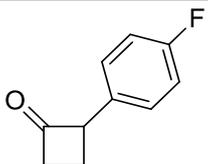
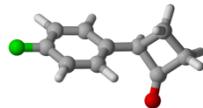
Sum of electronic and thermal Free Energies=

-921.677035

	E (Thermal) kCal/Mol	CV cal/Mol-Kelvin	S cal/Mol-kelvin
Total	109.379	39.133	104.975

#M062X/6-311+G\*\*

(32d)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

21

XYZ file generated by gabedit : coordinates in Angstrom

H	3.9769490000	-0.6343920000	1.1251270000
O	2.3693620000	-1.4996080000	-1.1075770000
C	3.4731730000	0.0878000000	0.4838570000
C	2.4548960000	-0.4754760000	-0.5031330000
H	0.2594310000	-1.5638030000	0.7609280000
H	1.8469700000	0.4426600000	1.9279500000
H	4.2151470000	0.7036680000	-0.0295620000
C	2.3045250000	0.9289920000	1.0656510000
H	-2.1798520000	-2.0152070000	0.9661750000
C	-0.4562510000	-0.8218860000	0.4233270000
H	2.5124650000	1.9710160000	1.2995760000
C	1.4625180000	0.6663580000	-0.2246880000
C	-1.8135300000	-1.0899460000	0.5398420000
C	-0.0044710000	0.3746950000	-0.1390510000
H	1.6585250000	1.4643770000	-0.9486830000
C	-2.7153140000	-0.1443210000	0.0837310000
C	-0.9461010000	1.2969820000	-0.5949490000
F	-4.0311680000	-0.3974630000	0.1942660000
C	-2.3097990000	1.0476460000	-0.4862400000
H	-0.6106610000	2.2263860000	-1.0425130000
H	-3.0512400000	1.7542630000	-0.8368640000

Zero-point correction=  
(Hartree/Particle)

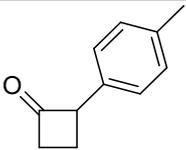
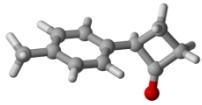
0.165211

Thermal correction to Energy=	0.175217
Thermal correction to Enthalpy=	0.176161
Thermal correction to Gibbs Free Energy=	0.128179
Sum of electronic and zero-point Energies=	-561.278079
Sum of electronic and thermal Energies=	-561.268073
Sum of electronic and thermal Enthalpies=	-561.267129
Sum of electronic and thermal Free Energies=	-561.315111

	E (Thermal) kCal/Mol	CV cal/Mol-Kelvin	S cal/Mol-kelvin
Total	109.950	38.284	100.987

#M062X/6-311+G\*\*

(32b)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

24

XYZ file generated by gabedit : coordinates in Angstrom

O	2.3998920000	-1.4847930000	-1.1500860000
H	-2.1353700000	-1.9714130000	0.9930520000
H	0.2768190000	-1.5405670000	0.7974620000
H	3.9983000000	-0.6996530000	1.1195950000
C	-1.7916810000	-1.0428250000	0.5485790000
H	-4.5264250000	-1.0182950000	-0.6835810000
C	-0.4299680000	-0.7968750000	0.4430250000
C	2.4889370000	-0.4802930000	-0.5138500000
H	-4.4478730000	-0.9613690000	1.0772390000
H	1.8846940000	0.3960550000	1.9384880000
C	3.5099280000	0.0449730000	0.4920130000
C	-4.2057720000	-0.4101470000	0.1669560000
C	-2.7299590000	-0.1188990000	0.0831880000
C	0.0385900000	0.3878240000	-0.1293390000
C	2.3517980000	0.8913160000	1.0865310000
C	1.5084080000	0.6653970000	-0.2098860000
H	4.2651740000	0.6593800000	-0.0036940000
H	-4.7909970000	0.5105080000	0.1574000000
C	-2.2596990000	1.0612920000	-0.4890760000
C	-0.8954240000	1.3099900000	-0.5968420000
H	2.5740440000	1.9258780000	1.3400410000
H	1.7127540000	1.4766970000	-0.9168690000
H	-2.9689520000	1.7950810000	-0.8581910000
H	-0.5522530000	2.2355290000	-1.0480460000

Zero-point correction=  
(Hartree/Particle)

0.201063

Thermal correction to Energy=

0.211999

Thermal correction to Enthalpy=

0.212943

Thermal correction to Gibbs Free Energy=

0.163095

Sum of electronic and zero-point Energies=

-501.307187

Sum of electronic and thermal Energies=

-501.296251

Sum of electronic and thermal Enthalpies=

-501.295307

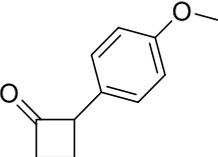
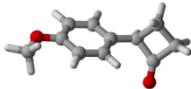
Sum of electronic and thermal Free Energies=

-501.345155

	E (Thermal) kCal/Mol	CV cal/Mol-Kelvin	S cal/Mol-Kelvin
Total	133.032	41.375	104.916

#M062X/6-311+G\*\*

(32a)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

25

XYZ file generated by gabedit : coordinates in Angstrom

O	2.6979530000	-1.5935170000	-1.1095580000
H	-4.0739710000	-1.8048790000	-0.3150670000
H	-1.9536400000	-1.7982790000	0.5787440000
H	0.4760140000	-1.5800080000	0.4614250000
H	4.2917370000	-0.9426780000	1.2008110000
H	-4.0537930000	-1.2571940000	1.3864110000
C	2.8474010000	-0.5979690000	-0.4693880000
C	-1.5255980000	-0.8509860000	0.2803650000
C	-4.3263150000	-0.9829660000	0.3622480000
C	-0.1397590000	-0.7204510000	0.2188760000
H	2.2322430000	0.2855790000	1.9662420000
H	-5.3953360000	-0.7887150000	0.3125920000
C	3.8754350000	-0.1587030000	0.5694310000
C	2.7637020000	0.7618120000	1.1415640000
H	4.6853900000	0.4059270000	0.1016010000
C	-2.3341420000	0.2339940000	-0.0538710000
O	-3.6920940000	0.2156520000	-0.0307530000
C	0.4610310000	0.4731350000	-0.1681180000
C	1.9517210000	0.6180880000	-0.1874040000
H	3.0518910000	1.7723860000	1.4235670000
H	2.2549670000	1.4174650000	-0.8728110000
C	-1.7461440000	1.4370910000	-0.4505670000
C	-0.3683560000	1.5471980000	-0.5073750000
H	-2.3920380000	2.2657560000	-0.7133900000
H	0.0758170000	2.4861100000	-0.8222170000

Zero-point correction=  
(Hartree/Particle)

0.206393

Thermal correction to Energy=

0.218086

Thermal correction to Enthalpy=

0.219031

Thermal correction to Gibbs Free Energy=

0.167234

Sum of electronic and zero-point Energies=

-576.507886

Sum of electronic and thermal Energies=

-576.496193

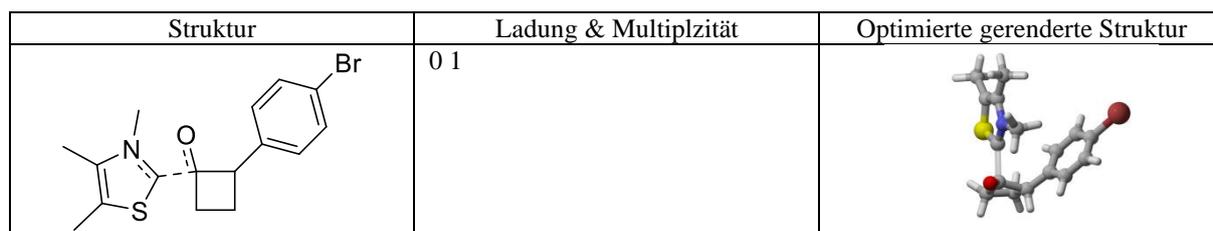
Sum of electronic and thermal Enthalpies=

-576.495248

Sum of electronic and thermal Free Energies=

-576.547045

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	136.851	44.365	109.015



38

XYZ file generated by gabedit : coordinates in Angstrom

H	-4.2432840000	3.5926410000	-0.8096010000
H	-2.7144860000	4.4314690000	-0.5438070000
H	-1.2959710000	3.2545320000	2.4226010000
C	-3.1659390000	3.5411220000	-0.9805360000
S	-3.0770550000	0.7129620000	-0.9178810000
C	-2.5891660000	2.2990830000	-0.3785560000
H	-3.4253690000	-3.5666320000	-0.0217160000
C	-1.6802090000	2.1626150000	0.6130950000
H	-0.5351550000	1.0690400000	2.7882420000
H	-3.9752840000	-1.9589480000	-0.5406810000
C	-2.0517930000	-0.1060410000	0.1817130000
C	-0.9746990000	3.2353450000	1.3780740000
H	-2.9947780000	3.5696410000	-2.0584670000
N	-1.4192830000	0.8112520000	0.9033930000
C	-3.0981050000	-2.5705500000	-0.3301920000
O	-2.0987470000	-2.1204870000	1.9398880000
C	-2.0649180000	-2.0775120000	0.7158470000
H	0.1063840000	3.0808600000	1.3598960000
C	-0.4198850000	0.4321530000	1.9123560000
H	-0.5994660000	-0.6036530000	2.1905080000
H	-1.1841110000	4.2103090000	0.9425640000
H	-0.1868790000	-0.5329320000	-1.9364140000
H	0.5798310000	0.5529960000	1.4886660000
C	-1.9584030000	-2.6411390000	-1.3770540000
C	0.5806600000	-0.7853020000	-1.2140840000
H	1.8893350000	0.7900220000	-1.8825790000
H	-1.9290070000	-3.5317620000	-2.0032900000
C	-0.9115410000	-2.5872030000	-0.2415570000
H	-1.9370720000	-1.7626250000	-2.0216040000
C	1.7471980000	-0.0284710000	-1.1883810000
C	0.3812600000	-1.8459490000	-0.3263960000
H	-0.7229600000	-3.6057480000	0.1160130000
C	2.7355220000	-0.3391970000	-0.2630690000
C	1.4061730000	-2.1443880000	0.5774180000
H	1.2731230000	-2.9650870000	1.2744440000
C	2.5803800000	-1.4001480000	0.6192890000
Br	4.3254620000	0.7035710000	-0.2125190000
H	3.3625980000	-1.6378600000	1.3288310000

Zero-point correction=  
(Hartree/Particle)

0.305517

Thermal correction to Energy=

0.324897

Thermal correction to Enthalpy=

0.325841

Thermal correction to Gibbs Free Energy=

0.256280

Sum of electronic and zero-point Energies=

-3722.364178

Sum of electronic and thermal Energies=

-3722.344798

Sum of electronic and thermal Enthalpies=

-3722.343854

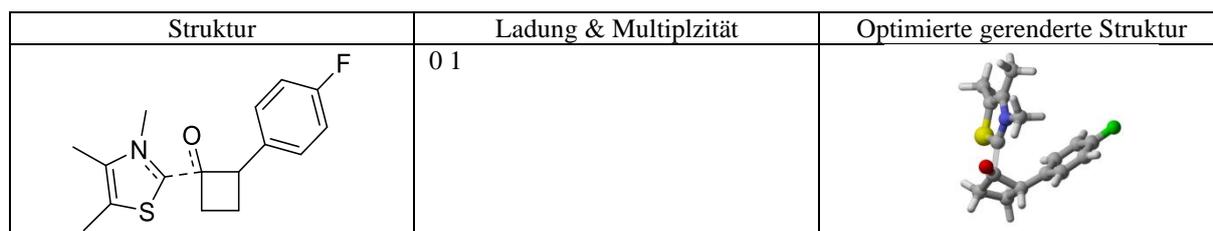
Sum of electronic and thermal Free Energies=

-3722.413415

	E (Thermal) kCal/Mol	CV Cal/Mol-kelvin	S Cal/Mol-kelvin
Total	203.876	73.787	146.403

#M062X/6-311+G\*\*

(40d-syn-syn)



38

XYZ file generated by gabedit : coordinates in Angstrom

H	4.9785530000	-1.2884710000	-0.7545660000
H	1.8341120000	3.2338720000	-0.3345780000
C	4.0501510000	-1.8223580000	-0.9677800000
H	3.9524080000	-1.9067420000	-2.0521470000
H	4.1408110000	-2.8277750000	-0.5574710000
S	2.4698140000	0.5230190000	-0.8482250000
C	2.8763970000	-1.1076140000	-0.3770220000
H	0.2274080000	2.1019820000	-1.9314300000
C	0.7613690000	3.2912330000	-0.1516080000
H	0.5169220000	4.2924770000	0.2124390000
C	-0.2218120000	2.8304310000	-1.2565170000
H	-0.6871180000	3.6152330000	-1.8512920000
C	1.1194870000	0.6153640000	0.2005670000
C	1.9912310000	-1.5260250000	0.5554190000
H	-0.6388270000	0.1340240000	-1.9686260000
C	0.1003940000	2.2734010000	0.8145020000
H	2.6530500000	-3.5373480000	0.8128190000
N	1.0392010000	-0.5353350000	0.8576030000
O	0.0788280000	2.2462530000	2.0399590000
C	-1.1235380000	2.1822830000	-0.1814590000
C	1.9297220000	-2.8497790000	1.2465630000
C	-1.4596910000	-0.0734250000	-1.2920450000
H	2.1520410000	-2.7524080000	2.3120940000
H	-1.7860190000	-2.0676380000	-2.0758090000
H	-1.8149820000	2.9406960000	0.2029180000
H	0.3410110000	-1.3426630000	2.6635530000
C	-1.8591330000	0.8946220000	-0.3662250000
C	-2.0882790000	-1.3129550000	-1.3601870000
C	-0.0506820000	-0.7914290000	1.8101440000
H	0.9371660000	-3.2952080000	1.1478000000
H	-0.4362310000	0.1688580000	2.1448010000
H	-0.8324170000	-1.3711070000	1.3138500000
C	-2.9288940000	0.5898890000	0.4824590000
C	-3.1319360000	-1.5752710000	-0.4904180000
H	-3.2536370000	1.3294650000	1.2066180000
C	-3.5711410000	-0.6424510000	0.4315810000
F	-3.7412030000	-2.7764570000	-0.5464530000
H	-4.3973380000	-0.8855930000	1.0879650000

Zero-point correction=  
(Hartree/Particle)

0.307239

Thermal correction to Energy=

0.326058

Thermal correction to Enthalpy=

0.327002

Thermal correction to Gibbs Free Energy=

0.260013

Sum of electronic and zero-point Energies=

-1248.030702

Sum of electronic and thermal Energies=

-1248.011883

Sum of electronic and thermal Enthalpies=

-1248.010939

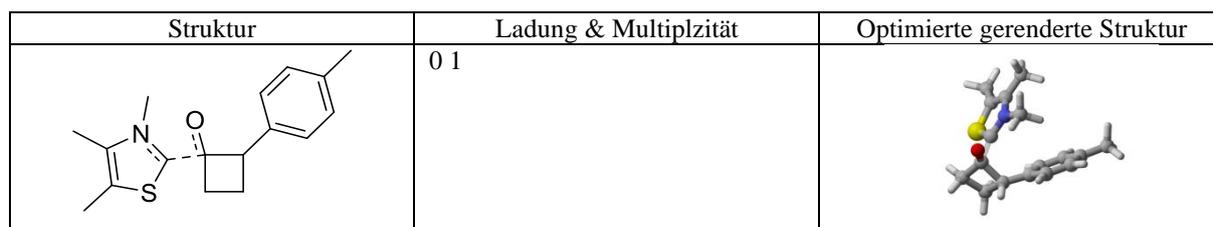
Sum of electronic and thermal Free Energies=

-1248.077928

	E (Thermal) kCal/Mol	CV Cal/Mol-kelvin	S Cal/Mol-kelvin
Total	204.604	72.642	140.991

#M062X/6-311+G\*\*

(40b-syn-syn)



41

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.6211940000	0.1705940000	-1.9721370000
H	0.3886490000	2.0845500000	-1.9379680000
H	3.9629340000	-3.0677970000	-0.5411660000
H	-1.8942930000	-1.9265700000	-2.0641730000
H	3.8382890000	-2.1377840000	-2.0368810000
H	-0.4298680000	3.6528390000	-1.8774990000
C	3.9389140000	-2.0589450000	-0.9522760000
C	-0.0179360000	2.8461600000	-1.2726700000
C	-1.4512650000	0.0245670000	-1.2898310000
C	-2.1692900000	-1.1669940000	-1.3385750000
H	2.0534700000	3.1311640000	-0.3404920000
S	2.5246430000	0.3894350000	-0.8308750000
H	4.8999140000	-1.5865960000	-0.7381420000
C	0.9848320000	3.2544370000	-0.1649650000
C	2.8131850000	-1.2677100000	-0.3657580000
C	-1.7816510000	1.0265010000	-0.3752030000
H	0.7988740000	4.2706810000	0.1922140000
C	-0.9645840000	2.2645200000	-0.1980130000
C	-3.2435140000	-1.4005490000	-0.4790870000
C	-4.0035430000	-2.7019370000	-0.5151500000
C	1.1726140000	0.5682430000	0.2042500000
H	-1.6059760000	3.0697970000	0.1783300000
C	0.2578470000	2.2840940000	0.8033410000
C	1.8909490000	-1.6290510000	0.5549760000
C	-2.8704290000	0.7978270000	0.4727140000
C	-3.5857610000	-0.3924030000	0.4238280000
H	2.4121500000	-3.6817470000	0.8037790000
N	1.0073880000	-0.5768920000	0.8548520000
C	1.7302300000	-2.9507620000	1.2338770000
H	-3.1478530000	1.5646170000	1.1888870000
O	0.2304130000	2.2659310000	2.0296990000
H	0.7110380000	-3.3262560000	1.1174340000
H	-4.4249700000	-0.5413100000	1.0963170000
H	1.9431030000	-2.8774520000	2.3032650000
C	-0.1091770000	-0.7625190000	1.7928630000
H	-0.4270490000	0.2201460000	2.1338050000
H	-0.9263590000	-1.2753500000	1.2799660000
H	0.2315550000	-1.3500500000	2.6441100000
H	-3.8983670000	-3.1918780000	-1.4845830000
H	-5.0667620000	-2.5416730000	-0.3273940000
H	-3.6351090000	-3.3929720000	0.2488440000

Zero-point correction=  
(Hartree/Particle)

0.343193

Thermal correction to Energy=

0.362860

Thermal correction to Enthalpy=

0.363804

Thermal correction to Gibbs Free Energy=

0.294561

Sum of electronic and zero-point Energies=

-1188.058961

Sum of electronic and thermal Energies=

-1188.039294

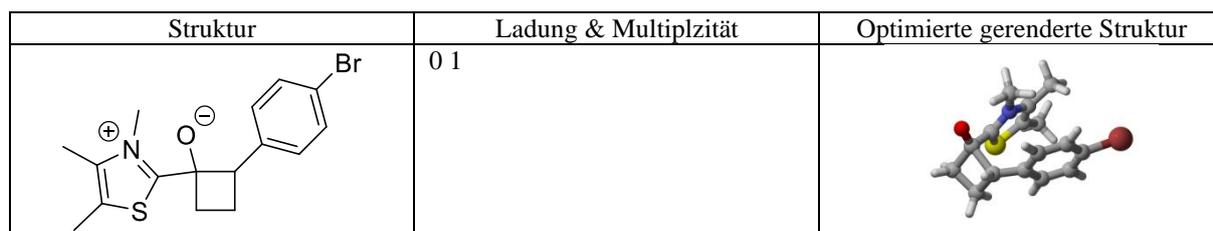
Sum of electronic and thermal Enthalpies=

-1188.038350

Sum of electronic and thermal Free Energies=

-1188.107594

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	227.698	75.518	145.736



38

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.0125080000	4.0630530000	-1.7704590000
H	0.3334960000	4.2273560000	-0.6459640000
H	0.5724360000	2.6527140000	2.5727990000
C	-0.2176000000	3.5163860000	-1.2609020000
S	-2.1395540000	1.4773220000	-0.9665100000
C	-0.7792230000	2.4124050000	-0.4217240000
H	-4.6703610000	-1.7214660000	-0.2272810000
C	-0.3451790000	1.9324900000	0.7647460000
H	-1.0354380000	1.0359010000	3.2983560000
H	-4.4655390000	-0.1021940000	-0.9270980000
C	-2.0725860000	0.4459070000	0.3954230000
C	0.8430050000	2.3766050000	1.5517250000
H	0.4616550000	3.1194890000	-2.0197410000
N	-1.1098680000	0.8486270000	1.2181760000
C	-3.9394850000	-1.0033620000	-0.5977160000
O	-3.1437740000	-1.1978380000	1.7574120000
C	-2.8752820000	-0.8581690000	0.5458870000
H	1.5864020000	1.5750510000	1.5975830000
C	-0.8559280000	0.2626770000	2.5498730000
H	-1.5609800000	-0.5602580000	2.6766440000
H	1.3077820000	3.2362150000	1.0731200000
H	-0.4313910000	-0.7161540000	-2.4035630000
H	0.1803300000	-0.0682380000	2.5926620000
C	-2.9281410000	-1.6499630000	-1.5684420000
C	0.1295350000	-0.9871690000	-1.5170230000
H	1.9221230000	-0.0190320000	-2.2189830000
H	-3.2730810000	-2.5286170000	-2.1139000000
C	-1.9569520000	-1.9259070000	-0.4158830000
H	-2.5396220000	-0.9383630000	-2.2985140000
C	1.4578500000	-0.5861620000	-1.4215850000
C	-0.4930140000	-1.7071000000	-0.4886320000
H	-2.2001740000	-2.8601990000	0.0918380000
C	2.1881640000	-0.9201770000	-0.2890740000
C	0.2953500000	-2.0799650000	0.6103750000
H	-0.1633700000	-2.6538730000	1.4097970000
C	1.6240150000	-1.6896190000	0.7219510000
Br	3.9851260000	-0.3142050000	-0.1242700000
H	2.2138000000	-1.9723080000	1.5858070000

Zero-point correction=  
(Hartree/Particle)

0.306104

Thermal correction to Energy=

0.325789

Thermal correction to Enthalpy=

0.326733

Thermal correction to Gibbs Free Energy=

0.256668

Sum of electronic and zero-point Energies=

-3722.370916

Sum of electronic and thermal Energies=

-3722.351232

Sum of electronic and thermal Enthalpies=

-3722.350287

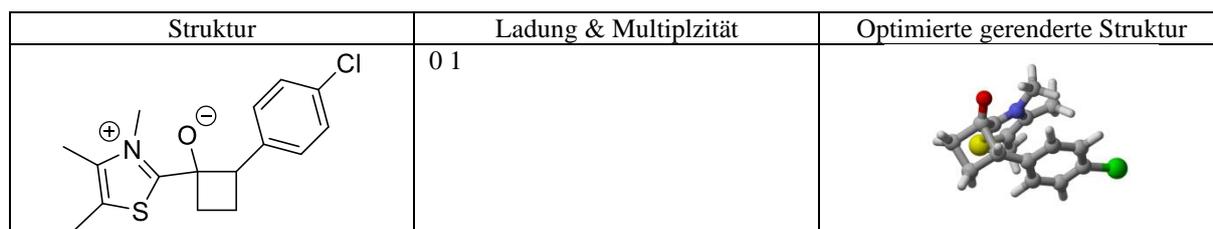
Sum of electronic and thermal Free Energies=

-3722.420353

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-kelvin	Cal/Mol-kelvin
Total	204.436	75.253	147.465

#M062X/6-311+G\*\*

(41e-syn-syn)



38

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.9269400000	4.2270090000	-1.5165500000
H	0.5807660000	4.3064030000	-0.6093730000
H	1.0310580000	2.6479630000	2.5434240000
C	-0.0609980000	3.6471040000	-1.1926050000
S	-1.8165680000	1.4695130000	-0.8844610000
C	-0.4839690000	2.4643310000	-0.3799270000
H	-4.1459420000	-1.8607660000	-0.1348410000
C	0.0523050000	1.9621760000	0.7548210000
H	-0.3890390000	0.9103180000	3.2752660000
H	-4.0339970000	-0.2162200000	-0.7948320000
C	-1.6040520000	0.3884940000	0.4230660000
C	1.2555960000	2.4471930000	1.4941650000
H	0.4890910000	3.3333000000	-2.0830440000
N	-0.6153150000	0.8128920000	1.2010750000
C	-3.4594330000	-1.1038990000	-0.5131000000
O	-2.5556830000	-1.3030770000	1.8094030000
C	-2.3490460000	-0.9524580000	0.5867140000
H	2.0531120000	1.6995480000	1.4507420000
C	-0.2359180000	0.1795150000	2.4799470000
H	-0.8976090000	-0.6760010000	2.6225220000
H	1.6295150000	3.3634510000	1.0421870000
H	-0.0132370000	-0.5842920000	-2.3472630000
H	0.8126410000	-0.1084150000	2.4280330000
C	-2.4620640000	-1.6868320000	-1.5378770000
C	0.5850070000	-0.9284210000	-1.5118910000
H	2.3514420000	0.0976860000	-2.2043020000
H	-2.7968680000	-2.5553060000	-2.1053320000
C	-1.4546180000	-1.9727970000	-0.4181680000
H	-2.1119490000	-0.9385500000	-2.2508200000
C	1.9170250000	-0.5364880000	-1.4410940000
C	0.0063350000	-1.7357530000	-0.5238650000
H	-1.6679970000	-2.9289780000	0.0623970000
C	2.6964790000	-0.9702390000	-0.3775360000
C	0.8383870000	-2.1962630000	0.5064020000
H	0.4145090000	-2.8361730000	1.2738360000
C	2.1731150000	-1.8199160000	0.5889060000
Cl	4.3618340000	-0.4470690000	-0.2592700000
H	2.8031140000	-2.1731320000	1.3964220000

Zero-point correction=  
(Hartree/Particle)

0.307062

Thermal correction to Energy=

0.326320

Thermal correction to Enthalpy=

0.327264

Thermal correction to Gibbs Free Energy=

0.258467

Sum of electronic and zero-point Energies=

-1608.398278

Sum of electronic and thermal Energies=

-1608.379020

Sum of electronic and thermal Enthalpies=

-1608.378075

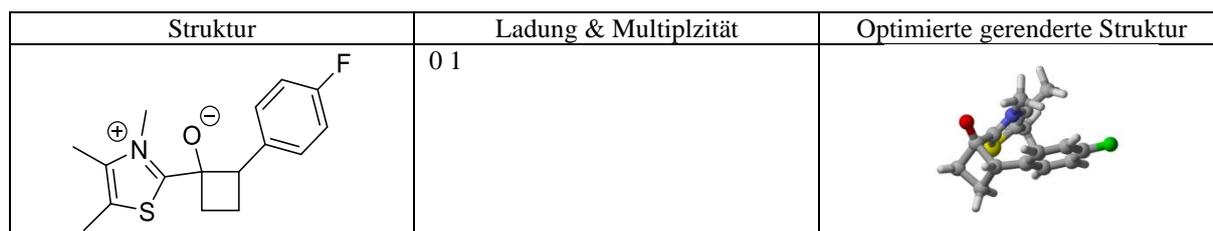
Sum of electronic and thermal Free Energies=

-1608.446873

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.769	74.519	144.797

#M062X/6-311+G\*\*

(41d-syn-syn)



38

XYZ file generated by gabedit : coordinates in Angstrom

H	-4.0995380000	2.5551850000	-1.0207230000
H	-2.6770970000	-2.6947930000	-0.6294690000
C	-3.0278180000	2.7571280000	-1.0669760000
H	-2.7413620000	2.8217260000	-2.1189540000
H	-2.8524890000	3.7282540000	-0.6059530000
S	-2.4901090000	0.0110890000	-0.7561290000
C	-2.2527220000	1.6884540000	-0.3627440000
H	-0.7615680000	-1.8798990000	-2.0924460000
C	-1.6400320000	-2.9104790000	-0.3552640000
H	-1.5919790000	-3.9105640000	0.0759220000
C	-0.5237710000	-2.6880690000	-1.3967840000
H	-0.2025800000	-3.5522190000	-1.9781650000
C	-1.3192670000	-0.4979300000	0.3803720000
C	-1.3195710000	1.7976980000	0.6113670000
H	0.3866110000	0.0079750000	-1.8654600000
C	-0.9087770000	-1.9688170000	0.6692910000
H	-1.1806890000	3.9201060000	0.7398970000
N	-0.8268540000	0.5531010000	1.0191230000
O	-0.8779620000	-2.2107650000	1.9399360000
C	0.4177070000	-2.2375410000	-0.2678080000
C	-0.7792770000	3.0408370000	1.2387320000
C	1.2712550000	-0.0618950000	-1.2405790000
H	-1.0415520000	3.0989020000	2.2976250000
H	2.0439210000	1.8558440000	-1.8907550000
H	0.8405000000	-3.1167100000	0.2241300000
H	-0.0743830000	1.0595630000	2.9015430000
C	1.4614090000	-1.1862830000	-0.4270890000
C	2.1862560000	0.9851290000	-1.2622610000
C	0.2196980000	0.4460050000	2.0506840000
H	0.3096990000	3.0688380000	1.1560120000
H	0.2681060000	-0.6036950000	2.3450890000
H	1.1611400000	0.8038060000	1.6297650000
C	2.6294570000	-1.2396720000	0.3447100000
C	3.3156800000	0.8939220000	-0.4666990000
H	2.7992890000	-2.1021270000	0.9800510000
C	3.5611800000	-0.2075570000	0.3327080000
F	4.2061500000	1.9061910000	-0.4804150000
H	4.4635960000	-0.2444970000	0.9303820000

Zero-point correction=  
(Hartree/Particle)

0.308343

Thermal correction to Energy=

0.327169

Thermal correction to Enthalpy=

0.328113

Thermal correction to Gibbs Free Energy=

0.261764

Sum of electronic and zero-point Energies=

-1248.038022

Sum of electronic and thermal Energies=

-1248.019196

Sum of electronic and thermal Enthalpies=

-1248.018252

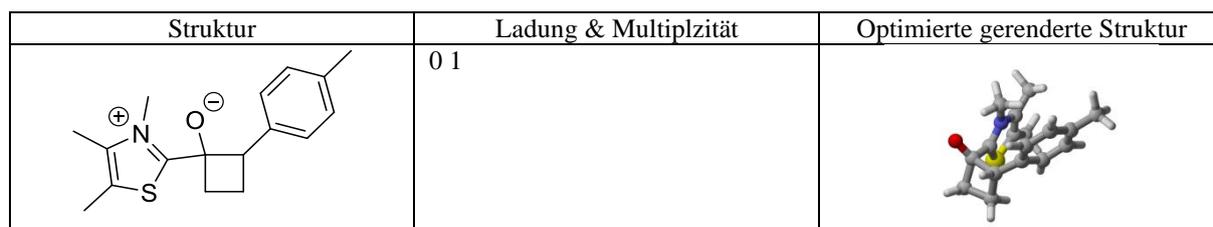
Sum of electronic and thermal Free Energies=

-1248.084601

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-kelvin	Cal/Mol-kelvin
Total	205.301	73.558	139.643

#M062X/6-311+G\*\*

(41b-syn-syn)



41

XYZ file generated by gabedit : coordinates in Angstrom

H	0.3808270000	-0.0044490000	-1.8534600000
H	-0.8857180000	-1.8380650000	-2.0957350000
H	-2.7617870000	2.8673620000	-2.1280110000
H	2.1197000000	1.7231730000	-1.8570640000
H	-3.9868360000	2.8467290000	-0.8545260000
H	-0.4247480000	-3.5409400000	-1.9879950000
C	-2.9139120000	2.9087640000	-1.0476340000
C	-0.6954140000	-2.6616360000	-1.4034570000
C	1.2600920000	-0.1395960000	-1.2304300000
C	2.2427270000	0.8449290000	-1.2299580000
H	-2.8449070000	-2.5490280000	-0.6324130000
S	-2.5165140000	0.1382000000	-0.7492700000
H	-2.5657520000	3.8784660000	-0.6944820000
C	-1.8208420000	-2.8228530000	-0.3606700000
C	-2.1821840000	1.8004340000	-0.3590250000
C	1.3766930000	-1.2825810000	-0.4309340000
H	-1.8287710000	-3.8248600000	0.0687770000
C	0.2721810000	-2.2697980000	-0.2747740000
C	3.3917500000	0.7203890000	-0.4465410000
C	4.4742460000	1.7685930000	-0.4719060000
C	-1.3631600000	-0.4343200000	0.3754000000
H	0.6420350000	-3.1738590000	0.2153020000
C	-1.0352860000	-1.9254430000	0.6634910000
C	-1.2334590000	1.8572410000	0.6047510000
C	2.5395260000	-1.4103340000	0.3389600000
C	3.5244440000	-0.4308690000	0.3321410000
H	-0.9749060000	3.9688480000	0.7334280000
N	-0.8065070000	0.5875890000	1.0083060000
C	-0.6182640000	3.0676200000	1.2271750000
H	2.6551750000	-2.2861650000	0.9691000000
O	-1.0199140000	-2.1668080000	1.9351130000
H	0.4698160000	3.0329550000	1.1344750000
H	4.4109770000	-0.5581910000	0.9460990000
H	-0.8674670000	3.1394650000	2.2883960000
C	0.2483650000	0.4212760000	2.0234460000
H	0.2397830000	-0.6285590000	2.3203460000
H	1.2030470000	0.7197790000	1.5854440000
H	0.0030330000	1.0521180000	2.8772530000
H	4.9106890000	1.9103790000	0.5188760000
H	4.0872760000	2.7289600000	-0.8170920000
H	5.2825880000	1.4751260000	-1.1476630000

Zero-point correction=  
(Hartree/Particle)

0.343776

Thermal correction to Energy=

0.363579

Thermal correction to Enthalpy=

0.364523

Thermal correction to Gibbs Free Energy=

0.295815

Sum of electronic and zero-point Energies=

-1188.066906

Sum of electronic and thermal Energies=

-1188.047103

Sum of electronic and thermal Enthalpies=

-1188.046159

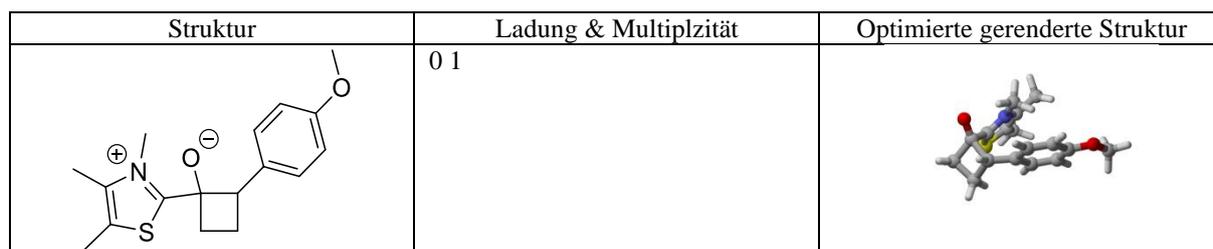
Sum of electronic and thermal Free Energies=

-1188.114867

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	228.149	76.709	144.608

#M062X/6-311+G\*\*

(41a-syn-syn)



42

XYZ file generated by gabedit : coordinates in Angstrom

H	-2.9216690000	-3.3451320000	-0.2010650000
H	-3.5446330000	-1.8381850000	-0.9028210000
C	-2.6401320000	-2.3622600000	-0.5794580000
S	-2.5794510000	0.6923440000	-0.8577970000
H	0.2951870000	-0.1345370000	-1.7956460000
C	-1.7363270000	-1.7184320000	0.5349800000
H	-1.3677280000	-1.5822120000	-2.2015190000
C	-1.4341780000	-2.4480210000	-1.5380510000
O	-1.8751750000	-1.9944770000	1.7933110000
H	-1.3403050000	-3.3484760000	-2.1450170000
C	-1.6794580000	-0.1822280000	0.3027180000
C	-2.2952890000	3.5113200000	-0.9833890000
C	-1.9157650000	2.2104470000	-0.3416850000
H	2.3921890000	1.1007960000	-1.6387230000
C	1.0626750000	-0.4994430000	-1.1192880000
C	-0.4902420000	-2.3390310000	-0.3286350000
N	-0.9548830000	0.6557660000	1.0319230000
C	-1.0575080000	2.0030900000	0.6835320000
H	-0.3308530000	-0.8128100000	2.3544100000
C	2.2575910000	0.2168750000	-1.0290010000
H	-0.5801230000	3.1267280000	2.4509130000
C	0.8307140000	-1.6489500000	-0.3645070000
H	-0.3859120000	-3.3233430000	0.1350420000
H	-0.1935120000	0.8630740000	2.9649390000
C	-0.0481840000	0.2112150000	2.1040690000
C	-0.2592390000	3.0339280000	1.4104610000
H	4.6864280000	1.3175320000	-1.8490250000
H	3.9998230000	2.3390630000	-0.5544010000
H	0.8028480000	2.7773910000	1.4045700000
C	4.7186440000	1.5429630000	-0.7780620000
H	0.9790470000	0.2807140000	1.7409030000
C	3.2627600000	-0.2276200000	-0.1710960000
H	-0.3841380000	4.0025890000	0.9279670000
C	1.8667490000	-2.0802300000	0.4787980000
H	5.7188940000	1.8750460000	-0.5085420000
O	4.4650540000	0.3914630000	-0.0053570000
H	1.7156800000	-2.9724670000	1.0773370000
C	3.0611400000	-1.3887040000	0.5788380000
H	3.8577010000	-1.7257370000	1.2312880000
H	-1.4314440000	3.9763410000	-1.4635060000
H	-2.6955290000	4.2083440000	-0.2445350000
H	-3.0592930000	3.3620120000	-1.7462480000

Zero-point correction=  
(Hartree/Particle)

0.349226

Thermal correction to Energy=

0.369840

Thermal correction to Enthalpy=

0.370784

Thermal correction to Gibbs Free Energy=

0.300415

Sum of electronic and zero-point Energies=

-1263.266424

Sum of electronic and thermal Energies=

-1263.245810

Sum of electronic and thermal Enthalpies=

-1263.244866

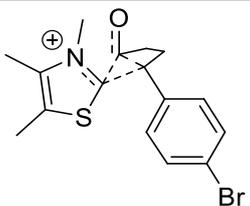
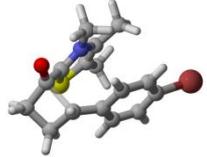
Sum of electronic and thermal Free Energies=

-1263.315235

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	232.078	79.761	148.104

#M062X/6-311+G\*\*

(42f-syn-syn)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.3869000000	3.8368240000	-2.0084150000
H	1.0304710000	3.6693090000	-0.9720640000
H	0.5810110000	2.6989800000	2.4823250000
C	0.2666430000	3.1144660000	-1.5153360000
S	-1.9404170000	1.4149030000	-1.1530920000
C	-0.5064970000	2.2306670000	-0.5911210000
H	-4.7860270000	-1.5038440000	-0.3243760000
C	-0.2429720000	1.8667110000	0.6816390000
H	-1.3154480000	1.4043270000	3.2316930000
H	-4.4310720000	0.0066150000	-1.1826340000
C	-2.1202780000	0.5657640000	0.3249840000
C	0.9138800000	2.2737830000	1.5331250000
H	0.7628990000	2.5212330000	-2.2879280000
N	-1.1831330000	0.9572280000	1.1904160000
C	-3.9847020000	-0.8687530000	-0.7000000000
O	-3.4532170000	-0.8476700000	1.7078080000
C	-3.0664280000	-0.5898140000	0.5265750000
H	1.5507230000	1.4107670000	1.7471710000
C	-1.1256420000	0.5338310000	2.6011690000
H	-1.9035350000	-0.2135090000	2.7498530000
H	1.5183360000	3.0165770000	1.0175120000
H	-0.3850230000	-1.0316840000	-2.4120950000
H	-0.1332330000	0.1349860000	2.8059130000
C	-2.9397810000	-1.6621050000	-1.5078020000
C	0.1310370000	-1.1588030000	-1.4683830000
H	1.9828700000	-0.3880510000	-2.2527220000
H	-3.2993210000	-2.5877360000	-1.9600780000
C	-2.0119330000	-1.8468580000	-0.3119090000
H	-2.4936500000	-1.0630280000	-2.3022800000
C	1.4707980000	-0.7939740000	-1.3889080000
C	-0.5556740000	-1.6762550000	-0.3583080000
H	-2.3246170000	-2.6619010000	0.3395000000
C	2.1501360000	-0.9525890000	-0.1894030000
C	0.1873840000	-1.8857150000	0.8174000000
H	-0.3128830000	-2.3162010000	1.6797720000
C	1.5227650000	-1.5226820000	0.9141910000
Br	3.9626790000	-0.3879320000	-0.0553850000
H	2.0735520000	-1.6797930000	1.8339390000

Zero-point correction=  
(Hartree/Particle)

0.305097

Thermal correction to Energy=

0.324318

Thermal correction to Enthalpy=

0.325262

Thermal correction to Gibbs Free Energy=

0.257420

Sum of electronic and zero-point Energies=

-3722.371401

Sum of electronic and thermal Energies=

-3722.352179

Sum of electronic and thermal Enthalpies=

-3722.351235

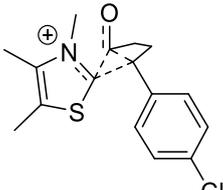
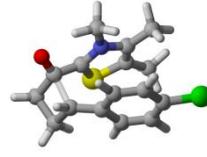
Sum of electronic and thermal Free Energies=

-3722.419078

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	203.513	74.019	142.787

#M062X/6-311+G\*\*

(42e-syn-syn)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	0.3713010000	3.7453790000	-2.0096850000
H	1.7445930000	3.5350830000	-0.9241000000
H	1.3201090000	2.4683660000	2.5035580000
C	0.9709060000	3.0043710000	-1.4777700000
S	-1.3837190000	1.5128700000	-1.1144220000
C	0.1248680000	2.1852630000	-0.5575910000
H	-4.4460510000	-1.1885200000	-0.3158290000
C	0.3713160000	1.7724340000	0.7034190000
H	-0.7092270000	1.3684060000	3.2578180000
H	-3.9795330000	0.3078620000	-1.1450080000
C	-1.6185580000	0.6507320000	0.3488860000
C	1.5829200000	2.0387960000	1.5346860000
H	1.4589030000	2.3656950000	-2.2191240000
N	-0.6413490000	0.9430520000	1.2093680000
C	-3.5999950000	-0.6103180000	-0.6853780000
O	-3.0445280000	-0.6856470000	1.7172180000
C	-2.6502320000	-0.4328810000	0.5369230000
H	2.1342560000	1.1091510000	1.7062870000
C	-0.6065440000	0.4938720000	2.6127570000
H	-1.4461470000	-0.1838440000	2.7606970000
H	2.2464670000	2.7305180000	1.0202140000
H	-0.0416740000	-1.0038980000	-2.4343380000
H	0.3486100000	0.0052580000	2.7993790000
C	-2.6273900000	-1.4657580000	-1.5203380000
C	0.4723360000	-1.1949920000	-1.5004130000
H	2.3750730000	-0.5455690000	-2.2810970000
H	-3.0615220000	-2.3504480000	-1.9886400000
C	-1.7072960000	-1.7473420000	-0.3374320000
H	-2.1393710000	-0.8870340000	-2.3053810000
C	1.8359880000	-0.9321530000	-1.4245130000
C	-0.2419180000	-1.6882970000	-0.3968500000
H	-2.0746150000	-2.5508420000	0.2996500000
C	2.5094990000	-1.1672070000	-0.2350200000
C	0.4924310000	-1.9821890000	0.7663900000
H	-0.0317040000	-2.3964440000	1.6224300000
C	1.8508910000	-1.7191070000	0.8589280000
Cl	4.2094040000	-0.7732630000	-0.1086310000
H	2.4004790000	-1.9371010000	1.7672260000

Zero-point correction=  
(Hartree/Particle)

0.305900

Thermal correction to Energy=

0.324671

Thermal correction to Enthalpy=

0.325616

Thermal correction to Gibbs Free Energy=

0.259664

Sum of electronic and zero-point Energies=

-1608.398716

Sum of electronic and thermal Energies=

-1608.379945

Sum of electronic and thermal Enthalpies=

-1608.379000

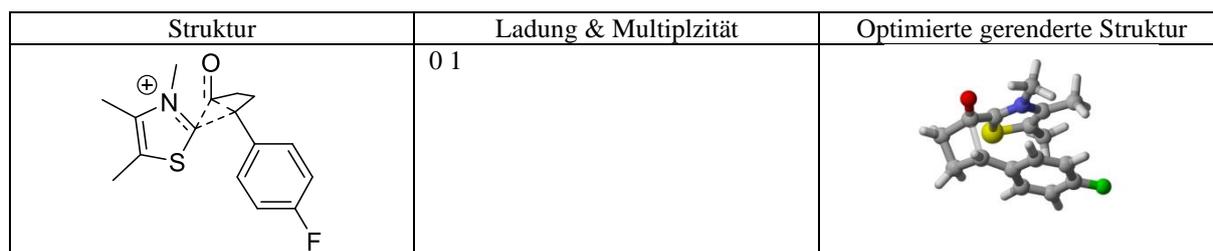
Sum of electronic and thermal Free Energies=

-1608.444952

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	203.734	73.419	138.806

#M062X/6-311+G\*\*

(42d-syn-syn)



38

XYZ file generated by gabedit : coordinates in Angstrom

H	1.8347520000	2.1841000000	-2.2620760000
H	-3.7220090000	0.4822630000	-1.1796680000
C	1.3932830000	2.8648310000	-1.5290630000
H	2.2021820000	3.3500600000	-0.9840550000
H	0.8446530000	3.6377660000	-2.0708210000
S	-1.0516830000	1.5333010000	-1.1512830000
C	0.4942320000	2.1199170000	-0.5963730000
H	-1.9318770000	-0.8244010000	-2.2889720000
C	-3.3924760000	-0.4408470000	-0.6922540000
H	-4.2696450000	-0.9685010000	-0.3196310000
C	-2.4543190000	-1.3616760000	-1.4965360000
H	-2.9278740000	-2.2334050000	-1.9512980000
C	-1.3517330000	0.7219200000	0.3318430000
C	0.7043060000	1.7231490000	0.6755920000
H	0.1564210000	-1.0824120000	-2.4134650000
C	-2.4563200000	-0.2707250000	0.5384680000
H	2.6338750000	2.5680180000	0.9822170000
N	-0.3622860000	0.9730390000	1.1945840000
O	-2.8774670000	-0.4786770000	1.7160380000
C	-1.5556580000	-1.6653160000	-0.3044890000
C	1.9204940000	1.9422260000	1.5139480000
C	0.6583270000	-1.2976790000	-1.4782660000
H	1.6755670000	2.4279230000	2.4607290000
H	2.6230880000	-0.8471450000	-2.2741820000
H	-1.9766580000	-2.4208890000	0.3575470000
H	-0.3993460000	1.4498930000	3.2332640000
C	-0.0891410000	-1.7084540000	-0.3623880000
C	2.0419500000	-1.1592860000	-1.4146450000
C	-0.3663970000	0.5562460000	2.6074430000
H	2.4065380000	0.9869170000	1.7320450000
H	-1.2577820000	-0.0482790000	2.7682040000
H	0.5443630000	-0.0051870000	2.8114120000
C	0.6208140000	-2.0335130000	0.8079960000
C	2.6856770000	-1.4403930000	-0.2247270000
H	0.0640060000	-2.3783820000	1.6740250000
C	1.9992480000	-1.8965690000	0.8893590000
F	4.0246200000	-1.2858990000	-0.1479940000
H	2.5471130000	-2.1429130000	1.7913710000

Zero-point correction=  
(Hartree/Particle)

0.307907

Thermal correction to Energy=

0.326171

Thermal correction to Enthalpy=

0.327115

Thermal correction to Gibbs Free Energy=

0.263087

Sum of electronic and zero-point Energies=

-1248.035797

Sum of electronic and thermal Energies=

-1248.017534

Sum of electronic and thermal Enthalpies=

-1248.016589

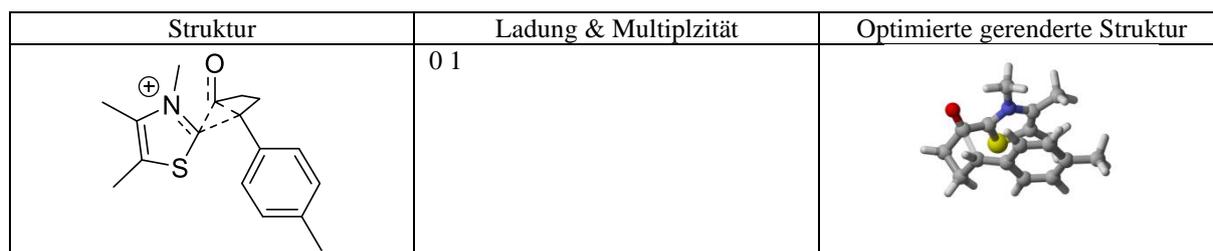
Sum of electronic and thermal Free Energies=

-1248.080618

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.675	72.421	134.759

#M062X/6-311+G\*\*

(42b-syn-syn)



41

XYZ file generated by gabedit : coordinates in Angstrom

H	0.1485700000	-1.0222070000	-2.4183260000
H	-1.9454390000	-0.8231360000	-2.3005630000
H	1.7827060000	2.2229070000	-2.2301850000
H	2.5800070000	-0.7514610000	-2.2841130000
H	0.7743210000	3.6638450000	-2.0357220000
H	-2.9227330000	-2.2490290000	-1.9786720000
C	1.3310920000	2.8955710000	-1.4956680000
C	-2.4606820000	-1.3761430000	-1.5143910000
C	0.6531490000	-1.2548380000	-1.4881050000
C	2.0342750000	-1.0989010000	-1.4113980000
H	-3.7508840000	0.4481280000	-1.1686650000
S	-1.1014930000	1.5384860000	-1.1275290000
H	2.1318120000	3.3891830000	-0.9458420000
C	-3.4095500000	-0.4787210000	-0.6964100000
C	0.4395880000	2.1336770000	-0.5696700000
C	-0.0894270000	-1.7001840000	-0.3846020000
H	-4.2797930000	-1.0223500000	-0.3304830000
C	-1.5577220000	-1.6813050000	-0.3247430000
C	2.7352160000	-1.3849700000	-0.2412170000
C	4.2321760000	-1.2284950000	-0.1628210000
C	-1.3849260000	0.6984760000	0.3423600000
H	-1.9648350000	-2.4574700000	0.3223680000
C	-2.4702390000	-0.3202920000	0.5345790000
C	0.6595540000	1.7178490000	0.6943810000
C	0.6306630000	-2.0343310000	0.7766010000
C	2.0056060000	-1.8719090000	0.8487290000
H	2.5859750000	2.5686710000	1.0036850000
N	-0.3959280000	0.9480490000	1.2052190000
C	1.8797890000	1.9288170000	1.5286350000
H	0.0818480000	-2.4022210000	1.6389590000
O	-2.8883590000	-0.5484650000	1.7116530000
H	2.3691860000	0.9699230000	1.7232170000
H	2.5290090000	-2.1308020000	1.7653440000
H	1.6391530000	2.3946610000	2.4864960000
C	-0.3883460000	0.5044480000	2.6098330000
H	-1.2703100000	-0.1165530000	2.7613730000
H	0.5312090000	-0.0476620000	2.7985970000
H	-0.4325890000	1.3859420000	3.2522300000
H	4.5412420000	-0.8545930000	0.8162020000
H	4.5972960000	-0.5354690000	-0.9228740000
H	4.7352020000	-2.1872020000	-0.3188670000

Zero-point correction=

0.343237

(Hartree/Particle)

Thermal correction to Energy=

0.362547

Thermal correction to Enthalpy=

0.363491

Thermal correction to Gibbs Free Energy=

0.296983

Sum of electronic and zero-point Energies=

-1188.064908

Sum of electronic and thermal Energies=

-1188.045598

Sum of electronic and thermal Enthalpies=

-1188.044653

Sum of electronic and thermal Free Energies=

-1188.111162

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	227.502	75.599	139.979

#M062X/6-311+G\*\*

(42a-syn-syn)



42

XYZ file generated by gabedit : coordinates in Angstrom

H	-4.4195950000	-1.2354650000	-0.5954360000
H	-3.8665710000	0.1862680000	-1.5000910000
C	-3.5389190000	-0.6832960000	-0.9211720000
S	-1.2826040000	1.4048300000	-1.2971640000
H	0.1810700000	-1.2340100000	-2.2749600000
C	-2.7288700000	-0.3855100000	0.3747510000
H	-1.9182070000	-1.0831470000	-2.3500760000
C	-2.4788930000	-1.5962090000	-1.5680550000
O	-3.2491420000	-0.5472580000	1.5234050000
H	-2.8556440000	-2.5280260000	-1.9932920000
C	-1.6789030000	0.6732750000	0.2041400000
C	1.1185360000	2.8477870000	-1.5393390000
C	0.1707190000	2.1153830000	-0.6456690000
H	2.5621370000	-0.8168940000	-1.9878940000
C	0.6060490000	-1.3357430000	-1.2833940000
C	-1.6807550000	-1.7518850000	-0.2784280000
N	-0.7927110000	1.0404580000	1.1347210000
C	0.2781200000	1.8153580000	0.6650350000
H	-1.7754330000	0.0648300000	2.6829530000
C	1.9719530000	-1.0927650000	-1.1234050000
H	1.0350170000	2.6817980000	2.4819340000
C	-0.2121380000	-1.6984770000	-0.2098740000
H	-2.1087000000	-2.4980160000	0.3905510000
H	-1.0479270000	1.6391310000	3.1246700000
C	-0.9069880000	0.7120840000	2.5659590000
C	1.3956010000	2.1578140000	1.5943050000
H	4.7413880000	-1.3003480000	-1.4400240000
H	4.3212600000	0.3978990000	-1.0775870000
H	1.9096190000	1.2476000000	1.9163410000
C	4.6856570000	-0.5435260000	-0.6508630000
H	0.0104230000	0.2200640000	2.8868730000
C	2.5527020000	-1.2157640000	0.1354040000
H	2.1201840000	2.7943000000	1.0906090000
C	0.4174900000	-1.8731880000	1.0390360000
H	5.6763450000	-0.3901480000	-0.2281090000
O	3.8651760000	-0.9711090000	0.4131530000
H	-0.1880940000	-2.1832510000	1.8858880000
C	1.7665190000	-1.6324620000	1.2154400000
H	2.2438760000	-1.7648230000	2.1801220000
H	1.8201690000	3.4431500000	-0.9556410000
H	0.5842800000	3.5242790000	-2.2092890000
H	1.6895070000	2.1440150000	-2.1516470000

Zero-point correction=  
(Hartree/Particle)

0.348501

Thermal correction to Energy=

0.368882

Thermal correction to Enthalpy=

0.369826

Thermal correction to Gibbs Free Energy=

0.300134

Sum of electronic and zero-point Energies=

-1263.265351

Sum of electronic and thermal Energies=

-1263.244971

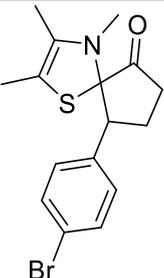
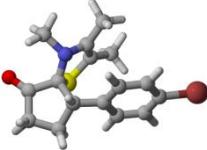
Sum of electronic and thermal Enthalpies=

-1263.244027

Sum of electronic and thermal Free Energies=

-1263.313719

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	231.477	78.686	146.679

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.3552490000	2.3298870000	-3.0257930000
H	0.6385470000	2.9245680000	-1.6923350000
H	-0.9862410000	3.7493820000	1.1511880000
C	0.1286750000	2.0464800000	-2.0870890000
S	-1.9579240000	0.2160980000	-1.6753620000
C	-0.8770610000	1.5199510000	-1.1167750000
H	-3.9392830000	-2.6708090000	1.0853250000
C	-1.0798150000	1.8314520000	0.1675210000
H	-3.7891730000	2.2998560000	0.5520130000
H	-4.1915030000	-2.7458380000	-0.6554160000
C	-2.3145410000	-0.1623260000	0.1150890000
C	-0.3561670000	2.8767820000	0.9583000000
H	0.8763020000	1.2802820000	-2.3136960000
N	-2.0661530000	1.0588510000	0.8533570000
C	-3.5637060000	-2.3097560000	0.1220370000
O	-4.7622650000	-0.2022470000	0.1290630000
C	-3.7209690000	-0.7943080000	0.1286990000
H	-0.0495120000	2.4616460000	1.9219350000
C	-3.1976740000	1.8480650000	1.3552350000
H	-3.8483750000	1.2230770000	1.9625580000
H	0.5348780000	3.2163950000	0.4330060000
H	0.2399440000	-1.9633600000	-1.4884440000
H	-2.7936980000	2.6332480000	1.9948050000
C	-2.0598940000	-2.5702720000	-0.0235780000
C	0.7499590000	-1.4696780000	-0.6708720000
H	2.6381180000	-1.4377530000	-1.7091960000
H	-1.7347690000	-3.4930320000	0.4568990000
C	-1.4312140000	-1.3340470000	0.6286850000
H	-1.7876410000	-2.6242430000	-1.0798590000
C	2.1020600000	-1.1696900000	-0.8076090000
C	0.0504710000	-1.1220530000	0.4854410000
H	-1.6567560000	-1.3718080000	1.7035050000
C	2.7587230000	-0.5171410000	0.2261650000
C	0.7482380000	-0.4946620000	1.5203150000
H	0.2168800000	-0.2242460000	2.4269190000
C	2.0960640000	-0.1828000000	1.4001080000
Br	4.6014670000	-0.0893710000	0.0417880000
H	2.6252580000	0.3131820000	2.2037760000

Zero-point correction=  
(Hartree/Particle)

0.307977

Thermal correction to Energy=

0.327620

Thermal correction to Enthalpy=

0.328564

Thermal correction to Gibbs Free Energy=

0.258823

Sum of electronic and zero-point Energies=

-3722.427868

Sum of electronic and thermal Energies=

-3722.408225

Sum of electronic and thermal Enthalpies=

-3722.407281

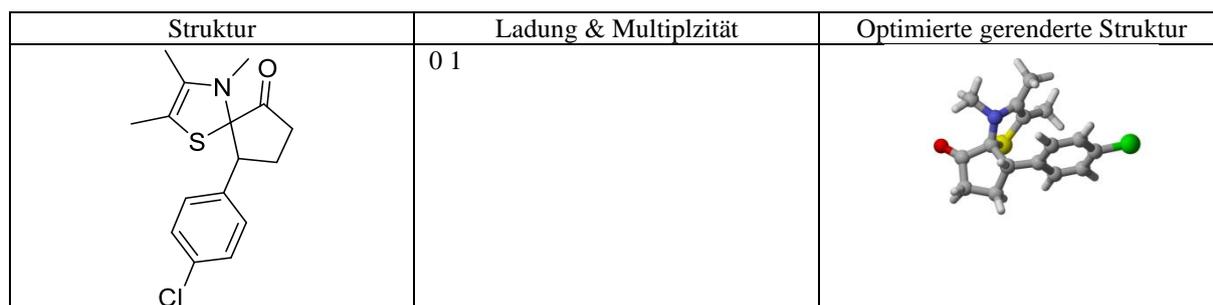
Sum of electronic and thermal Free Energies=

-3722.477022

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	205.585	74.450	146.782

#M062X/6-311+G\*\*

(38e-s)



38

XYZ file generated by gabedit : coordinates in Angstrom

H	0.2101790000	2.3194330000	-3.0166170000
H	1.2031510000	2.9022680000	-1.6773390000
H	-0.4297640000	3.7401650000	1.1639440000
C	0.6860700000	2.0300180000	-2.0756350000
S	-1.4214760000	0.2209190000	-1.6760460000
C	-0.3304430000	1.5134530000	-1.1111650000
H	-3.4369430000	-2.6478230000	1.0821850000
C	-0.5371790000	1.8272350000	0.1718890000
H	-3.2434720000	2.3223070000	0.5137010000
H	-3.6825490000	-2.7269290000	-0.6593690000
C	-1.7906320000	-0.1538000000	0.1130810000
C	0.1937030000	2.8635990000	0.9676320000
H	1.4265150000	1.2560440000	-2.2989910000
N	-1.5379970000	1.0665740000	0.8515660000
C	-3.0548950000	-2.2926980000	0.1192380000
O	-4.2390230000	-0.1774700000	0.1113830000
C	-3.2015560000	-0.7762300000	0.1200590000
H	0.4960190000	2.4419180000	1.9298180000
C	-2.6689190000	1.8718220000	1.3299080000
H	-3.3348400000	1.2591060000	1.9330680000
H	1.0877740000	3.1989090000	0.4447590000
H	0.7537550000	-1.9790460000	-1.4774900000
H	-2.2662200000	2.6586650000	1.9681550000
C	-1.5525120000	-2.5639990000	-0.0190490000
C	1.2659620000	-1.4879030000	-0.6598950000
H	3.1607660000	-1.4720830000	-1.6910500000
H	-1.2358590000	-3.4875950000	0.4654780000
C	-0.9175420000	-1.3305950000	0.6325450000
H	-1.2762020000	-2.6229960000	-1.0739980000
C	2.6203160000	-1.1993660000	-0.7933080000
C	0.5664930000	-1.1316490000	0.4939060000
H	-1.1473170000	-1.3640810000	1.7065920000
C	3.2798290000	-0.5496160000	0.2397870000
C	1.2671000000	-0.5081170000	1.5292810000
H	0.7356000000	-0.2316470000	2.4339380000
C	2.6174580000	-0.2076960000	1.4112520000
Cl	4.9758160000	-0.1682490000	0.0698840000
H	3.1527740000	0.2859050000	2.2127460000

Zero-point correction=  
(Hartree/Particle)

0.308481

Thermal correction to Energy=

0.327900

Thermal correction to Enthalpy=

0.328844

Thermal correction to Gibbs Free Energy=

0.260250

Sum of electronic and zero-point Energies=

-1608.455738

Sum of electronic and thermal Energies=

-1608.436318

Sum of electronic and thermal Enthalpies=

-1608.435374

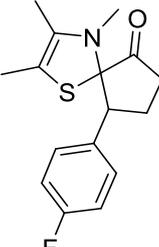
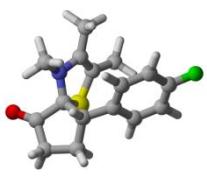
Sum of electronic and thermal Free Energies=

-1608.503968

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	205.760	74.066	144.368

#M062X/6-311+G\*\*

(38d-s)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

38

XYZ file generated by gabedit : coordinates in Angstrom

```

H      -0.4978290000      2.5394560000      3.0164360000
H      -1.5217550000      3.0072560000      1.6573870000
H      0.3459460000      3.7502940000     -1.2517170000
C      -0.9762560000      2.1748750000      2.1023030000
S       1.1096230000      0.3203840000      1.7340860000
C       0.0308610000      1.6230830000      1.1507240000
H       3.3743410000     -2.5744180000     -0.7891160000
C       0.2991970000      1.9260420000     -0.1252660000
H       1.7181420000      2.2809550000     -2.4244460000
H       3.4714680000     -2.4724460000      0.9643610000
C       1.5318710000     -0.0786770000     -0.0172270000
C      -0.3661950000      2.9749380000     -0.9555240000
H      -1.6996790000      1.4048770000      2.3881240000
N       1.3426740000      1.1726200000     -0.7007690000
C       2.8952240000     -2.1473270000      0.0966960000
O       3.9564350000      0.0199310000     -0.2077310000
C       2.9666330000     -0.6315970000     -0.0396630000
H      -0.7881770000      2.5386970000     -1.8660120000
C       1.6595240000      1.2385770000     -2.1132910000
H       2.6454190000      0.7994980000     -2.2720840000
H      -1.1726860000      3.4500680000     -0.4012200000
H      -0.9510520000     -1.9191580000      1.5701240000
H       0.9330330000      0.7253870000     -2.7584170000
C       1.3966620000     -2.4839120000      0.1613210000
C      -1.4729520000     -1.4903600000      0.7250400000
H      -3.3909450000     -1.5006660000      1.7301480000
H       1.1519060000     -3.4360240000     -0.3094250000
C       0.7196040000     -1.3028250000     -0.5507840000
H       1.0672970000     -2.5292040000      1.2013790000
C      -2.8391840000     -1.2540340000      0.8316780000
C      -0.7742910000     -1.1628300000     -0.4396260000
H       0.9723260000     -1.3753510000     -1.6184710000
C      -3.5022110000     -0.6885740000     -0.2415930000
C      -1.4908600000     -0.6212510000     -1.5094070000
H      -0.9724280000     -0.3821960000     -2.4320530000
C      -2.8553570000     -0.3739690000     -1.4225410000
F      -4.8230460000     -0.4515080000     -0.1393020000
H      -3.4156850000      0.0496670000     -2.2464710000

```

Zero-point correction=

0.309690

(Hartree/Particle)

```

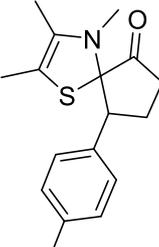
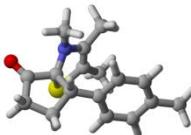
Thermal correction to Energy=      0.328690
Thermal correction to Enthalpy=    0.329635
Thermal correction to Gibbs Free Energy= 0.263111
Sum of electronic and zero-point Energies= -1248.095702
Sum of electronic and thermal Energies= -1248.076702
Sum of electronic and thermal Enthalpies= -1248.075758
Sum of electronic and thermal Free Energies= -1248.142282

```

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	206.256	73.362	140.011

#M062X/6-311+G\*\*

(38b-s)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

41

XYZ file generated by gabedit : coordinates in Angstrom

```

H      -0.9316700000      -1.9097040000      1.5704940000
H      1.0934150000      -2.5253290000      1.2008300000
H     -1.6958620000      1.3697720000      2.3595440000
H     -3.3424740000     -1.5097430000      1.7266080000
H     -0.5086760000      2.4990020000      3.0271210000
H      1.1819840000     -3.4315640000     -0.3099770000
C     -0.9717660000      2.1486430000      2.0996050000
C      1.4251730000     -2.4794580000      0.1616270000
C     -1.4519110000     -1.4873960000      0.7203860000
C     -2.8179520000     -1.2533210000      0.8110450000
H      3.4992010000     -2.4627820000      0.9679070000
S      1.1400480000      0.3223770000      1.7358450000
H     -1.5133540000      2.9869840000      1.6608740000
C      2.9235600000     -2.1412930000      0.0983880000
C      0.0508030000      1.6164850000      1.1536040000
C     -0.7477370000     -1.1628980000     -0.4426420000
H      3.4047980000     -2.5701040000     -0.7854520000
C      0.7468620000     -1.2992320000     -0.5509870000
C     -3.5318850000     -0.6921640000     -0.2493920000
C     -5.0107840000     -0.4314400000     -0.1252470000
C      1.5583750000     -0.0751190000     -0.0172590000
H      1.0012860000     -1.3709330000     -1.6185170000
C      2.9932580000     -0.6257920000     -0.0422430000
C      0.3158310000      1.9217560000     -0.1223260000
C     -1.4677400000     -0.6323850000     -1.5127780000
C     -2.8348190000     -0.3949130000     -1.4183690000
H     -1.1691860000      3.4328630000     -0.3967270000
N      1.3662920000      1.1778580000     -0.6978780000
C     -0.3645330000      2.9590130000     -0.9548420000
H     -0.9515640000     -0.3959890000     -2.4381370000
O      3.9825970000      0.0257090000     -0.2153630000
H     -0.7921830000      2.5104270000     -1.8567050000
H     -3.3662160000      0.0242470000     -2.2667470000
H      0.3387520000      3.7371010000     -1.2646920000
C      1.6745980000      1.2429230000     -2.1125030000
H      2.6594480000      0.8033530000     -2.2764590000
H      0.9436270000      0.7295840000     -2.7520220000
H      1.7320340000      2.2852420000     -2.4243960000
H     -5.4224490000     -0.0425210000     -1.0574340000
H     -5.2121110000      0.2978850000      0.6636510000
H     -5.5503760000     -1.3469470000      0.1283530000

```

Zero-point correction=

0.345176

(Hartree/Particle)

Thermal correction to Energy=

0.365315

Thermal correction to Enthalpy=

0.366259

Thermal correction to Gibbs Free Energy=

0.296078

Sum of electronic and zero-point Energies=

-1188.124718

Sum of electronic and thermal Energies=

-1188.104579

Sum of electronic and thermal Enthalpies=

-1188.103635

Sum of electronic and thermal Free Energies=

-1188.173816

E (Thermal)

CV

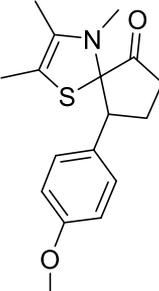
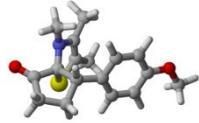
S

KCal/Mol  
229.239Cal/Mol-Kelvin  
76.536Cal/Mol-Kelvin  
147.709

Total

#M062X/6-311+G\*\*

(38a-s)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

42

XYZ file generated by gabedit : coordinates in Angstrom

```

H      -3.5927680000    -2.6741340000     0.7308110000
H      -3.5930500000    -2.6386780000    -1.0279410000
C      -3.0823510000    -2.2572460000    -0.1423730000
S      -1.3151170000     0.2326690000    -1.7668270000
H       0.8430810000    -1.9163840000    -1.3961480000
C      -3.2268790000    -0.7424900000    -0.0665040000
H      -1.1791840000    -2.5948340000    -1.1272280000
C      -1.5695700000    -2.5271230000    -0.1098560000
O      -4.2528070000    -0.1317630000     0.0226800000
H      -1.3107160000    -3.4497230000     0.4096370000
C      -1.8180390000    -0.1268280000    -0.0283970000
C       0.7048440000     2.1680560000    -2.0840730000
C      -0.3327680000     1.6047980000    -1.1731410000
H       3.2243330000    -1.4123970000    -1.4574540000
C       1.2905170000    -1.4303710000    -0.5386360000
C      -0.9844300000    -1.2928800000     0.5929310000
N      -1.7236250000     1.1545600000     0.6191180000
C      -0.6840690000     1.9359190000     0.0754730000
H      -3.0827500000     0.7533220000     2.1340240000
C       2.6533010000    -1.1342740000    -0.5816570000
H      -0.8689810000     3.7892640000     1.1387620000
C       0.5063500000    -1.0921270000     0.5598300000
H      -1.2943120000    -1.3384850000     1.6473740000
H      -2.2709930000     2.3014420000     2.2703230000
C      -2.1220080000     1.2542490000     2.0086630000
C      -0.1101150000     3.0364650000     0.9071550000
H       5.4099490000    -1.5161490000    -0.7599620000
H       5.0061310000     0.0760190000    -1.4640960000
H       0.2777750000     2.6440480000     1.8520500000
C       5.3724060000    -0.4387930000    -0.5698520000
H      -1.3994780000     0.8204600000     2.7134190000
C       3.2540520000    -0.4867990000     0.4949610000
H       0.7071200000     3.5284190000     0.3839260000
C       1.1393210000    -0.4656710000     1.6408100000
H       6.3704720000    -0.0796720000    -0.3289950000
O       4.5686480000    -0.1454080000     0.5527940000
H       0.5581910000    -0.2066250000     2.5205260000
C       2.4877860000    -0.1612350000     1.6168200000
H       2.9754050000     0.3258270000     2.4525980000
H       1.1903030000     3.0353660000    -1.6360850000
H       0.2666060000     2.4844930000    -3.0357160000
H       1.4732970000     1.4192660000    -2.3011450000

```

Zero-point correction=  
(Hartree/Particle)

0.350978

Thermal correction to Energy=

0.371709

Thermal correction to Enthalpy=

0.372653

Thermal correction to Gibbs Free Energy=

0.302035

Sum of electronic and zero-point Energies=

-1263.325055

Sum of electronic and thermal Energies=

-1263.304324

Sum of electronic and thermal Enthalpies=

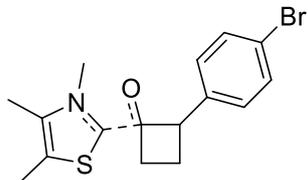
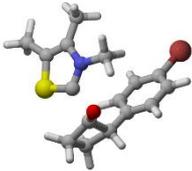
-1263.303380

Sum of electronic and thermal Free Energies=

-1263.373998

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.251	79.427	148.628

Substituierte TSs mit PCM-Lösungsmittelleffekten:

#M062X/6-311+G**	(40f-syn-syn)	
Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 scrf=(pcm,solvent=2-propanol)	

38

H	-1.7852540272	4.7077572063	-1.3194870653
H	-0.1187381534	4.7065760616	-0.7391746277
H	0.0644521053	3.1686629139	2.3979131816
C	-0.8648717161	4.1221073135	-1.2761803318
S	-2.2413566889	1.6463794883	-1.2272281561
C	-1.1008315372	2.8101739844	-0.5980751079
H	-4.7553027538	-2.0484722747	-0.6759820581
C	-0.5469367095	2.3082076927	0.5289240675
H	-0.5300396447	0.9348248785	2.8697913390
H	-4.3641737311	-0.3576092401	-1.0685060870
C	-1.9573247486	0.5007916669	0.0162564580
C	0.4822226928	2.9291741552	1.4168984818
H	-0.5119562349	3.9746027333	-2.2985799583
N	-1.0596511967	1.0335703630	0.8391318617
C	-3.9441032582	-1.3241097331	-0.7952176264
O	-3.2972317468	-1.39111110930	1.6393618274
C	-3.0372532697	-1.4101587092	0.4460982579
H	1.3278971153	2.2538562844	1.5656286702
C	-0.5565057017	0.2844744166	1.9963589556
H	-1.2307032833	-0.5479187672	2.1762552344
H	0.8577630814	3.8494135332	0.9744079640
H	-0.1883791640	-0.8467875030	-1.7440170997
H	0.4480199839	-0.0852450065	1.7794977057
C	-2.7768798979	-1.8986072510	-1.6393481485
C	0.2398399643	-1.4100388431	-0.9236024637
H	2.2148342942	-0.6273800624	-1.2742308735
H	-3.0325319606	-2.7079829118	-2.3210586385
C	-2.0494061712	-2.3324681270	-0.3436765210
H	-2.2481952938	-1.1231620094	-2.1903023494
C	1.5995557269	-1.2751062195	-0.6626784507
C	-0.5692873315	-2.2400803499	-0.1444882707
H	-2.3809308334	-3.3438067750	-0.0767091216
C	2.1570236709	-1.9855499179	0.3929077965
C	0.0292248024	-2.9549601302	0.8974620468
H	-0.5771475051	-3.6150839383	1.5089472571
C	1.3867981263	-2.8326832925	1.1779077792
Br	4.0164495222	-1.7937844707	0.7610734703
H	1.8347454731	-3.3871420657	1.9925816011

Zero-point correction= 0.304882  
(Hartree/Particle)

Thermal correction to Energy= 0.324498

Thermal correction to Enthalpy= 0.325442

Thermal correction to Gibbs Free Energy= 0.254814

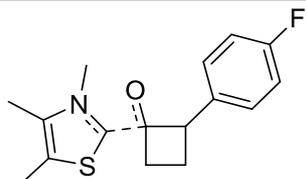
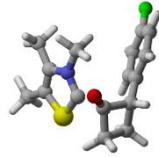
Sum of electronic and zero-point Energies= -3722.379158

Sum of electronic and thermal Energies= -3722.359543

Sum of electronic and thermal Enthalpies= -3722.358598

Sum of electronic and thermal Free Energies= -3722.429227

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	203.625	74.124	148.649

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 scrf=(pcm,solvent=2-propanol)	

38

H	-4.3276829485	2.8954307931	-0.9206487346
H	-2.6552951089	-2.4923659451	-0.4171548813
C	-3.2701264464	3.1093917953	-1.0869301568
H	-3.1014277754	3.1521028726	-2.1647704258
H	-3.0554916838	4.0924293406	-0.6693204015
S	-2.5342864549	0.3792746777	-0.9029934179
C	-2.4097761352	2.0630667415	-0.4529044612
H	-0.8378959066	-1.7291045866	-1.9809941226
C	-1.6486926923	-2.8877586137	-0.2904567153
H	-1.7087720828	-3.9531743400	-0.0487688300
C	-0.5874709534	-2.6049599433	-1.3855043330
H	-0.3519634527	-3.4336749824	-2.0511345953
C	-1.3148310916	-0.1364277382	0.1862163311
C	-1.4638843219	2.1862030577	0.5056857194
H	0.5439575822	-0.1001990704	-1.9432842684
C	-0.7126923845	-2.2172801315	0.7320609447
H	-1.4603630992	4.3037295072	0.7581794546
N	-0.8919594404	0.9421689505	0.8374657065
O	-0.6911553533	-2.2539929482	1.9533943252
C	0.4667631085	-2.3139521462	-0.2896533731
C	-0.9983724457	3.4241181646	1.2012322502
C	1.3853797464	-0.1572105307	-1.2629893034
H	-1.2578326192	3.4019508344	2.2624024240
H	2.2388191041	1.7103692332	-1.9518408298
H	0.9564223371	-3.2580352761	-0.0184791970
H	-0.0813041599	1.4102647769	2.7176561940
C	1.5065152968	-1.2408749564	-0.3888786234
C	2.3254971820	0.8687669481	-1.2756205129
C	0.1913054565	0.8518235855	1.8229938793
H	0.0855732078	3.5331998952	1.1205656739
H	0.3319238794	-0.1962935317	2.0698997249
H	1.1084136030	1.2629132755	1.3954781896
C	2.6111019321	-1.2791264239	0.4684055700
C	3.3932799908	0.7943139488	-0.3994698788
H	2.7277598561	-2.1165319796	1.1483239610
C	3.5610357672	-0.2629186693	0.4757420614
F	4.3107137586	1.7877655985	-0.4036772794
H	4.4163427479	-0.2853501838	1.1395589321

Zero-point correction=  
(Hartree/Particle)

0.307533

Thermal correction to Energy=

0.326209

Thermal correction to Enthalpy=

0.327153

Thermal correction to Gibbs Free Energy=

0.260610

Sum of electronic and zero-point Energies=

-1248.045455

Sum of electronic and thermal Energies=

-1248.026779

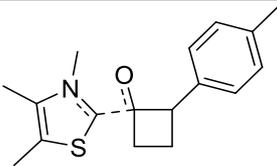
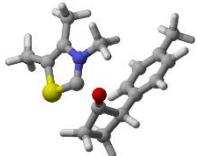
Sum of electronic and thermal Enthalpies=

-1248.025835

Sum of electronic and thermal Free Energies=

-1248.092377

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.699	72.573	140.051

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 scrf=(pcm,solvent=2-propanol)	

41

H	0.3884808705	-0.0888691349	-1.9237858551
H	-1.0661291510	-1.6748829022	-1.9345463979
H	-2.7447767962	4.2512451007	-0.6160263908
H	2.1369543753	1.6295336270	-1.9735850956
H	-2.9526726529	3.2774480137	-2.0754744536
H	-0.6588642215	-3.3974098944	-2.0451184897
C	-3.0727316792	3.2822170818	-0.9903625921
C	-0.8295627164	-2.5683817268	-1.3601229867
C	1.2585243245	-0.2034394008	-1.2866724589
C	2.2485680293	0.7764011511	-1.3115976881
H	-2.8450823468	-2.3797663016	-0.2975054401
S	-2.5879274461	0.5008982961	-0.7568768916
H	-4.1368695299	3.1767466229	-0.7702120346
C	-1.8527318896	-2.8218824566	-0.2222984828
C	-2.2873254000	2.1754488021	-0.3620183813
C	1.3662744427	-1.3106888711	-0.4442236388
H	-1.9505700899	-3.8875380627	0.0058439811
C	0.2838441994	-2.3372465310	-0.3096662585
C	3.3808747370	0.6824729270	-0.5014982979
C	4.4593741712	1.7345998975	-0.5326298041
C	-1.3711428568	-0.0993842961	0.2913241911
H	0.7430815533	-3.3058742334	-0.0727281707
C	-0.8426100820	-2.2106114904	0.7677107669
C	-1.2910501818	2.2327843209	0.5515068588
C	2.5105194329	-1.4130019854	0.3549832902
C	3.4958654528	-0.4335209999	0.3318790652
H	-1.0812664659	4.3459158758	0.7376624537
N	-0.8246991416	0.9500473107	0.8961740694
C	-0.6788246359	3.4396323562	1.1851678430
H	2.6209419763	-2.2696101434	1.0128150754
O	-0.7650175557	-2.2826265829	1.9863469387
H	0.4049153866	3.4435222499	1.0478513613
H	4.3679565380	-0.5340925032	0.9707659310
H	-0.8837535580	3.4706347047	2.2579304712
C	0.2917130188	0.7841259129	1.8341974293
H	0.3473928618	-0.2668169634	2.1025158751
H	1.2202544280	1.0950872899	1.3503940292
H	0.1136199620	1.3865783985	2.7242717656
H	4.1353751590	2.6145341709	-1.0896138314
H	5.3645242864	1.3484526477	-1.0090831467
H	4.7307811914	2.0475977227	0.4778893910

Zero-point correction=  
(Hartree/Particle)

0.342283

Thermal correction to Energy=

0.361457

Thermal correction to Enthalpy=

0.362401

Thermal correction to Gibbs Free Energy=

0.294360

Sum of electronic and zero-point Energies=

-1188.074746

Sum of electronic and thermal Energies=

-1188.055572

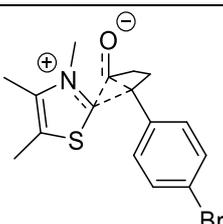
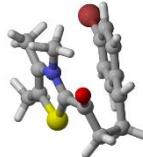
Sum of electronic and thermal Enthalpies=

-1188.054628

Sum of electronic and thermal Free Energies=

-1188.122669

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	226.818	73.998	143.204

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 scrf=(pcm,solvent=2-propanol)	

38

H	-0.3012127914	3.7014550301	-2.0547035016
H	1.0525756710	3.6160526816	-0.9261833085
H	0.5474418297	2.6317447114	2.5385412529
C	0.3304077978	3.0199743907	-1.4823565646
S	-1.9401703025	1.4066934813	-1.1383637240
C	-0.4862613190	2.1787264608	-0.5567666216
H	-4.8156208434	-1.4925234475	-0.3696334312
C	-0.2525968461	1.8176467779	0.7218152718
H	-1.4486210638	1.3022194783	3.2807710074
H	-4.4324422593	-0.0165899017	-1.2672835668
C	-2.1614195965	0.5668357536	0.3448768651
C	0.8942936181	2.2204485525	1.5884490345
H	0.8763559994	2.3883200250	-2.1886724226
N	-1.2195592925	0.9326860789	1.2258637967
C	-4.0000109566	-0.8597910023	-0.7186861881
O	-3.6600354128	-0.7024986024	1.6935992374
C	-3.2005041195	-0.4654491303	0.5414566623
H	1.5368308904	1.3613882059	1.8009948575
C	-1.1602757857	0.4800965172	2.6236574438
H	-1.8528142382	-0.3441543243	2.7475309589
H	1.4942772904	2.9758332080	1.0860859686
H	-0.4274519527	-1.0137191975	-2.4413108324
H	-0.1420325585	0.1688061340	2.8478741039
C	-2.9206278697	-1.6684808265	-1.4574530999
C	0.1135179956	-1.1237859523	-1.5102581120
H	1.9241364798	-0.3352173344	-2.3617511546
H	-3.2759652196	-2.6069355235	-1.8884732663
C	-1.9699125372	-1.8327831622	-0.2848981146
H	-2.4752242951	-1.0910858114	-2.2670513733
C	1.4492764943	-0.7400573722	-1.4763414507
C	-0.5330224656	-1.6378547840	-0.3687789481
H	-2.2823601601	-2.5761128939	0.4458122432
C	2.1669296781	-0.8748136236	-0.2961444504
C	0.2535843018	-1.8187287278	0.7879077118
H	-0.2076370351	-2.2422489778	1.6748193066
C	1.5851177420	-1.4379105064	0.8369687821
Br	3.9816206819	-0.2954551354	-0.2296784621
H	2.1621404505	-1.5668092499	1.7448180888

Zero-point correction=  
(Hartree/Particle)

0.305437

Thermal correction to Energy=

0.324535

Thermal correction to Enthalpy=

0.325479

Thermal correction to Gibbs Free Energy=

0.258331

Sum of electronic and zero-point Energies=

-3722.388204

Sum of electronic and thermal Energies=

-3722.369107

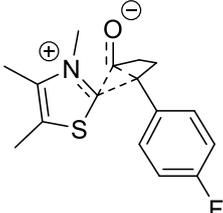
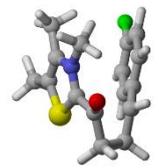
Sum of electronic and thermal Enthalpies=

-3722.368163

Sum of electronic and thermal Free Energies=

-3722.435311

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	203.649	74.162	141.325

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 scrf=(pcm,solvent=2-propanol)	

38

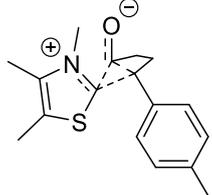
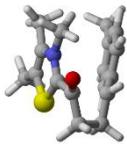
H	1.6393682045	1.8814182903	-3.3107233014
H	2.7361421644	2.1316927443	-1.9505423984
H	1.3465437982	3.4390967190	1.1388862051
C	1.9520387394	1.4855282061	-2.3425451625
S	-0.6777686858	0.6220739292	-1.8868323543
C	0.8012239503	1.4141021480	-1.3930596975
H	-4.2796089109	-0.9946612719	-0.5731813978
C	0.7014773477	1.8193757571	-0.1111308633
H	-1.0848669892	2.9760413998	1.8620623892
H	-3.3992295203	-0.3460859648	-1.9648189051
C	-1.3675383715	0.8021006572	-0.3200296779
C	1.7373405144	2.5141393002	0.7096817927
H	2.3760599626	0.4907175686	-2.5040827878
N	-0.5355391872	1.4970862998	0.4719417136
C	-3.2873842573	-0.7571065982	-0.9561318169
O	-3.3671548195	0.7380535285	0.9716391754
C	-2.6614381048	0.2154758831	0.0646067861
H	2.0757029878	1.8734758525	1.5283661612
C	-0.8489999769	1.9104800732	1.8466199073
H	-1.7090777166	1.3464376155	2.1878847799
H	2.5985944171	2.7598466407	0.0928905336
H	0.3959396307	-2.2592301995	-1.2022557283
H	0.0153946673	1.7147628275	2.4774358906
C	-2.3162168925	-1.9409926036	-0.8098271037
C	0.7158181315	-1.8919524689	-0.2356096483
H	2.8124564853	-1.9966890255	-0.7603964068
H	-2.7989920443	-2.9199052161	-0.7656470840
C	-1.6668036523	-1.4983308384	0.4883546439
H	-1.6016330929	-1.9713887885	-1.6320262925
C	2.0799276451	-1.7519990022	-0.0005153828
C	-0.2361910192	-1.5668794521	0.7501915144
H	-2.2896651363	-1.6430502010	1.3692649163
C	2.4979785062	-1.2896004916	1.2324492328
C	0.2505586845	-1.1487823954	2.0056456172
H	-0.4605734735	-0.9139550597	2.7914633534
C	1.6067442562	-1.0006472229	2.2537758617
F	3.8240844121	-1.1338073391	1.4613210987
H	1.9759323464	-0.6655033015	3.2157434364

Zero-point correction=  
(Hartree/Particle)

0.307416

Thermal correction to Energy=	0.325962
Thermal correction to Enthalpy=	0.326906
Thermal correction to Gibbs Free Energy=	0.262073
Sum of electronic and zero-point Energies=	-1248.053586
Sum of electronic and thermal Energies=	-1248.035040
Sum of electronic and thermal Enthalpies=	-1248.034096
Sum of electronic and thermal Free Energies=	-1248.098929

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	204.544	72.978	136.452

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1 scrf=(pcm,solvent=2-propanol)	

41

H	-0.3314449078	-1.0694011795	-2.3817329571
H	-2.3952632572	-1.1270519803	-2.2381390730
H	0.85938992950	2.3260433466	-2.2838286782
H	2.02686097850	-0.4403783323	-2.2854499330
H	-0.2434786930	3.6965809267	-2.0987462748
H	-3.1750659522	-2.6499440059	-1.8403258112
C	0.36903151590	2.9758166022	-1.5535401434
C	-2.8505456702	-1.6927401602	-1.4255778316
C	0.1944903931	-1.1593379158	-1.4389944197
C	1.5382296377	-0.8023593590	-1.3855495933
H	-4.4054351917	-0.0733896957	-1.3227035585
S	-1.9144603089	1.3867536182	-1.1935987877
H	1.1384752371	3.5268764100	-1.0144733456
C	-3.9643230332	-0.8862153386	-0.7363353561
C	-0.4608256222	2.1661364592	-0.6119595328
C	-0.4800047321	-1.6255743511	-0.2952900255
H	-4.7713515394	-1.5272170621	-0.3819775957
C	-1.9231718862	-1.8048121909	-0.2294683773
C	2.2718929763	-0.8944205934	-0.2026715069
C	3.7069321157	-0.4416016914	-0.1301905441
C	-2.1534346601	0.5785180269	0.3083054648
H	-2.2528077971	-2.5184409507	0.5239145142
C	-3.2048350876	-0.4259554596	0.5249893877
C	-0.2441896445	1.8351740132	0.6765677175
C	0.2865152168	-1.7769961512	0.8779262191
C	1.6230508205	-1.4138701463	0.9242971877
H	1.5287303536	2.9602767433	1.0169817724
N	-1.2227395300	0.9703434979	1.1939188684
C	0.9024091950	2.2424592804	1.5417397362
H	-0.1966300057	-2.1632628525	1.7710048243
O	-3.6893312953	-0.6241760259	1.6749020812
H	1.5169209180	1.3738181432	1.7946692641
H	2.1764555660	-1.5292585599	1.8520059461
H	0.5566059597	2.7012752566	2.4704206665
C	-1.1874838905	0.5511127228	2.6011704815
H	-1.8435184146	-0.3028599356	2.7223640110
H	-0.1646149809	0.2901307100	2.8636834556
H	-1.5359525123	1.3693402564	3.2341879925
H	4.2888622118	-1.0777821266	0.5394967447
H	3.7712502746	0.5823673602	0.2520291798
H	4.1762003132	-0.4566913092	-1.1152581697

Zero-point correction=  
(Hartree/Particle)

0.342830

Thermal correction to Energy=

0.362520

Thermal correction to Enthalpy=

0.363464

Thermal correction to Gibbs Free Energy=

0.295262

Sum of electronic and zero-point Energies=

-1188.082397

Sum of electronic and thermal Energies=

-1188.062707

Sum of electronic and thermal Enthalpies=

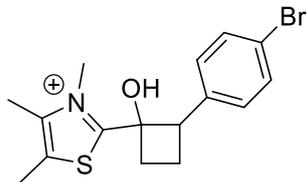
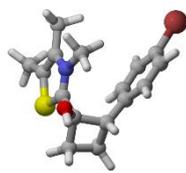
-1188.061763

Sum of electronic and thermal Free Energies=

-1188.129965

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	227.485	76.121	143.542

Protonierte substituierte Strukturen:

#M062X/6-311+G**	(41f-syn-syn-H)	
Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	1 1	

39

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.3028950000	3.5046130000	-1.8098330000
H	-2.9643540000	4.3322920000	-0.2896400000
C	-2.5647980000	3.6235530000	-1.0172840000
H	-1.6625110000	4.0499250000	-1.4589470000
C	-2.2571000000	2.3129620000	-0.3591270000
H	-0.5686240000	4.0164410000	0.8228380000
S	-3.0772720000	0.8595180000	-0.7969910000
C	-1.3612630000	2.0588940000	0.6303450000
C	-0.4459040000	3.0383410000	1.2850290000
H	-0.6648150000	3.1391970000	2.3504930000
H	-4.1478040000	-1.5875470000	-0.9024270000
H	0.5981650000	2.7355480000	1.1741670000
C	-2.1975880000	-0.0531360000	0.3316710000
N	-1.3526840000	0.7163250000	1.0041140000
H	-1.9585790000	-1.5877250000	-2.2134680000
H	-0.2904760000	-0.1577370000	-1.7969790000
C	-3.2931090000	-2.1731470000	-0.5618430000
H	1.9065320000	0.9451750000	-1.7044990000
C	-2.3246790000	-1.5507420000	0.4676620000
C	-2.0964030000	-2.4097150000	-1.5098420000
H	-0.5776400000	0.8256270000	2.9417010000
H	-3.6673980000	-3.1182110000	-0.1624370000
C	-0.4095570000	0.2463330000	2.0346060000
C	0.4755170000	-0.5643160000	-1.1434370000
O	-2.5232360000	-1.8009180000	1.8316640000
H	-2.0717540000	-3.3480480000	-2.0581880000
C	1.7114560000	0.0691780000	-1.0982400000
H	0.6053960000	0.3985690000	1.6641540000
C	-1.1540650000	-2.3033050000	-0.2886370000
H	-0.5905220000	-0.8017360000	2.2353870000
H	-2.7741740000	-2.7219130000	1.9573350000
C	0.2152180000	-1.6964220000	-0.3658470000
H	-1.0926900000	-3.2849610000	0.1921380000
C	2.7100290000	-0.4434900000	-0.2743320000
Br	4.3790710000	0.4376620000	-0.1748250000
C	1.2474930000	-2.2112530000	0.4204630000
C	2.4926640000	-1.5954230000	0.4729240000
H	1.0763210000	-3.1047590000	1.0121760000
H	3.2839030000	-2.0020080000	1.0899580000

Zero-point correction=  
(Hartree/Particle)

0.321273

Thermal correction to Energy=

0.340828

Thermal correction to Enthalpy=

0.341772

Thermal correction to Gibbs Free Energy=

0.273147

Sum of electronic and zero-point Energies=

-3722.794470

Sum of electronic and thermal Energies=

-3722.774915

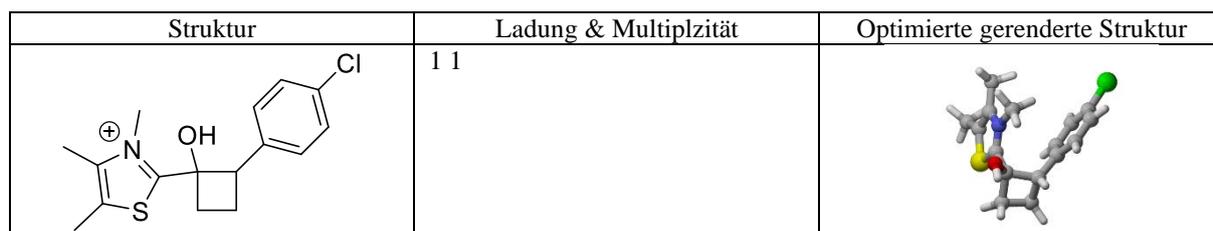
Sum of electronic and thermal Enthalpies=

-3722.773971

Sum of electronic and thermal Free Energies=

-3722.842596

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	213.873	75.679	144.434



39

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.2740940000	-1.7266340000	-2.1919340000
H	-1.1626560000	-3.4857680000	-2.0184690000
H	-3.2899120000	3.1760540000	-1.7757220000
H	0.1922560000	-0.0984320000	-1.8090980000
H	2.2418900000	1.2653920000	-1.7805220000
C	-1.3012350000	-2.5518570000	-1.4796480000
H	-1.6931690000	3.8864970000	-1.5386690000
C	1.0146180000	-0.3975430000	-1.1664350000
C	2.1638380000	0.3831530000	-1.1571860000
C	-2.5212750000	3.3865370000	-1.0328640000
H	-3.4351810000	-1.9859270000	-0.8659560000
S	-2.6766670000	0.5808170000	-0.7933370000
C	-2.5118740000	-2.4555460000	-0.5249930000
C	0.9098870000	-1.5397350000	-0.3678190000
C	-2.0489200000	2.1304020000	-0.3662050000
H	-2.9448000000	4.0730970000	-0.2978150000
C	-0.3711670000	-2.3136430000	-0.2673220000
C	3.2330840000	0.0102050000	-0.3479990000
Cl	4.6615420000	0.9914580000	-0.3143370000
H	-2.7615110000	-3.4352360000	-0.1119810000
H	-0.1831060000	-3.2738080000	0.2232420000
C	-1.6841750000	-0.2044990000	0.3383990000
C	2.0108280000	-1.9083620000	0.4081630000
C	-1.6222960000	-1.7047100000	0.4897740000
C	3.1715920000	-1.1437300000	0.4241680000
C	-1.1249830000	1.9996290000	0.6210220000
H	-0.5863380000	4.0429750000	0.7943960000
N	-0.9422610000	0.6712480000	1.0018750000
H	1.9624670000	-2.8048810000	1.0178090000
H	4.0222590000	-1.4353750000	1.0272430000
H	0.7300350000	2.9250430000	1.1671120000
C	-0.3445830000	3.0935990000	1.2691790000
H	1.0493290000	0.5817060000	1.6309010000
O	-1.7810820000	-1.9620020000	1.8578350000
H	-1.9280600000	-2.9037750000	1.9938910000
C	0.0630850000	0.3305550000	2.0248220000
H	0.0002520000	-0.7260040000	2.2531020000
H	-0.5817480000	3.1768090000	2.3324120000
H	-0.1515310000	0.9109790000	2.9210460000

Zero-point correction=  
(Hartree/Particle)

0.321689

Thermal correction to Energy=

0.341122

Thermal correction to Enthalpy=

0.342066

Thermal correction to Gibbs Free Energy=

0.274219

Sum of electronic and zero-point Energies=

-1608.822513

Sum of electronic and thermal Energies=

-1608.803080

Sum of electronic and thermal Enthalpies=

-1608.802136

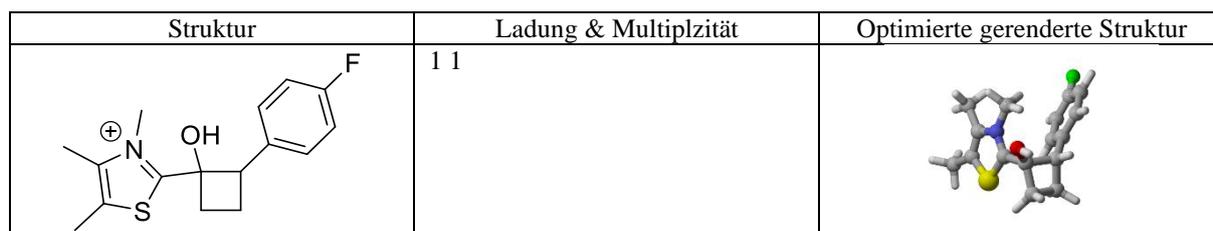
Sum of electronic and thermal Free Energies=

-1608.869983

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	214.057	75.355	142.796

#M062X/6-311+G\*\*

(41d-syn-syn-H)



39

XYZ file generated by gabedit : coordinates in Angstrom

H	3.6505860000	-2.3389150000	-1.9063190000
H	3.8231550000	-3.1643650000	-0.3558210000
C	3.1014170000	-2.7301380000	-1.0504680000
H	2.4438810000	-3.5231810000	-1.4095640000
C	2.3043780000	-1.6542860000	-0.3780290000
H	1.3866260000	-3.8992040000	0.7503890000
S	2.5135960000	0.0128420000	-0.7734970000
C	1.3718710000	-1.7837950000	0.6012640000
C	0.9031040000	-3.0516000000	1.2328720000
H	1.1542320000	-3.0824600000	2.2957310000
H	2.5775060000	2.6856510000	-0.8092760000
H	-0.1781150000	-3.1686660000	1.1296260000
C	1.3418170000	0.4942580000	0.3560410000
N	0.8463690000	-0.5546390000	0.9976530000
H	0.5678470000	1.8981640000	-2.1642290000
H	-0.4222170000	-0.0563790000	-1.8257790000
C	1.5617000000	2.8953320000	-0.4723760000
H	-2.0842680000	-1.8969550000	-1.8774230000
C	0.8894900000	1.9238580000	0.5226850000
C	0.3746820000	2.6896520000	-1.4389350000
H	0.1178930000	-1.0353580000	2.8965540000
H	1.5472610000	3.8994750000	-0.0432990000
C	-0.2247020000	-0.5041570000	2.0096270000
C	-1.3046630000	0.0070630000	-1.1967040000
O	0.9635190000	2.1957450000	1.8953870000
H	0.0017390000	3.5644840000	-1.9657030000
C	-2.2224820000	-1.0352850000	-1.2361670000
H	-1.1108240000	-0.9857610000	1.5930090000
C	-0.4700680000	2.1955390000	-0.2413030000
H	-0.4329690000	0.5279590000	2.2621650000
H	0.8293820000	3.1376140000	2.0437030000
C	-1.5071580000	1.1194740000	-0.3744360000
H	-0.9073020000	3.0651010000	0.2598230000
C	-3.3610840000	-0.9442200000	-0.4502000000
F	-4.2458940000	-1.9438710000	-0.4806220000
C	-2.6789960000	1.1813820000	0.3841260000
C	-3.6138750000	0.1534760000	0.3545470000
H	-2.8664830000	2.0461130000	1.0122240000
H	-4.5277450000	0.1932530000	0.9338240000

Zero-point correction=  
(Hartree/Particle)

0.322862

Thermal correction to Energy=

0.341919

Thermal correction to Enthalpy=

0.342864

Thermal correction to Gibbs Free Energy=

0.276332

Sum of electronic and zero-point Energies=

-1248.462212

Sum of electronic and thermal Energies=

-1248.443155

Sum of electronic and thermal Enthalpies=

-1248.442211

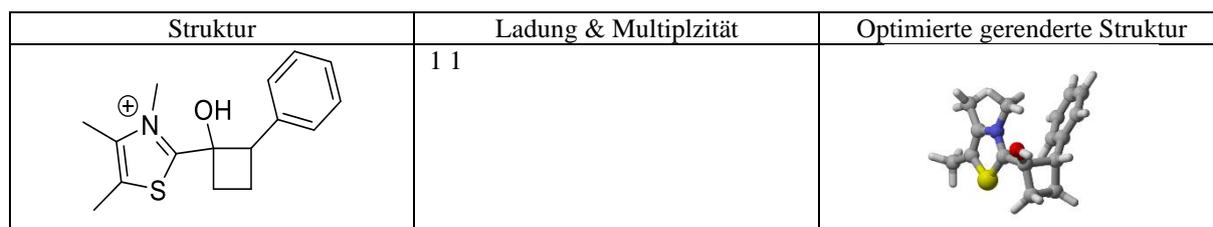
Sum of electronic and thermal Free Energies=

-1248.508743

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-kelvin	Cal/Mol-kelvin
Total	214.558	74.546	140.028

#M062X/6-311+G\*\*

(41c-syn-syn-H)



39

XYZ file generated by gabedit : coordinates in Angstrom

H	0.9914820000	3.3973510000	-0.5918450000
H	-0.3962260000	1.8725710000	-2.0949850000
H	0.2966260000	-1.2911710000	2.7712700000
H	-0.5050380000	3.9741900000	0.1503940000
C	-0.0235560000	3.1112490000	-0.3142620000
C	-0.9519980000	2.4582180000	-1.3618580000
H	-2.3332450000	2.1417960000	0.2685220000
C	-0.2107090000	-0.8875310000	1.8961850000
H	-1.6499930000	3.1065230000	-1.8856080000
H	-0.7853530000	-1.6658900000	1.3906440000
N	0.8129490000	-0.3874930000	0.9599110000
C	-1.5415750000	1.5778880000	-0.2355010000
C	-0.2320550000	1.8823120000	0.5981780000
C	0.8143000000	0.8134900000	0.3989280000
H	3.6553340000	-2.1342140000	-1.5114200000
H	-0.8535460000	-0.0689360000	2.1942410000
C	1.9617030000	-2.6137090000	1.0818560000
C	1.8482940000	-1.2252130000	0.5481410000
S	2.1264410000	0.9817160000	-0.6648630000
C	2.6681260000	-0.6272830000	-0.3552560000
H	-0.4549310000	-0.3569200000	-1.8754190000
C	3.8890050000	-1.1900070000	-1.0170010000
H	4.2809580000	-0.5064710000	-1.7695510000
O	-0.3344180000	2.0691220000	1.9831980000
C	-1.9984260000	0.1660510000	-0.4567430000
C	-1.3013290000	-0.7104680000	-1.2937460000
H	-3.6717980000	0.3560380000	0.8790410000
H	4.6758500000	-1.3673240000	-0.2813710000
C	-3.1066560000	-0.3170260000	0.2421290000
C	-1.6812050000	-2.0444750000	-1.3982140000
H	-1.1354130000	-2.7098230000	-2.0570890000
C	-3.4941660000	-1.6485790000	0.1349840000
C	-2.7746530000	-2.5192820000	-0.6771530000
H	-4.3599340000	-2.0035180000	0.6810460000
H	-3.0765480000	-3.5558280000	-0.7657400000
H	1.0466780000	-3.1806750000	0.8954320000
H	2.1555810000	-2.6130360000	2.1569930000
H	2.7880320000	-3.1258090000	0.5917050000
H	-0.8974520000	2.8293550000	2.1625970000

Zero-point correction=  
(Hartree/Particle)

0.331340

Thermal correction to Energy=

0.349537

Thermal correction to Enthalpy=

0.350481

Thermal correction to Gibbs Free Energy=

0.286049

Sum of electronic and zero-point Energies=

-1149.215268

Sum of electronic and thermal Energies=

-1149.197071

Sum of electronic and thermal Enthalpies=

-1149.196127

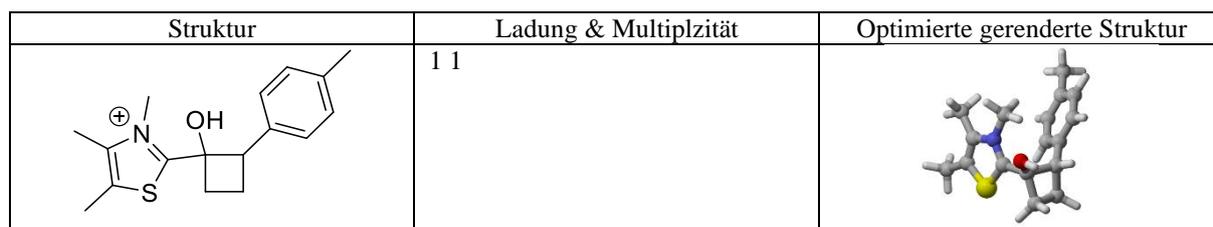
Sum of electronic and thermal Free Energies=

-1149.260559

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	219.338	71.526	135.609

#M062X/6-311+G\*\*

(41b-syn-syn-H)



42

XYZ file generated by gabedit : coordinates in Angstrom

H	0.4102920000	0.0505910000	-1.8072330000
H	-0.7109330000	-1.8519680000	-2.1706730000
H	-3.5810880000	2.5405210000	-1.8506660000
H	2.1588500000	1.7658850000	-1.8283540000
H	-3.6052330000	3.4154620000	-0.3189960000
H	-0.2488500000	-3.5525070000	-1.9914850000
C	-2.9583340000	2.9025420000	-1.0332700000
C	-0.5650700000	-2.6616670000	-1.4544070000
C	1.2881410000	-0.0841630000	-1.1816560000
C	2.2774380000	0.8928600000	-1.1946870000
H	-2.7613260000	-2.5322830000	-0.8126960000
S	-2.5412140000	0.1266360000	-0.7618960000
H	-2.2528450000	3.6257590000	-1.4454110000
C	-1.7577660000	-2.8040960000	-0.4832930000
C	-2.2259470000	1.7775630000	-0.3678000000
C	1.4160640000	-1.2219590000	-0.3817270000
H	-1.8007090000	-3.8099780000	-0.0603940000
C	0.3136930000	-2.2312210000	-0.2568450000
C	3.4367740000	0.7573630000	-0.4263990000
C	4.5300200000	1.7906250000	-0.4746940000
C	-1.3887940000	-0.4264570000	0.3545140000
H	0.6961470000	-3.1312430000	0.2360440000
C	-1.0235790000	-1.8811770000	0.5142470000
C	-1.2752530000	1.8478450000	0.5999220000
C	2.5819970000	-1.3664860000	0.3730480000
C	3.5738610000	-0.3940680000	0.3520760000
H	-1.1485940000	3.9603760000	0.7398170000
N	-0.8234520000	0.5890340000	0.9917920000
C	-0.7160480000	3.0843250000	1.2198990000
H	2.7138290000	-2.2504920000	0.9893550000
O	-1.1103010000	-2.1535540000	1.8864680000
H	0.3690200000	3.1265820000	1.1005560000
H	4.4723920000	-0.5324870000	0.9442230000
H	-0.9491570000	3.1359950000	2.2859810000
C	0.2534490000	0.4710470000	1.9918160000
H	0.3900190000	-0.5716660000	2.2494770000
H	1.1675180000	0.8834450000	1.5606070000
H	-0.0419640000	1.0311440000	2.8778780000
H	4.9876370000	1.9286000000	0.5061230000
H	4.1533560000	2.7534940000	-0.8213220000
H	5.3178890000	1.4747330000	-1.1635570000
H	-0.9941110000	-3.0981960000	2.0323230000

Zero-point correction=  
(Hartree/Particle)

0.358146

Thermal correction to Energy=

0.378247

Thermal correction to Enthalpy=

0.379192

Thermal correction to Gibbs Free Energy=

0.309912

Sum of electronic and zero-point Energies=

-1188.496397

Sum of electronic and thermal Energies=

-1188.476296

Sum of electronic and thermal Enthalpies=

-1188.475351

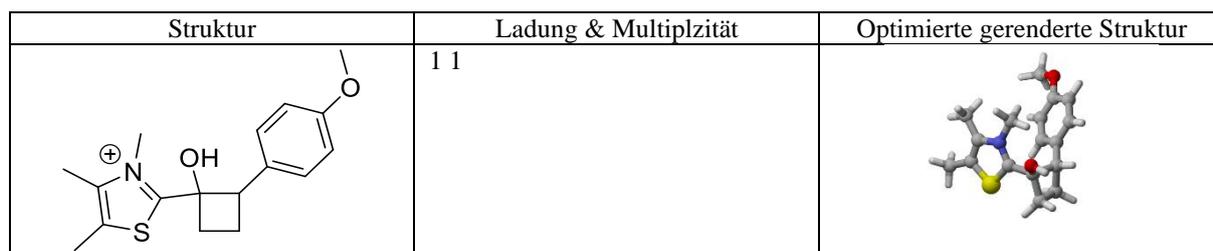
Sum of electronic and thermal Free Energies=

-1188.544631

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	237.354	77.810	145.812

#M062X/6-311+G\*\*

(41a-syn-syn-H)



43

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.0777480000	3.3685100000	-1.7458590000
H	-2.7350540000	4.1985730000	-0.2291830000
C	-2.3231400000	3.5153450000	-0.9737840000
H	-1.4553130000	3.9881280000	-1.4372810000
C	-1.9367390000	2.2153840000	-0.3364880000
S	-2.6097040000	0.7122000000	-0.8522420000
H	-3.4757090000	-1.8095650000	-1.0622770000
H	-0.4344680000	4.0127480000	0.9543910000
C	-1.0664410000	2.0059820000	0.6851160000
C	-0.2736540000	3.0387670000	1.4137190000
H	-0.5745610000	3.1049460000	2.4620410000
C	-1.7071460000	-0.1578850000	0.2923870000
C	-2.5928070000	-2.3334450000	-0.6941310000
N	-0.9586450000	0.6578500000	1.0214210000
H	-2.9076290000	-3.3140740000	-0.3311590000
H	-1.2377060000	-1.6024550000	-2.2670750000
C	-1.7234730000	-1.6623890000	0.3915690000
H	0.7945800000	2.8136410000	1.3756610000
C	-1.3394680000	-2.4512450000	-1.5895680000
O	-1.9662600000	-1.9581890000	1.7402780000
H	0.3232620000	-0.0757720000	-1.7560820000
H	-0.2335990000	0.8019620000	2.9753750000
H	-2.1230100000	-2.9031960000	1.8370830000
H	-1.2153600000	-3.3702730000	-2.1569970000
C	-0.0156860000	0.2337790000	2.0721330000
C	-0.4639210000	-2.3011650000	-0.3238400000
C	1.0875160000	-0.4479690000	-1.0795290000
H	-0.1475570000	-0.8230310000	2.2660380000
H	2.4333740000	1.1346190000	-1.6100090000
H	0.9983940000	0.4355970000	1.7230460000
H	-0.3509760000	-3.2882640000	0.1370580000
C	0.8599360000	-1.5983870000	-0.3283040000
C	2.2892470000	0.2544300000	-0.9978230000
C	1.8948750000	-2.0542340000	0.4992380000
C	3.3021840000	-0.2096900000	-0.1541110000
H	1.7536200000	-2.9598070000	1.0809220000
C	3.0956740000	-1.3767410000	0.5916850000
O	4.5013640000	0.3835240000	-0.0008590000
C	4.7942900000	1.5243320000	-0.7890920000
H	3.9003520000	-1.7323230000	1.2233080000
H	4.1082390000	2.3461120000	-0.5612170000
H	4.7465900000	1.2857500000	-1.8552690000
H	5.8077450000	1.8161260000	-0.5270020000

Zero-point correction= 0.364460

Thermal correction to Energy= 0.385084

Thermal correction to Enthalpy= 0.386028

Thermal correction to Gibbs Free Energy= 0.316193

Sum of electronic and zero-point Energies= -1263.695988

Sum of electronic and thermal Energies= -1263.675365

Sum of electronic and thermal Enthalpies= -1263.674420

Sum of electronic and thermal Free Energies= -1263.744255

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	241.644	80.501	146.979

Von den Strukturen der protonierten Primäraddukte **41-H** ausgehend, wurden die Energien der Übergangszustände **40-H** und **42-H** mit Hilfe von relaxierten PES-Scans abgeschätzt. Um zu **42-H** zu gelangen wurde die Bindungslänge C2–C3 schrittweise verkleinert. Um zu Struktur **40-H** zu gelangen wurde die Bindungslänge zwischen C1 und C3 schrittweise vergrößert und außerdem die Länge der OH-Bindung auf den Anfangswert fixiert, um die Protonierung beizubehalten.

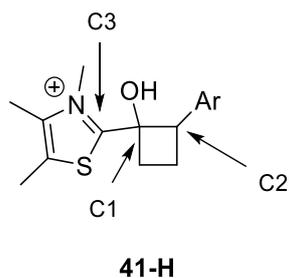


Abbildung A 144: Struktura **41-H** mit Definition der Atome C1, C2 und C3.

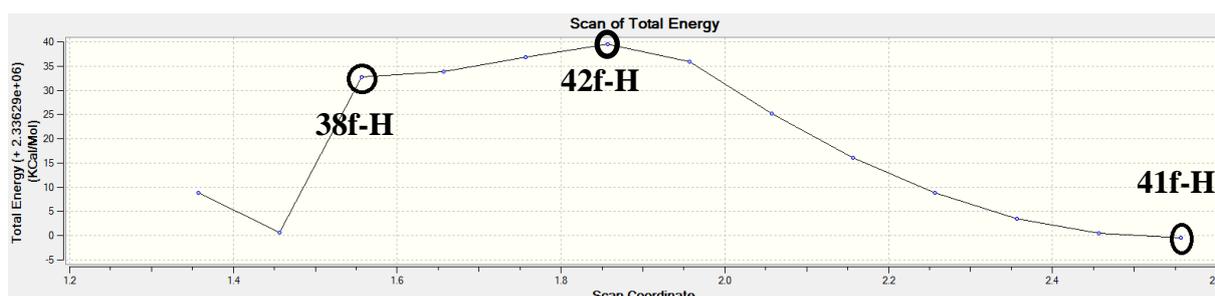


Abbildung A 145: Relaxierter PES-Scan von Struktur **41f-H** entlang der Bindung C2–C3.

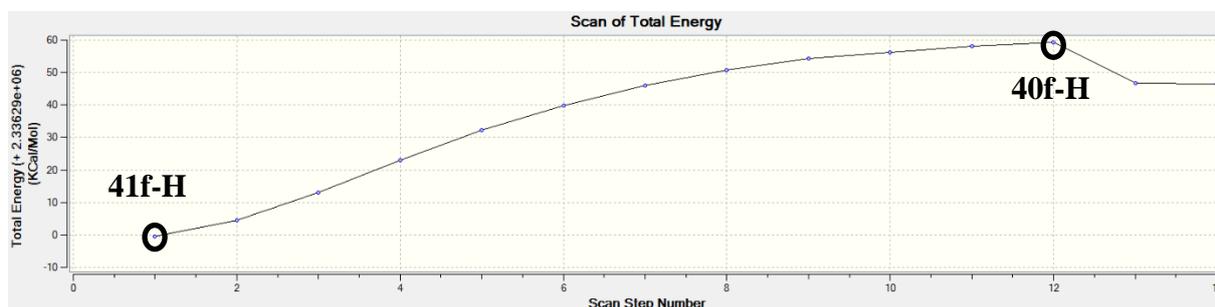


Abbildung A 146: Relaxierter PES-Scan von Struktur **41f-H** entlang der Bindung C1–C3.

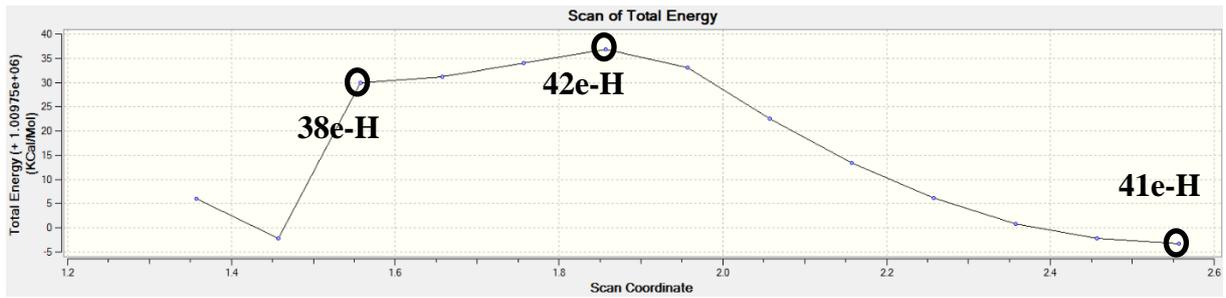


Abbildung A 147: Relaxierter PES-Scan von Struktur **41e-H** entlang der Bindung C2–C3.

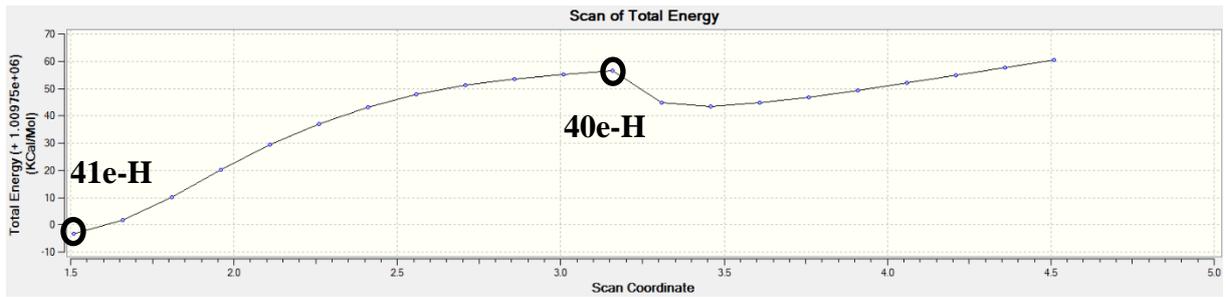


Abbildung A 148: Relaxierter PES-Scan von Struktur **41e-H** entlang der Bindung C1–C3.

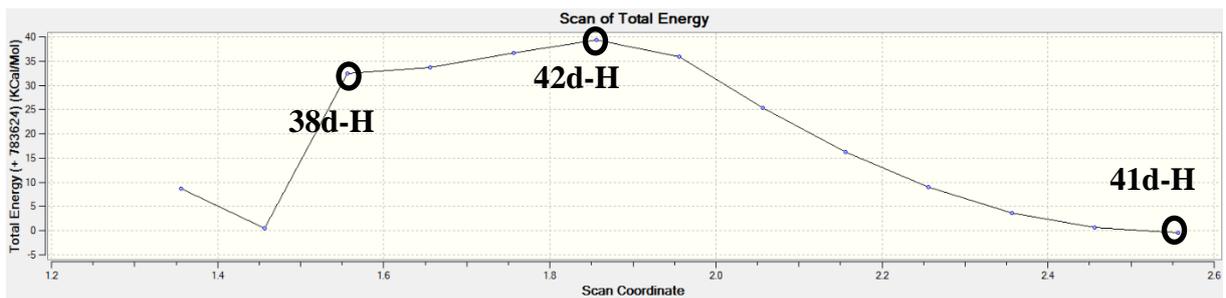


Abbildung A 149: Relaxierter PES-Scan von Struktur **41d-H** entlang der Bindung C2–C3.

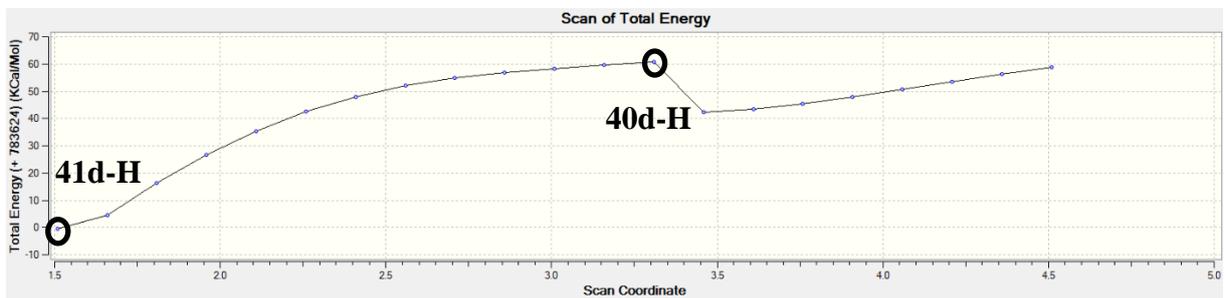


Abbildung A 150: Relaxierter PES-Scan von Struktur **41d-H** entlang der Bindung C1–C3.

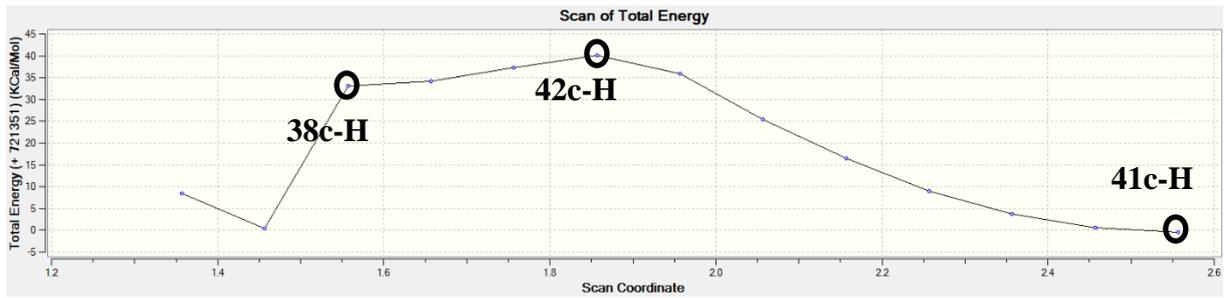


Abbildung A 151: Relaxierter PES-Scan von Struktur **41c-H** entlang der Bindung C2–C3.

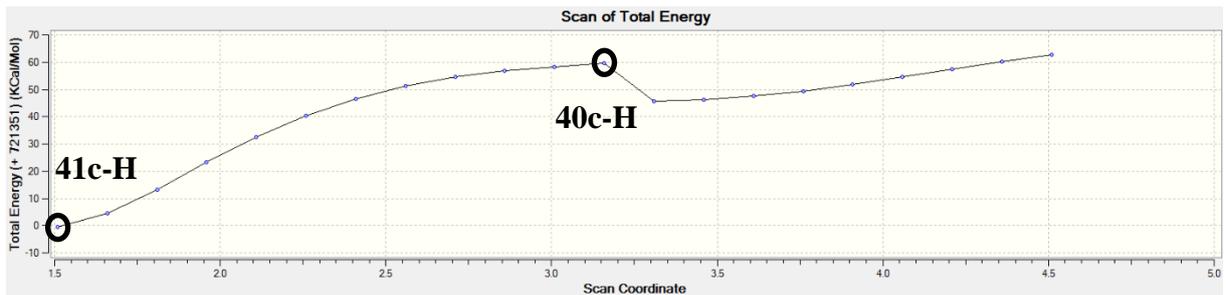


Abbildung A 152: Relaxierter PES-Scan von Struktur **41c-H** entlang der Bindung C1–C3.

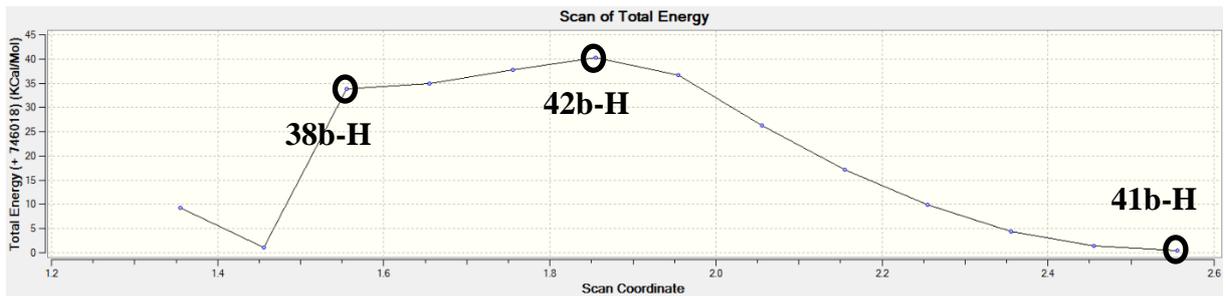


Abbildung A 153: Relaxierter PES-Scan von Struktur **41b-H** entlang der Bindung C2–C3.

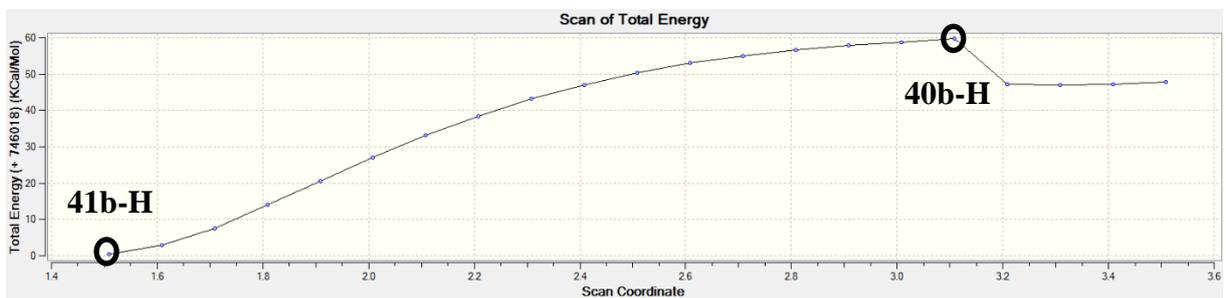


Abbildung A 154: Relaxierter PES-Scan von Struktur **41b-H** entlang der Bindung C1–C3.

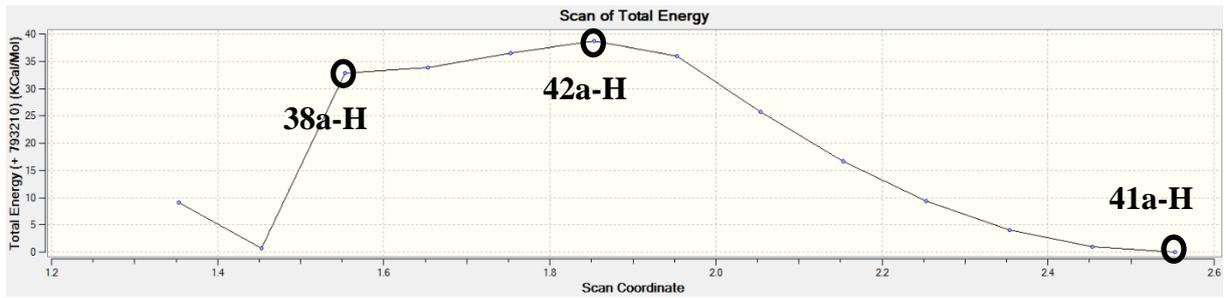


Abbildung A 155: Relaxierter PES-Scan von Struktur **41a-H** entlang der Bindung C2-C3.

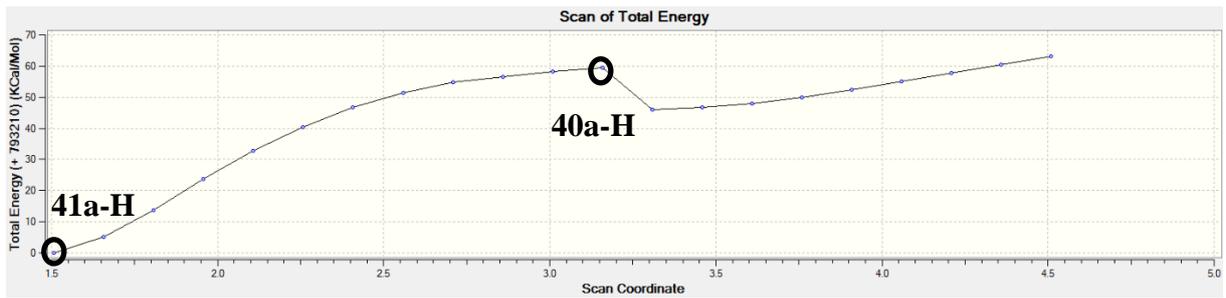
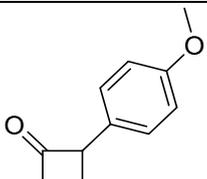
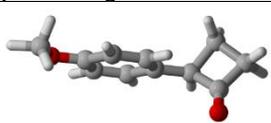


Abbildung A 156: Relaxierter PES-Scan von Struktur **41a-H** entlang der Bindung C1-C3.

## Mit der Methode B3LYP optimierte Strukturen (für berechnete IR-Spektren):

#B3LYP/6-311+G**	(32a)	
Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

25

XYZ file generated by gabedit : coordinates in Angstrom

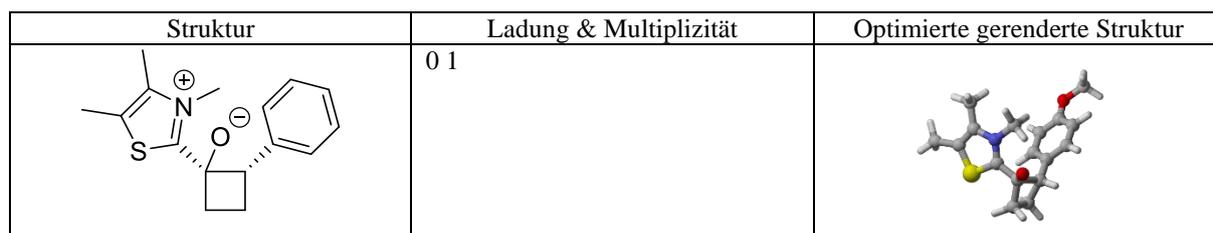
O	2.7862640000	-1.3799610000	-1.3814320000
H	-4.1097410000	-1.8288840000	-0.3386450000
H	-1.9744040000	-1.7846860000	0.6498740000
H	0.4529240000	-1.5590560000	0.6068350000
H	4.2124590000	-1.1469970000	1.1394320000
H	-4.1547340000	-1.2527110000	1.3542220000
C	2.8771290000	-0.5292970000	-0.5430410000
C	-1.5412440000	-0.8445160000	0.3360040000
C	-4.3779550000	-0.9911210000	0.3140790000
C	-0.1531560000	-0.7083480000	0.3137200000
H	2.2450060000	0.1185070000	2.0489430000
H	-5.4423120000	-0.7841010000	0.2156190000
C	3.8700780000	-0.2648540000	0.5950730000
C	2.7792510000	0.6337450000	1.2496310000
H	4.7437600000	0.2917670000	0.2436420000
C	-2.3484190000	0.2265440000	-0.0566040000
O	-3.7129970000	0.2030070000	-0.0752850000
C	0.4607940000	0.4781990000	-0.0921380000
C	1.9552000000	0.6291530000	-0.0890450000
H	3.0988120000	1.6125680000	1.6058690000
H	2.2383340000	1.5085760000	-0.6801820000
C	-1.7507630000	1.4216250000	-0.4712730000
C	-0.3686380000	1.5369520000	-0.4887040000
H	-2.3873480000	2.2423260000	-0.7794180000
H	0.0774450000	2.4698340000	-0.8186660000

Zero-point correction=(Hartree/Particle)	0.203771
Thermal correction to Energy=	0.215688
Thermal correction to Enthalpy=	0.216632
Thermal correction to Gibbs Free Energy=	0.164097
Sum of electronic and zero-point Energies=	-576.757112
Sum of electronic and thermal Energies=	-576.745195
Sum of electronic and thermal Enthalpies=	-576.744251
Sum of electronic and thermal Free Energies=	-576.796786

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	135.346	45.044	110.570

#B3LYP/6-311+G\*\*

(41aa'-syn-syn)



42

XYZ file generated by gabedit : coordinates in Angstrom

H	-3.0022780000	-2.5863000000	-0.7706190000
H	-0.8807130000	-2.1245930000	-2.0705330000
H	-0.6564370000	1.2943790000	2.8990340000
H	-2.1458700000	-3.8044000000	0.1888020000
C	-2.0323510000	-2.8581080000	-0.3411380000
C	-0.7861160000	-2.8439740000	-1.2528160000
H	0.3723230000	-3.1425820000	0.5503740000
C	-0.3536580000	0.5740020000	2.1411140000
H	-0.4694850000	-3.7966520000	-1.6825420000
H	0.6656880000	0.7763940000	1.8115210000
N	-1.2735600000	0.6786400000	0.9895260000
C	0.0657920000	-2.3061930000	-0.0830090000
C	-1.3469270000	-1.8643510000	0.6807210000
C	-1.6747800000	-0.3962600000	0.3037220000
H	-3.1610830000	3.8238690000	-0.8878180000
H	-0.4598620000	-0.4491870000	2.5164160000
C	-1.3817860000	3.1746760000	1.2429670000
C	-1.7867050000	1.9109180000	0.5512220000
S	-2.7644230000	0.0899600000	-0.9405480000
C	-2.6294110000	1.7813850000	-0.5048290000
H	0.4453620000	-0.3419020000	-2.0078950000
C	-3.3954320000	2.8251460000	-1.2572640000
H	-3.1581220000	2.8014170000	-2.3245690000
O	-1.4820060000	-2.0311470000	1.9681750000
C	1.2201070000	-1.3783710000	-0.2778200000
C	1.2556420000	-0.4017230000	-1.2898150000
H	2.3269060000	-2.1645930000	1.3852720000
H	-4.4744870000	2.6778740000	-1.1540570000
C	2.3119390000	-1.4177080000	0.5982100000
C	2.3121990000	0.4902520000	-1.4094540000
H	2.3332940000	1.2314590000	-2.2001940000
C	3.3838150000	-0.5277780000	0.4959100000
C	3.3859670000	0.4372270000	-0.5132190000
H	4.2040180000	-0.6054990000	1.1976260000
H	-0.2941380000	3.2739950000	1.2832850000
H	-1.7596630000	3.2119550000	2.2689530000
H	-1.7775790000	4.0390930000	0.7123440000
O	4.3801370000	1.3584560000	-0.7125900000
C	5.5170390000	1.3181210000	0.1364840000
H	6.1757730000	2.1141850000	-0.2076570000
H	5.2454930000	1.5011960000	1.1824740000
H	6.0394930000	0.3580010000	0.0612760000

Zero-point correction=  
(Hartree/Particle)

0.344966

Thermal correction to Energy=

0.366177

Thermal correction to Enthalpy=

0.367121

Thermal correction to Gibbs Free Energy=

0.294176

Sum of electronic and zero-point Energies=

-1263.664169

Sum of electronic and thermal Energies=

-1263.642958

Sum of electronic and thermal Enthalpies=

-1263.642013

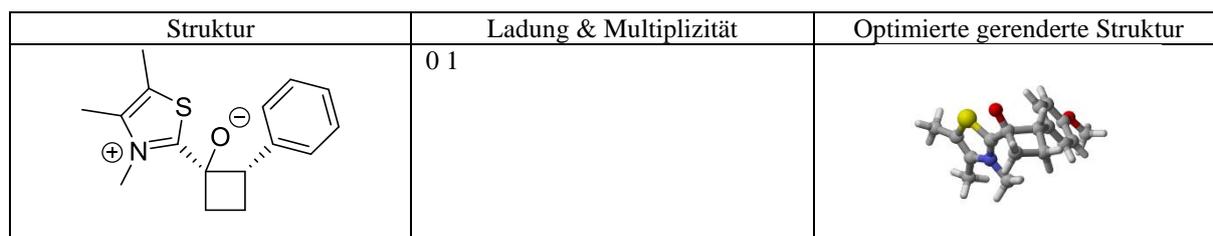
Sum of electronic and thermal Free Energies=

-1263.714959

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	229.780	80.925	153.526

#B3LYP/6-311+G\*\*

(41aa'-syn-anti)



42

XYZ file generated by gabedit : coordinates in Angstrom

H	-2.2951290000	2.5495550000	1.6991050000
H	0.1820530000	2.8117410000	1.8785090000
H	0.2869880000	-0.4421580000	2.3075210000
H	-2.3332400000	3.7109790000	0.3591130000
C	-1.7651700000	2.8957010000	0.8060070000
C	-0.2536470000	3.2011650000	0.9548550000
H	0.0967570000	2.9936550000	-1.1837000000
C	-0.7244430000	-0.0359030000	2.2815440000
H	0.0274670000	4.2540980000	0.8912910000
H	-1.2886790000	-0.3893160000	3.1448010000
N	-1.4031240000	-0.4539920000	1.0505120000
C	0.0665600000	2.3531790000	-0.2995000000
C	-1.4903960000	1.8423700000	-0.3546350000
C	-1.6894150000	0.3662940000	0.0334870000
H	-3.0070180000	-4.0317980000	-0.2040910000
H	-0.6737310000	1.0450480000	2.3127440000
C	-1.5209030000	-2.8139110000	1.9148520000
C	-1.8073030000	-1.7917590000	0.8576230000
S	-2.5165410000	-0.4377300000	-1.2278610000
C	-2.4315280000	-1.9588920000	-0.3372420000
H	2.1371980000	1.9400820000	1.5181570000
C	-3.0049110000	-3.2124860000	-0.9242970000
H	-4.0368260000	-3.0559110000	-1.2504670000
O	-2.1243320000	1.9774410000	-1.5046160000
C	1.2136880000	1.3851830000	-0.3428820000
C	2.1792740000	1.2808930000	0.6580280000
H	0.6265500000	0.6065840000	-2.2636880000
H	-2.4322520000	-3.5368800000	-1.7985180000
C	1.3480310000	0.5317220000	-1.4569010000
C	3.2326290000	0.3597310000	0.5819970000
H	3.9650760000	0.3280450000	1.3782500000
C	2.3773470000	-0.3902200000	-1.5452320000
C	3.3305330000	-0.4856010000	-0.5218560000
H	2.4743380000	-1.0417560000	-2.4059840000
H	-2.0502880000	-2.6013490000	2.8492940000
H	-0.4524050000	-2.8735990000	2.1421090000
H	-1.8384430000	-3.7983880000	1.5748890000
O	4.3106860000	-1.4248410000	-0.7035980000
C	5.3355530000	-1.5272510000	0.2721000000
H	4.9322270000	-1.8089240000	1.2518530000
H	6.0056990000	-2.3109370000	-0.0783140000
H	5.8939510000	-0.5892200000	0.3673350000

Zero-point correction=  
(Hartree/Particle)

0.344797

Thermal correction to Energy=

0.366302

Thermal correction to Enthalpy=

0.367247

Thermal correction to Gibbs Free Energy=

0.292528

Sum of electronic and zero-point Energies=

-1263.656122

Sum of electronic and thermal Energies=

-1263.634616

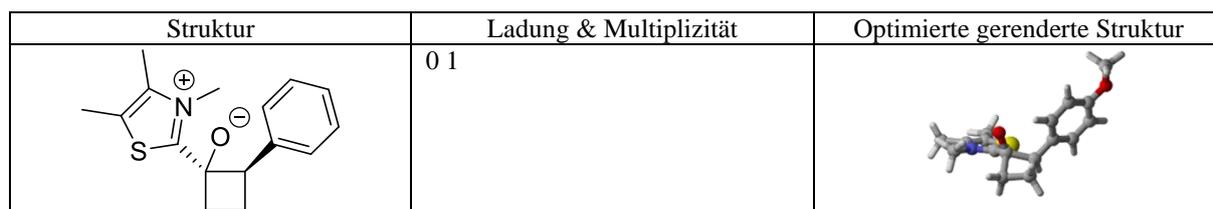
Sum of electronic and thermal Enthalpies=

-1263.633672

Sum of electronic and thermal Free Energies=

-1263.708391

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	229.858	81.132	157.258



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XYZ file generated by gabedit : coordinates in Angstrom

H	-1.7425630000	2.7726770000	1.5495690000
H	0.6332760000	3.2365920000	2.2317220000
H	-3.8783370000	2.2921780000	-0.6405920000
H	-1.3187330000	3.6283780000	0.0336460000
C	-1.0217850000	2.8385140000	0.7262230000
C	0.4394590000	2.8437360000	1.2309950000
H	0.1197050000	0.8527650000	1.9965050000
C	-3.3750360000	1.5691030000	-1.2847850000
H	1.1038770000	3.3375460000	0.5206610000
H	-4.0452690000	1.2608330000	-2.0829850000
N	-2.9708370000	0.3853720000	-0.5053140000
C	0.4969430000	1.2994250000	1.0678220000
C	-0.7201550000	1.4517010000	0.0220140000
C	-1.7946540000	0.3648160000	0.1348550000
H	-3.5205420000	-3.4036770000	1.5866200000
H	-2.4526120000	1.9845860000	-1.7007460000
C	-5.0354560000	-0.8970470000	-1.1474830000
C	-3.7073800000	-0.8106250000	-0.4621570000
S	-1.5456570000	-1.1768150000	0.8538090000
C	-3.0747200000	-1.7847650000	0.2398730000
H	1.8741630000	-0.6111590000	2.4407860000
C	-3.4907580000	-3.1969240000	0.5130250000
H	-4.4834880000	-3.3977080000	0.1090000000
O	-0.4300520000	1.4855630000	-1.2756720000
C	1.7605000000	0.6038380000	0.6639250000
C	2.3454470000	-0.3655470000	1.4932500000
H	1.9442300000	1.6027920000	-1.2211350000
H	-2.7965430000	-3.9093240000	0.0577890000
C	2.4013050000	0.8904240000	-0.5464990000
C	3.5206760000	-1.0168160000	1.1418840000
H	3.9703450000	-1.7589550000	1.7912220000
C	3.5809540000	0.2422560000	-0.9164910000
C	4.1472300000	-0.7140830000	-0.0703410000
H	4.0396170000	0.4884250000	-1.8653370000
H	-4.9352930000	-0.8233100000	-2.2345660000
H	-5.7083750000	-0.1005620000	-0.8181120000
H	-5.5138310000	-1.8494470000	-0.9248630000
O	5.3025860000	-1.4034180000	-0.3362930000
C	5.9828180000	-1.1336270000	-1.5515470000
H	6.3036730000	-0.0872800000	-1.6093240000
H	6.8603700000	-1.7791200000	-1.5528870000
H	5.3601180000	-1.3682290000	-2.4223680000

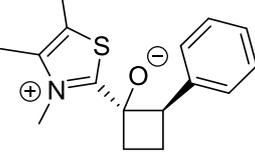
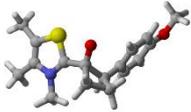
Zero-point correction= 0.344717  
(Hartree/Particle)

Thermal correction to Energy= 0.366177  
 Thermal correction to Enthalpy= 0.367121  
 Thermal correction to Gibbs Free Energy= 0.293153  
 Sum of electronic and zero-point Energies= -1263.661792  
 Sum of electronic and thermal Energies= -1263.640332  
 Sum of electronic and thermal Enthalpies= -1263.639388  
 Sum of electronic and thermal Free Energies= -1263.713356

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	229.779	80.990	155.679

#B3LYP/6-311+G\*\*

(41aa'-anti-anti)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

42

XYZ file generated by gabedit : coordinates in Angstrom

H	-1.7951040000	3.2527860000	-0.2315910000
H	0.5100050000	3.9294900000	0.5204730000
H	-2.6307590000	0.9084290000	2.6628850000
H	-1.1193110000	3.2522010000	-1.8802010000
C	-0.9712850000	2.8973350000	-0.8600700000
C	0.4170920000	3.1270550000	-0.2160320000
H	-0.0509060000	1.6801920000	1.3333560000
C	-2.8431320000	1.3352720000	1.6816680000
H	1.1885420000	3.2576110000	-0.9751970000
H	-3.8642430000	1.7191470000	1.6676080000
N	-2.6805740000	0.3108740000	0.6447230000
C	0.4181600000	1.6791750000	0.3433710000
C	-0.6992890000	1.3413150000	-0.8206960000
C	-1.8012910000	0.3935330000	-0.3625940000
H	-4.1900500000	-2.9612830000	-1.7819710000
H	-2.1558190000	2.1510280000	1.4923590000
C	-4.4938680000	-1.0682270000	1.7096180000
C	-3.4690060000	-0.8592810000	0.6370790000
S	-1.8741400000	-0.9621550000	-1.3980020000
C	-3.1585900000	-1.6659770000	-0.4114910000
H	1.4707180000	0.3968650000	2.5002170000
C	-3.7527750000	-2.9910490000	-0.7797580000
H	-2.9916370000	-3.7767090000	-0.7793070000
O	-0.2320060000	0.8277260000	-1.9487010000
C	1.6617330000	0.8557190000	0.4023210000
C	2.0660160000	0.2504750000	1.6029650000
H	2.1353780000	1.0521280000	-1.6774460000
H	-4.5380380000	-3.2892330000	-0.0838810000
C	2.4554220000	0.6393800000	-0.7299500000
C	3.2169080000	-0.5217420000	1.6825460000
H	3.5281190000	-0.9768730000	2.6155740000
C	3.6131320000	-0.1379000000	-0.6677430000
C	4.0006900000	-0.7193850000	0.5415980000
H	4.1949680000	-0.2851910000	-1.5682220000
H	-5.2541600000	-0.2809250000	1.7083180000
H	-4.0438090000	-1.0951590000	2.7068800000
H	-5.0052590000	-2.0170130000	1.5560190000
O	5.1202270000	-1.4922620000	0.7109120000
C	5.9562270000	-1.7224930000	-0.4122050000
H	6.7735640000	-2.3469090000	-0.0534180000
H	5.4215860000	-2.2495800000	-1.2104470000
H	6.3638240000	-0.7855830000	-0.8084970000

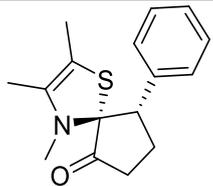
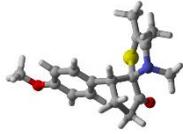
Zero-point correction= 0.344650  
(Hartree/Particle)

Thermal correction to Energy=	0.366188
Thermal correction to Enthalpy=	0.367132
Thermal correction to Gibbs Free Energy=	0.292619
Sum of electronic and zero-point Energies=	-1263.657514
Sum of electronic and thermal Energies=	-1263.635975
Sum of electronic and thermal Enthalpies=	-1263.635031
Sum of electronic and thermal Free Energies=	-1263.709545

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	229.787	81.163	156.827

#B3LYP/6-311+G\*\*

(38aa'-s)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

42

XYZ file generated by gabedit : coordinates in Angstrom

H	-0.3576690000	-2.2205020000	2.2483920000
H	-5.6425470000	2.1322670000	0.0593540000
H	0.0424120000	-3.4605290000	0.2026200000
C	0.5223800000	-1.9001210000	1.6902040000
H	1.3519510000	-1.8041910000	2.3926670000
H	0.5314760000	0.2834860000	1.6917080000
H	-3.5442540000	-1.3978610000	-1.6403350000
C	-3.0891480000	-0.8463470000	-0.8263450000
O	-5.1735090000	0.1824840000	-0.5181210000
H	-1.1873560000	-1.7444670000	-1.0830400000
C	-1.7561770000	-1.0343570000	-0.4941630000
C	-3.8723800000	0.0713680000	-0.1172470000
C	0.8941130000	-2.8740100000	0.5583500000
C	-3.2946380000	0.7990830000	0.9230820000
H	1.6740170000	-3.5921650000	0.8258960000
C	-1.1510330000	-0.3181190000	0.5521190000
H	-3.8678000000	1.5217950000	1.4882740000
C	-1.9488790000	0.5965980000	1.2390030000
C	-6.0141130000	1.1063060000	0.1579960000
H	-1.5149790000	1.1761850000	2.0477550000
C	0.2856620000	-0.5204520000	0.9974770000
H	-6.9884560000	1.0288960000	-0.3218800000
H	-6.1128770000	0.8554140000	1.2200250000
C	1.3787480000	-2.0027810000	-0.5967890000
C	1.3801430000	-0.5276270000	-0.1187860000
O	1.6615240000	-2.3867450000	-1.7016710000
N	2.6681700000	-0.1715030000	0.5104710000
H	3.3499490000	1.7192910000	2.4712000000
H	3.8041370000	-1.9292610000	0.1735120000
S	1.1113880000	0.7179150000	-1.4742970000
C	2.8061410000	1.2654400000	0.4469940000
C	3.8665610000	-0.8564510000	-0.0160850000
H	1.0030950000	3.7181240000	-0.6780810000
C	2.0938670000	1.8694670000	-0.5185930000
C	3.7107780000	1.9084950000	1.4545300000
H	4.7385910000	-0.4834910000	0.5207400000
H	3.7713670000	2.9868220000	1.3076470000
C	2.0055030000	3.3218330000	-0.8691380000
H	4.0138210000	-0.6933300000	-1.0906590000
H	4.7303950000	1.5130630000	1.3991610000
H	2.7235880000	3.9165190000	-0.3027650000
H	2.2124450000	3.4719460000	-1.9340310000

Zero-point correction=  
(Hartree/Particle)

0.346302

Thermal correction to Energy=

0.367496

Thermal correction to Enthalpy=

0.368440

Thermal correction to Gibbs Free Energy=

0.295925

Sum of electronic and zero-point Energies=

-1263.709915

Sum of electronic and thermal Energies=

-1263.688721

Sum of electronic and thermal Enthalpies=

-1263.687777

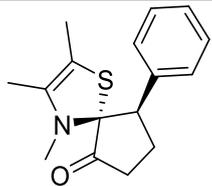
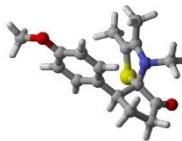
Sum of electronic and thermal Free Energies=

-1263.760292

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	230.607	80.460	152.621

#B3LYP/6-311+G\*\*

(38aa'-r)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

42

XYZ file generated by gabedit : coordinates in Angstrom

H	0.8670160000	-3.5434800000	-0.0508140000
H	-5.7792830000	-0.8171130000	-1.1679920000
H	3.0559040000	-3.0416410000	-1.0258930000
C	1.3255500000	-2.5983390000	0.2449490000
H	1.1730820000	-2.4822680000	1.3206260000
H	0.7832570000	-1.6367060000	-1.5884420000
H	-3.0169640000	-0.8281200000	2.3089940000
C	-2.6106850000	-0.8212780000	1.3043190000
O	-4.7670890000	-0.2625390000	0.5704700000
H	-0.6310710000	-1.3214000000	1.9139350000
C	-1.2731390000	-1.1034240000	1.0698090000
C	-3.4675940000	-0.5254980000	0.2379090000
C	2.8197860000	-2.5167940000	-0.0927500000
C	-2.9646560000	-0.5250940000	-1.0639600000
H	3.4934990000	-2.9133740000	0.6701780000
C	-0.7420500000	-1.1007790000	-0.2297530000
H	-3.6019890000	-0.3097870000	-1.9112580000
C	-1.6154370000	-0.8140740000	-1.2799280000
C	-5.6879740000	0.0242450000	-0.4722180000
H	-1.2379690000	-0.8081520000	-2.2969640000
C	0.7079840000	-1.4042010000	-0.5189570000
H	-6.6468260000	0.1941040000	0.0151050000
H	-5.3991570000	0.9243350000	-1.0262580000
C	3.1008100000	-1.0354140000	-0.3224090000
C	1.7488240000	-0.2565840000	-0.2800410000
O	4.1805950000	-0.5464880000	-0.5247260000
N	1.5331410000	0.4293350000	1.0046950000
H	-0.4113870000	1.5725270000	2.5437310000
H	3.0405020000	-0.4748780000	2.1783830000
S	1.6733080000	1.0502100000	-1.6002240000
C	0.8288530000	1.6596600000	0.7986290000
C	2.6627190000	0.5219280000	1.9443730000
H	-0.7167570000	3.0222590000	-1.7044900000
C	0.7851860000	2.1088150000	-0.4652520000
C	0.1940750000	2.3015680000	1.9969750000
H	2.3012850000	0.9531060000	2.8777860000
H	-0.4554900000	3.1245830000	1.7011150000
C	0.0975380000	3.3101880000	-1.0309930000
H	3.4928950000	1.1318800000	1.5672900000
H	0.9367980000	2.7071500000	2.6921060000
H	-0.3177730000	3.9417660000	-0.2446850000
H	0.7987390000	3.9191770000	-1.6119180000

Zero-point correction=  
(Hartree/Particle)

0.346304

Thermal correction to Energy=

0.367539

Thermal correction to Enthalpy=

0.368484

Thermal correction to Gibbs Free Energy=

0.295912

Sum of electronic and zero-point Energies=

-1263.713977

Sum of electronic and thermal Energies=

-1263.692742

Sum of electronic and thermal Enthalpies=

-1263.691797

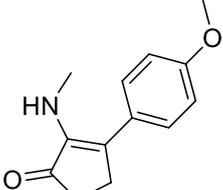
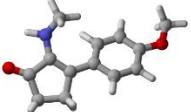
Sum of electronic and thermal Free Energies=

-1263.764369

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	230.634	80.503	152.740

#B3LYP/6-311+G\*\*

(37aa')

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

31

XYZ file generated by gabedit : coordinates in Angstrom

O	-4.5204450000	0.5358110000	-0.3912690000
H	-2.9872150000	2.2231400000	-0.1066960000
H	-1.4938500000	3.5523310000	1.0145810000
N	-2.0576930000	1.8272580000	-0.0047630000
C	-3.5020720000	-0.1241320000	-0.2822010000
C	-1.2819540000	2.4825610000	1.0475070000
H	-3.6421900000	-1.9741930000	-1.3488440000
C	-2.1550490000	0.4473260000	-0.0666060000
H	-0.2105980000	2.3464080000	0.8951100000
H	0.3367770000	1.3698590000	-1.0823010000
C	-3.3770390000	-1.6349530000	-0.3432360000
H	-4.0882730000	-2.0950920000	0.3465160000
H	-1.5312460000	2.1055210000	2.0485940000
C	-1.2278580000	-0.5519070000	0.0212360000
C	0.9092790000	0.6101700000	-0.5635660000
H	2.7775970000	1.5078190000	-1.0955680000
C	-1.9010800000	-1.9168760000	-0.0118200000
H	-1.4230870000	-2.5652760000	-0.7525560000
C	0.2318290000	-0.4428040000	0.0702010000
C	2.3002800000	0.6846990000	-0.5809040000
H	-1.8061510000	-2.4266780000	0.9536390000
C	1.0193750000	-1.4386200000	0.6830970000
H	4.9475230000	0.7428100000	-1.6045740000
C	3.0565330000	-0.3045080000	0.0547400000
H	6.1952450000	0.4953540000	-0.3572060000
H	0.5393480000	-2.2762940000	1.1754150000
O	4.4178630000	-0.3260980000	0.1083550000
C	2.4018600000	-1.3692430000	0.6870800000
C	5.1434650000	0.7187860000	-0.5273050000
H	4.9049390000	1.6943460000	-0.0902290000
H	3.0002720000	-2.1315510000	1.1714450000

Zero-point correction= 0.256214

(Hartree/Particle)

Thermal correction to Energy= 0.271423

Thermal correction to Enthalpy= 0.272367

Thermal correction to Gibbs Free Energy= 0.212997

Sum of electronic and zero-point Energies= -709.538603

Sum of electronic and thermal Energies= -709.523394

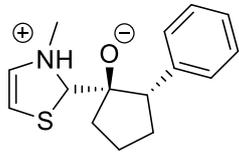
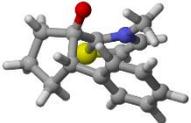
Sum of electronic and thermal Enthalpies= -709.522449

Sum of electronic and thermal Free Energies= -709.581820

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	170.320	57.059	124.955

# Cyclopentanon

#M062X/6-311+G\*\* (SI-1-syn-syn)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

35

XYZ file generated by gabedit : coordinates in Angstrom

H	4.7050300000	1.0012160000	-0.6579690000
C	3.7726000000	0.4547920000	-0.5776520000
H	2.8590370000	1.4407910000	-2.2563240000
H	4.4035040000	-0.7057380000	1.1190840000
C	2.7352620000	0.7006140000	-1.4734940000
C	3.6034320000	-0.5068190000	0.4152170000
C	1.5409460000	-0.0080590000	-1.3757260000
C	2.4080390000	-1.2098700000	0.5121940000
H	0.7473090000	0.2017520000	-2.0857150000
H	2.2630020000	-1.9379770000	1.3022700000
C	1.3560940000	-0.9750130000	-0.3806050000
S	-2.3426850000	1.0039390000	-0.6428260000
H	-2.3269800000	3.4255990000	-1.1554150000
H	-3.0393970000	-1.7457520000	-1.3180790000
C	0.0528460000	-1.6775780000	-0.1563500000
C	-1.8169300000	2.6463390000	-0.6133480000
C	-1.0776640000	0.5100680000	0.4098300000
C	-0.8666710000	-0.9524730000	0.9435040000
C	-2.1987280000	-1.7423880000	0.7223750000
C	-2.2507520000	-2.2346290000	-0.7405870000
C	-0.8540250000	-1.9478370000	-1.3527310000
H	-3.0738560000	-1.1642300000	1.0286080000
H	-0.4900550000	-2.7789970000	-1.9595400000
H	0.2561220000	-2.6231490000	0.3581710000
O	-0.3961400000	-0.9333450000	2.1626770000
H	-0.9036810000	-1.0800810000	-2.0153390000
C	-0.7372770000	2.7629080000	0.1805220000
H	-2.1117240000	-2.5769430000	1.4189720000
H	-2.4681980000	-3.3034020000	-0.7721590000
N	-0.3424120000	1.5638490000	0.7492010000
H	-0.1766480000	3.6554810000	0.4129970000
C	0.8464590000	1.5277440000	1.6286100000
H	1.7370280000	1.5623260000	0.9993190000
H	0.7880440000	0.5952620000	2.1948040000
H	0.7986390000	2.4038500000	2.2751630000

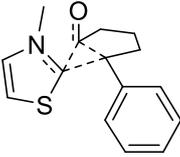
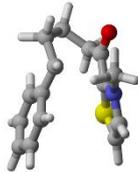
Zero-point correction= 0.291142  
(Hartree/Particle)

Thermal correction to Energy=	0.306541
Thermal correction to Enthalpy=	0.307485
Thermal correction to Gibbs Free Energy=	0.249182
Sum of electronic and zero-point Energies=	-1109.521073
Sum of electronic and thermal Energies=	-1109.505674
Sum of electronic and thermal Enthalpies=	-1109.504730
Sum of electronic and thermal Free Energies=	-1109.563032

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	192.357	62.602	122.708

#M062X/6-311+G\*\*

(SI-2-syn-syn)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

35

XYZ file generated by gabedit : coordinates in Angstrom

```

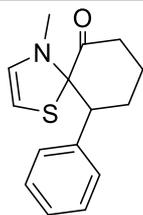
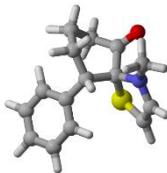
H      -0.6676140000    3.4583120000    1.3395250000
H      1.0480710000    3.6780440000    -0.6804060000
C     -0.0076720000    2.7035620000    0.9471410000
C      0.8497140000    2.8054640000    -0.0753430000
H      3.1134450000    2.4540690000    -1.4671060000
S      0.0172360000    1.0903580000    1.6064580000
N      1.5481150000    1.6389790000    -0.3526170000
H     -1.0584680000    1.1778410000    -1.8958320000
C      2.4626530000    1.5795970000    -1.4960000000
H     -3.3179090000    1.9563370000    -1.3024610000
H      1.8867050000    1.5859970000    -2.4250020000
C      1.1761270000    0.5715290000    0.4082950000
H      0.6281560000    -0.4957340000    -1.8891440000
C     -1.6846010000    0.5723090000    -1.2456640000
H      3.0531050000    0.6710420000    -1.4224090000
C     -2.9547990000    1.0125970000    -0.9103810000
C      0.1933020000    -1.0395640000    -1.0525320000
O      2.9106570000    -0.9475050000    -0.1264070000
C      1.8199010000    -0.7369650000    0.4256520000
C     -1.1778240000    -0.6490450000    -0.7632530000
C     -3.7693390000    0.2444650000    -0.0780830000
H      1.4607270000    -2.6309210000    -1.6505510000
C      0.5820350000    -2.5100840000    -1.0180140000
H     -4.7638540000    0.5850870000    0.1830320000
C      0.9382880000    -3.0227750000    0.4015430000
C      1.1960100000    -1.8057310000    1.3025780000
C     -2.0157390000    -1.4105820000    0.0691180000
C     -3.2910080000    -0.9689710000    0.4047240000
H     -0.2180480000    -3.1156180000    -1.4574410000
H      1.8328430000    -3.6443850000    0.3473710000
H      0.2537230000    -1.4665010000    1.7406080000
H      1.8876830000    -2.0401570000    2.1152510000
H     -1.6672840000    -2.3650550000    0.4486780000
H      0.1449590000    -3.6416010000    0.8275570000
H     -3.9163730000    -1.5801390000    1.0458950000

```

Zero-point correction= 0.289119  
(Hartree/Particle)

Thermal correction to Energy= 0.304882  
Thermal correction to Enthalpy= 0.305826  
Thermal correction to Gibbs Free Energy= 0.246451  
Sum of electronic and zero-point Energies= -1109.505938  
Sum of electronic and thermal Energies= -1109.490176  
Sum of electronic and thermal Enthalpies= -1109.489231  
Sum of electronic and thermal Free Energies= -1109.548606

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	191.316	62.720	124.964

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

35

XYZ file generated by gabedit : coordinates in Angstrom

```

H      0.6044430000    -3.6319170000    -0.9837220000
H      2.2372820000    -3.0911740000     1.0007540000
C      0.9047510000    -2.6591090000    -0.6333310000
C      1.7398180000    -2.3691300000     0.3667340000
H      3.5574440000    -1.2882190000     1.9140210000
S      0.3758520000    -1.1897180000    -1.4716190000
N      2.0282000000    -1.0261010000     0.5434200000
H     -1.3488440000    -1.8915840000     1.1086360000
C      2.7799080000    -0.5578000000     1.6884260000
H     -3.6938630000    -2.4065840000     0.5447970000
H      2.1649920000    -0.4172110000     2.5885850000
C      1.0655610000    -0.1458220000    -0.0957540000
H      0.1282600000    -0.1848740000     1.8274620000
C     -1.9971840000    -1.1092180000     0.7247490000
H      3.2736090000     0.3814610000     1.4361770000
C     -3.3131530000    -1.4022260000     0.4002480000
C     -0.0262510000     0.4175040000     0.9276960000
O      2.9570370000     1.0856310000    -0.9455330000
C      1.7657220000     1.0274830000    -0.8016840000
C     -1.4739480000     0.1755720000     0.5468110000
C     -4.1428800000    -0.4077670000    -0.1126270000
H      1.2579770000     1.8415540000     1.8673190000
C      0.3143800000     1.8728730000     1.3144550000
H     -5.1717450000    -0.6318460000    -0.3685560000
C      0.4835640000     2.8640110000     0.1376740000
C      0.8133920000     2.1314580000    -1.1784160000
C     -2.3180860000     1.1635700000     0.0445440000
C     -3.6416580000     0.8745820000    -0.2857540000
H     -0.4386490000     2.2393220000     2.0159300000
H      1.3032850000     3.5471660000     0.3693330000
H     -0.0990250000     1.6985130000    -1.6020190000
H      1.2758020000     2.7935080000    -1.9089500000
H     -1.9594230000     2.1757740000    -0.0893000000
H     -0.4029780000     3.4840640000    -0.0014220000
H     -4.2795070000     1.6593040000    -0.6754460000

```

Zero-point correction= 0.291205  
(Hartree/Particle)

```

Thermal correction to Energy= 0.307186
Thermal correction to Enthalpy= 0.308130
Thermal correction to Gibbs Free Energy= 0.247882
Sum of electronic and zero-point Energies= -1109.546000
Sum of electronic and thermal Energies= -1109.530019
Sum of electronic and thermal Enthalpies= -1109.529075
Sum of electronic and thermal Free Energies= -1109.589323

```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	192.762	63.284	126.803

## Python-Skripte:

Skript zum Erstellen der Input-files für MD-Simulationen. Autor: Simon Malcherek

```
import os
import math
import random

amount=int(input('How many MDs?'))

os.makedirs('created inputs')

h = open('seed_list.txt', 'a')

counter = []

while len(counter) < (amount*2):
    seed = random.randint(100000,9999999)

    h.write(str(seed)+'\n')

    g = open('sample.com', 'r')

    content = g.read()
    content = content.replace('replace', str(seed))
#    print(content)

    f = open('created inputs\MD_'+str(seed)+'.com', 'w')
    f.write(content)
    f.close()

    g = open('sample.pbs', 'r')

    content = g.read()
    content = content.replace('replace', str(seed))
#    print(content)
```

```
f = open('created inputs\MD_'+str(seed)+'.pbs', 'w')
f.write(content)
f.close()
```

```
counter=os.listdir('created inputs')
```

```
h.write('\n')
h.close()
```

Skript zur Auswertung einer Bindungslänge entlang einer MD-Trajektorie. Autor: Daniel Harms-Pollak

```
import math
import os
```

```
Atomzahl=int(input('Anzahl der Atome:'))
print('\n')
A2=int(input('Atom 1:'))
print('\n')
A1=int(input('Atom 2:'))
print('\n')
```

```
Zeile=0
Spalte=1+A2%5
if Spalte==1:
    Spalte=6
```

```
Dateienliste=[]
```

```
Dateienliste_komplett=os.listdir()
```

```
for entry in Dateienliste_komplett:
    if '.log' in entry:
        Dateienliste.append(entry)
        print(entry)
```

```
Matrix=math.ceil(A2/5)-1
```

```

if Matrix>0:
    for i in range(Matrix):
        Zeile=Zeile+1+(Atomzahl-i*5)
Zeile=Zeile+A1+1-Matrix*5

Ausgabe=[]

for i in range(len(Dateienliste)):
    Ausgabe.append([])
    file=Dateienliste[i]
    f = open(file, 'r')
    modus=0
    z=0
    for line in f:
        if modus==1:
            z=z+1
        if z==Zeile:
            #print(line.split()[Spalte])
            Ausgabe[i].append(line.split()[Spalte])
            modus=0
            z=0
        if "Distance matrix " in line:
            modus=1
    f.close()

#print(Ausgabe)

f = open('Bindungslaengen.txt', 'w')
string=""
for i in range(len(Dateienliste)):
    string=string+str(Dateienliste[i])+'\t'
f.write(string+'\n')
for i in range(len(Ausgabe[0])):
    string=""
    for j in range(len(Dateienliste)):
        string=string+str(Ausgabe[j][i])+'\t'
    f.write(string+'\n')

```

```
f.close()
```

Skript zur Bestimmung der Produktbildungszeiten in MD-Trajektorien. Autor: Simon Malcherek

```
import math
```

```
import os
```

```
def erstes_Prod (a,b,c):
```

```
    Spalte=1+b%5
```

```
    if Spalte==1:
```

```
        Spalte=6
```

```
    Zeile=0
```

```
    Matrix=math.ceil(b/5)-1
```

```
    if Matrix>0:
```

```
        for i in range(Matrix):
```

```
            Zeile=Zeile+1+(Atomzahl-i*5)
```

```
    Zeile=Zeile+a+1-Matrix*5
```

```
    Liste1=[]
```

```
    Liste1.append(c)
```

```
    for i in range(len(Dateienliste)):
```

```
        file>Dateienliste[i]
```

```
        f = open(file, 'r')
```

```
        modus=0
```

```
        z=0
```

```
        Liste1.append(Dateienliste[i])
```

```
        for line in f:
```

```
            if modus==1:
```

```
                z=z+1
```

```
            if z==Zeile and modus==1:
```

```

temp=line.split()[Spalte]
#print(temp)
trigger = float(temp)-threashold
#print(trigger)
z=0
modus=0
if trigger <=0 :
    #print('Hallo!')

    modus=2
if modus==2 and 'Time' in line:
    Liste1.append('Zeit gebildet: '+str(line.split()[2]))
    modus=3
if "Distance matrix " in line and modus==0:
    modus=1
if "Distance matrix " in line and modus==3:
    modus=4
if modus==4 and line.split()[0]==str(a):
    temp=line.split()[Spalte]
    z=0
    modus=3

f.close()
Liste1.append('Last structure '+str(temp))

return Liste1

```

```

Atomzahl=int(input('Anzahl der Atome:'))
print('\n')
A2=int(input('Atom 1 für Startmaterial:'))
print('\n')
A1=int(input('Atom 2 für Startmaterial:'))
print('\n')
A4=int(input('Atom 1 für Spiro:'))
print('\n')
A3=int(input('Atom 2 für Spiro:'))
print('\n')

```

```
threshold=float(1.75)
```

```
Dateienliste=[]
```

```
Dateienliste_komplett=os.listdir()
```

```
for entry in Dateienliste_komplett:
```

```
    if '.log' in entry:
```

```
        Dateienliste.append(entry)
```

```
        print(entry)
```

```
Ausgabe=[]
```

```
Liste_temp = erstes_Prod (A1,A2,'Startmaterial')
```

```
Ausgabe.append(Liste_temp)
```

```
Liste_temp = erstes_Prod (A3,A4,'Spiro')
```

```
Ausgabe.append(Liste_temp)
```

```
#print(Ausgabe)
```

```
f = open('first-product.txt', 'w')
```

```
string=""
```

```
for i in range(len(Ausgabe)):
```

```
    for j in range(len(Ausgabe[i])):
```

```
        string=string+str(Ausgabe[i][j])+'\n'
```

```
    string=string+'\n'
```

```
f.write(string+'\n')
```

```
f.close()
```

Skript zur Auswertung der Gesamtenergie entlang einer MD-Trajektorie. Autor: Daniel Harms-Pollak, Simon Malcherek

```
import math
import os

Atomzahl=int(input('Anzahl der Atome:'))
print('\n')
#A2=int(input('Atom 1:'))
#print('\n')
#A1=int(input('Atom 2:'))
#print('\n')

#Zeile=0
Spalte=8
#if Spalte==1:
#    Spalte=6

Dateienliste=[]

Dateienliste_komplett=os.listdir()

for entry in Dateienliste_komplett:
    if '.log' in entry:
        Dateienliste.append(entry)
        print(entry)

#Matrix=math.ceil(A2/5)-1
#if Matrix>0:
#    for i in range(Matrix):
#        Zeile=Zeile+1+(Atomzahl-i*5)
#Zeile=Zeile+A1+1-Matrix*5

Ausgabe=[]

for i in range(len(Dateienliste)):
```

```
Ausgabe.append([])
file=Dateienliste[i]
f = open(file, 'r')
modus=0
z=0
for line in f:
    if modus==2:
        z=z+1
        #print(line)
        Ausgabe[i].append(line.split()[Spalte])
        modus=0
        z=0
    if "Summary information " in line:
        modus=1
    if "Time " in line and modus==1:
        modus=2
f.close()
```

```
print(Ausgabe)
```

```
f = open('Energieliste.txt', 'w')
string=""
for i in range(len(Dateienliste)):
    string=string+str(Dateienliste[i])+'\t'
f.write(string+'\n')
for i in range(len(Ausgabe[0])):
    string=""
    for j in range(len(Dateienliste)):
        string=string+str(Ausgabe[j][i])+'\t'
    f.write(string+'\n')

f.close()
```

Skript zur Auswertung der Spinkontamination entlang von MD-Trajektorien. Autor: Simon Malcherek

```
import math
```

```
import os
```

```
Dateienliste=[]
```

```
Dateienliste_komplett=os.listdir()
```

```
for entry in Dateienliste_komplett:
```

```
    if '.log' in entry:
```

```
        Dateienliste.append(entry)
```

```
        print(entry)
```

```
Ausgabe=[]
```

```
for i in range(len(Dateienliste)):
```

```
    Ausgabe.append(['before'],['after'])
```

```
    file=Dateienliste[i]
```

```
    f = open(file, 'r')
```

```
    modus=0
```

```
    z=0
```

```
    for line in f:
```

```
        if modus==1:
```

```
            z=z+1
```

```
            #print(line)
```

```
            #print(line.split())
```

```
            Ausgabe[i][0].append(line.split()[3])
```

```
            Ausgabe[i][1].append(line.split()[5])
```

```
            modus=0
```

```
            z=0
```

```
        if "spin contaminant" in line:
```

```
            modus=1
```

```
    f.close()
```

```
print(Ausgabe)
```

```

f = open('spinliste.txt', 'w')
string=""
for i in range(len(Dateienliste)):
    string=string+'{: <20}'.format(str(Dateienliste[i]))
f.write(string+'\n')
for i in range(len(Ausgabe[0][0])):
    string=""
    for j in range(len(Dateienliste)):
        string=string+'{: <10}'.format(str(Ausgabe[j][0][i]))+'{: <10}'.format(str(Ausgabe[j][1][i]))
    f.write(string+'\n')

f.close()

```

Skript zum Mitteln einer Struktur eines Rechenschrittes über mehrere MD-Trajektorien. Autor:  
Daniel Harms-Pollak, Simon Malcherek

```

import math
import os

```

```

Atomzahl=int(input('Anzahl der Atome:'))
print('\n')

```

```

def Matrix_Mittel (Matrixnummer):

```

```

    counter = 1

```

```

#Einlesen der Dateien im Ordner

```

```

    Dateienliste=[]

```

```

    Dateienliste_komplett=os.listdir()

```

```

    for entry in Dateienliste_komplett:

```

```
if '.log' in entry:
```

```
    Dateienliste.append(entry)
```

```
Matrix=[]
```

```
Atomliste=[]
```

```
for i in range(Atomzahl):
```

```
    Matrix.append([])
```

```
    Atomliste.append('a')
```

```
    for j in range(4):
```

```
        Matrix[i].append([])
```

```
#öffnen der Dateien und lesen der gesuchten Matrix
```

```
for i in range(len(Dateienliste)):
```

```
    file=Dateienliste[i]
```

```
    f = open(file, 'r')
```

```
    z=0
```

```
    Modus=0
```

```
    for line in f:
```

```
        if Modus==1:
```

```
            a=line.split()
```

```
            if a[0]=="Distance" or a[0]=="Stoichiometry":
```

```
                Modus=0
```

```
            else:
```

```
                if '.' in line:
```

```
                    Atomliste[int(a[0])-1]=a[1]
```

```
                    #print(line)
```

```
                    for j in range(3):
```

```
                        Matrix[int(a[0])-1][j].append(float(a[j+3]))
```

```
                else:
```

```
                    b=line.split()
```

```
            if "Input orientation" in line:
```

```
                z=z+1
```

```
            if z==Matrixnummer+1:
```

```
Modus=1
counter = 0
```

```
f.close()
```

```
#averagen der Matrizen
```

```
for i in range(Atomzahl):
    for j in range(3):
        x=0
        z=0
        #print(i, j)
        for k in range(len(Matrix[i][j])):
            x=x+Matrix[i][j][k]
            z=z+1
        if z>0:
            Matrix[i][j][0]=x/z
```

```
#schreiben der Matrizen in output datei
```

```
f = open('BindungslaengenMatrix_Mittelwerte'+str(Matrixnummer)+'.txt', 'w')
```

```
for i in range(Atomzahl):
    Text=Atomliste[i]+'\\t'
    for j in range(3):
        if len(Matrix[i][j])!=0:
            Text=Text+str(Matrix[i][j][0]+'\\t'
    Text=Text+'\\n'
    f.write(Text)
```

```
f.close()
```

```
return counter
```

```
Matrixnummer = 1
counter = 0
```

```
while counter == 0:
    counter = Matrix_Mittel (Matrixnummer)
    Matrixnummer += 5    # jede fünfte Matrix
```

Skript zum Berechnen der Bindungsabstände aus gemittelten Md-Strukturen. Autor: Simon Malcherek

```
import math
import os
```

```
def BerechnungderAbstaende (Atomabstaende,Atom1,Atom2):
```

```
    #print(len(Dateienliste))
    for i in range (len(Dateienliste)):
        Atomabstaende[0].append(Dateienliste[i])
        file=Dateienliste[i]
        #print(file)
        f=open(file)
        #print(f)
        f_lines=f.readlines()
        #print(f_lines)
        f.close()
        a1=f_lines[Atom1].split()
        a2=f_lines[Atom2].split()
        #Abstände der Atome
        a=float(a1[1])-float(a2[1])
        b=float(a1[2])-float(a2[2])
        c=float(a1[3])-float(a2[3])
        #print(a,b,c)

        Abstand=pow(pow(a,2)+pow(b,2)+pow(c,2),0.5)
        Atomabstaende[1].append(Abstand)
```

```
    return Atomabstaende
```

```
#Einlesen der Matrizen
```

```
Dateienliste=[]
```

```
Dateienliste_komplett=os.listdir()
```

```
for entry in Dateienliste_komplett:
```

```
    if ('BindungslaengenMatrix_Mittelwerte' in entry) and ('.txt' in entry):
```

```
        Dateienliste.append(entry)
```

```
#print(Dateienliste)
```

```
#Erstellen der Listen für die Abstände
```

```
Atomabstaende=[[[],[]]]
```

```
#Abfrage der Atome deren Abstand berechnet werden soll.
```

```
Atom1=(int(input('Atom 1:'))-1)
```

```
print('\n')
```

```
Atom2=(int(input('Atom 2:'))-1)
```

```
print('\n')
```

```
Atomabstaende=BerechnungderAbstaende (Atomabstaende,Atom1,Atom2)
```

```
#print(Atomabstaende)
```

```
#print(len(Atomabstaende[0]))
```

```
#print(len(Atomabstaende[1]))
```

```
#schreiben der Matrizen in output datei
```

```
output=open('Atomabstaende Atom'+str(Atom1+1)+'Atom'+str(Atom2+1)+'.txt','w')
```

```
Text=str("")
```

```
for i in range(len(Atomabstaende[0])):
```

```
    for j in range (2):
```

```
        if j==0:
```

```
            #print(Atomabstaende[i][j])
```

```
            Text=Text+str(Atomabstaende[j][i])+'\t'
```

```
        else:
```

```
#print(Atomabstaende[i][j])
Text=Text+str(Atomabstaende[j][i])+'\n'
output.write(Text)
output.close()
```

Skript zum Auslesen einer Bindungslänge entlang einer IRC. Autor: Simon Malcherek

```
import math
import os

#Definieren der Atome und Matrixlänge
Atomzahl=int(input('Anzahl der Atome:'))
print('\n')
A2=int(input('Atom 1:'))
print('\n')
A1=int(input('Atom 2:'))
print('\n')

#Lesemodus für Tabelle 'Distance Matrix'
Zeile=0
Spalte=1+A2%5
if Spalte==1:
    Spalte=6

#Erfassen der Dateien

Dateienliste_komplett=os.listdir()

for i in range (len(Dateienliste_komplett)):
    print(i, Dateienliste_komplett[i])

choice = int(input('Welche Datei?'))

file = Dateienliste_komplett[choice]
```

```

Matrix=math.ceil(A2/5)-1
if Matrix>0:
    for i in range(Matrix):
        Zeile=Zeile+1+(Atomzahl-i*5)
Zeile=Zeile+A1+1-Matrix*5

#Lesen des Bindungsabstands
Ausgabe=[]

f = open(file, 'r')
modus=0
z=0
for line in f:
    if modus==1:
        z=z+1
    if z==Zeile and modus==1:
        #print(line.split()[Spalte])
        temp=(line.split()[Spalte])
        modus=2
    if "Convergence NOT Met" in line:
        modus=0
        z=0
    if "Convergence Met" in line and modus==2:
        Ausgabe.append(temp)
        modus=0
        z=0
    if "Calculating another point on the path" in line and modus==2:
        Ausgabe.append(temp)
        modus=0
        z=0
    if "Distance matrix " in line:
        modus=1
f.close()

#print(Ausgabe)

f = open('Bindungslaengen_IRC.txt', 'w')
string=""

```

```
for i in range(len(Ausgabe)):
    string=string+str(Ausgabe[i])+'\n'
f.write(string+'\n')

f.close()
```

Skript zum Berechnen eines Bindungswinkels entlang einer IRC. Autor: Simon Malcherek

```
import math
import os

#Erfassen der Dateien

Dateienliste_komplett=os.listdir()

for i in range (len(Dateienliste_komplett)):
    print(i, Dateienliste_komplett[i])

choice = int(input('Welche Datei?'))

file = Dateienliste_komplett[choice]

#Definieren der Atome und Matrixlänge
Bx=[]
Cx=[]
Atomzahl=int(input('Anzahl der Atome:'))
print('\n')
print('Es wird der Winkel zwischen zwei Bindungen berechnet:')
Cx.append(int(input('Bindung 1 Atom 1:')))
print('\n')
Bx.append(int(input('Bindung 1 Atom 2:')))
print('\n')
Cx.append(int(input('Bindung 2 Atom 1:')))
print('\n')
Bx.append(int(input('Bindung 2 Atom 2:')))
print('\n')
```

```
Beträge=[[[],[]]]
```

```
for i in range (2):
```

```
    #print(i)
```

```
    A1=Bx[i]
```

```
    A2=Cx[i]
```

```
    #print(A1,A2)
```

```
    #Lesemodus für Tabelle 'Distance Matrix'
```

```
    Zeile=0
```

```
    Spalte=1+A2%5
```

```
    if Spalte==1:
```

```
        Spalte=6
```

```
    Matrix=math.ceil(A2/5)-1
```

```
    if Matrix>0:
```

```
        for i in range(Matrix):
```

```
            Zeile=Zeile+1+(Atomzahl-i*5)
```

```
    Zeile=Zeile+A1+1-Matrix*5
```

```
#Lesen des Bindungsabstands (Vektorbeträge)
```

```
f = open(file, 'r')
```

```
modus=0
```

```
z=0
```

```
for line in f:
```

```
    if modus==1:
```

```
        z=z+1
```

```
    if z==Zeile and modus==1:
```

```
        #print(line.split()[Spalte])
```

```
        temp=(line.split()[Spalte])
```

```
        modus=2
```

```
    if "Convergence NOT Met" in line:
```

```
        modus=0
```

```
        z=0
```

```
    if "Convergence Met" in line and modus==2:
```

```
        Beträge[i-1].append(temp)
```

```
        modus=0
```

```
        z=0
        if "Calculating another point on the path" in line and modus==2:
            Beträge[i-1].append(temp)
            modus=0
            z=0
        if "Distance matrix " in line:
            modus=1
    f.close()
```

```
#print(Beträge)
```

```
# Lesen der Vektoren
```

```
if Bx[0]==Cx[0]:
```

```
    A=Bx[0]
```

```
    B=Bx[1]
```

```
    C=Cx[1]
```

```
elif Bx[0]==Cx[1]:
```

```
    A=Bx[0]
```

```
    B=Bx[1]
```

```
    C=Cx[0]
```

```
elif Bx[0]==Bx[1]:
```

```
    A=Bx[0]
```

```
    B=Cx[0]
```

```
    C=Cx[1]
```

```
elif Bx[1]==Cx[0]:
```

```
    A=Bx[1]
```

```
    B=Bx[0]
```

```
    C=Cx[1]
```

```
elif Bx[1]==Cx[1]:
```

```
    A=Bx[1]
```

```
    B=Bx[0]
```

```
    C=Cx[0]
```

```
elif Cx[0]==Cx[1]:
```

```
    A=Cx[0]
```

```
    B=Bx[0]
```

```
C=Bx[1]
```

```
#print(A,B,C)
```

```
PunkteA=[[],[],[[
```

```
PunkteB=[[],[],[[
```

```
PunkteC=[[],[],[[
```

```
f = open(file, 'r')
```

```
modus=0
```

```
for line in f:
```

```
    if modus==1:
```

```
        #print(line.split())
```

```
        temp=(line.split())
```

```
        if temp[0]==str(A):
```

```
            tempA0=temp[3]
```

```
            tempA1=temp[4]
```

```
            tempA2=temp[5]
```

```
        elif temp[0]==str(B):
```

```
            tempB0=temp[3]
```

```
            tempB1=temp[4]
```

```
            tempB2=temp[5]
```

```
        elif temp[0]==str(C):
```

```
            tempC0=temp[3]
```

```
            tempC1=temp[4]
```

```
            tempC2=temp[5]
```

```
    if "Distance matrix" in line:
```

```
        modus=2
```

```
    if "Convergence Met" in line and modus==2:
```

```
        PunkteA[0].append(tempA0)
```

```
        PunkteA[1].append(tempA1)
```

```
        PunkteA[2].append(tempA2)
```

```
        PunkteB[0].append(tempB0)
```

```
        PunkteB[1].append(tempB1)
```

```
        PunkteB[2].append(tempB2)
```

```
        PunkteC[0].append(tempC0)
```

```
        PunkteC[1].append(tempC1)
```

```
        PunkteC[2].append(tempC2)
```

```
    modus=0
```

```

if "Calculating another point on the path" in line and modus==2:
    PunkteA[0].append(tempA0)
    PunkteA[1].append(tempA1)
    PunkteA[2].append(tempA2)
    PunkteB[0].append(tempB0)
    PunkteB[1].append(tempB1)
    PunkteB[2].append(tempB2)
    PunkteC[0].append(tempC0)
    PunkteC[1].append(tempC1)
    PunkteC[2].append(tempC2)
    modus=0
if "Input orientation" in line:
    modus=1
f.close()

#print(Beträge)
#print(PunkteA)
#print(PunkteB)
#print(PunkteC)

#Berechnung des Winkels mit dem Skalarprodukt
Produkt=[]

for i in range(len(Beträge[0])):
    Winkel=(float(PunkteB[0][i])-float(PunkteA[0][i]))*(float(PunkteC[0][i])-float(PunkteA[0][i]))
    Winkel=Winkel+(float(PunkteB[1][i])-float(PunkteA[1][i]))*(float(PunkteC[1][i])-float(PunkteA[1][i]))
    Winkel=Winkel+(float(PunkteB[2][i])-float(PunkteA[2][i]))*(float(PunkteC[2][i])-float(PunkteA[2][i]))
    Winkel=Winkel/(float(Beträge[0][i])*float(Beträge[1][i]))
    Winkel=math.acos(Winkel)
    Winkel=math.degrees(Winkel)
    Produkt.append(Winkel)

f = open('Bindungswinkel_IRC.txt', 'w')
string=""
for i in range(len(Produkt)):
    string=string+str(Produkt[i])+'\n'
f.write(string+'\n')
f.close()

```

Skript zum Erstellen von Input-files zur Berechnung der orthogonalen Frequenzen der Strukturen entlang einer IRC. Autor: Simon Malcherek

```
import math
import os
```

```
Dateienliste = []
```

```
Dateienliste_komplett=os.listdir()
```

```
for i in range (len(Dateienliste_komplett)):
    print(i, Dateienliste_komplett[i])
```

```
choice = int(input('Welche Datei?'))
```

```
file = Dateienliste_komplett[choice]
```

```
f = open(file,'r')
```

```
Text_pbs = '#!/bin/bash'+'\n'+###+'\n'+### queue/job setup, adapt these to your
needs!'+'\n'+###+'\n'+\t'+# desired queue'+'\n'+#PBS -q rehbein'+'\n'+\t'+# number of nodes, cores per
node'+'\n'
```

```
Text_pbs = Text_pbs +'#PBS -l nodes=1:ppn=6'+'\n'+# estimated runtime'+'\n'+#PBS -l
walltime=00:05:00'+'\n'+\t'+# max. memory per process'+'\n'+#PBS -l
pmem=700mB'+'\n'+\n'+#ATHOS -deps athos-gaussian'+'\n'+\n'
```

```
Text_pbs = Text_pbs +'#ATHOS -o req-cpuset'+'\n'+\n'+source
/software/g09.ifort.avx.mkl/bsd/g09.profile'+'\n'+PATH=$PATH:/software/g09.ifort.avx.mkl:/software/N
BO6/bin'+'\n'+export PATH'+'\n'
```

```
modus = 0
```

```
z = 0
```

```
n = 0
```

```
matrix_temp = []
```

```
for line in f:
```

```
    if modus == 3:
```

```
        matrix_temp.append(line)
```

```
        #print(line)
```

```
    if '----' in line and modus == 3:
```

```
        modus = 4
```

```
    if 'Input orientation:' in line:
```

```

matrix_temp = []
modus = 1
#print(line)
if '-----' in line and modus == 2:
    modus = 3
if '-----' in line and modus == 1:
    modus = 2
    #print(line)
if 'Calculating another point on the path.' in line and modus == 4:
    Text = '%mem=6GB'+'\n'
    Text = Text+'%nprocs=4'+'\n'
    Text = Text+'%nosave'+'\n'
    Text = Text+'#M062X/6-311+G** projected'+'\n'
    Text = Text+'\n'
    Text = Text+'projected frequencies step'+str(n)+'\n'
    Text = Text+'\n'
    Text = Text+'0 1'+'\n'
    for j in range (len(matrix_temp)-1):
        Text = Text+str(matrix_temp[j])
    Text = Text+'\n'
    g = open('IRC_projected'+str(n)+'.com', 'w')
    g.write(Text)
    g.close()

    Text_pbs_X = Text_pbs +'\n'+'\n'+cd "${PBS_O_WORKDIR}"+'\t'+# change work directory
to the job-submit directory'+'\n'+g09 IRC_projected'+str(n)+'.com > IRC_projected'+str(n)+'.com'+'\t'+#
start Gaussian09'

    h = open('IRC_projected'+str(n)+'.pbs', 'w')
    h.write(Text_pbs_X)
    h.close()

n=n+1

```





```
h.write(Text_pbs_X)
h.close()

n=n+1
```

Skript zum Auslesen der NBO-Ladungen aus mehreren NBO-Analysen entlang einer IRC.  
Autor: Simon Malcherek

```
import math
import os

Dateienliste_komplett=os.listdir()

Dateienliste = []

for i in range (len(Dateienliste_komplett)):
    if '.log' in Dateienliste_komplett[i]:
        Dateienliste.append(Dateienliste_komplett[i])

Ergebnisse = []

for i in range (len(Dateienliste)):
    file = Dateienliste[i]

    f = open(file,'r')

    modus = 0
    Ergebnisse.append([])
    for line in f:
        if '===' in line and modus == 3:
            modus = 0
        if modus == 3:
            temp = line.split()
            Ergebnisse[i].append(temp[2])
            # print(Ergebnisse[i])
        if 'Summary of Natural Population Analysis:' in line:
```

```

matrix_temp = []
modus = 1
#print(line)
if '----' in line and modus == 2:
    modus = 3
if 'Charge' in line and modus == 1:
    modus = 2
#print(line)
f.close()

# output

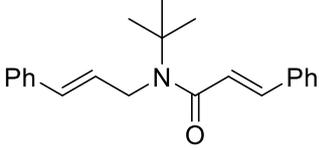
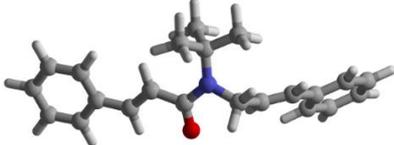
f = open('charges.txt', 'w')
string='\t'
for i in range(len(Dateienliste)):
    string=string+'{: <25}'.format(str(Dateienliste[i]))
f.write(string+'\n')
for i in range(len(Ergebnisse[0])):
    string=str(i+1)+'\t'
    for j in range(len(Dateienliste)):
        string=string+'{: <25}'.format(str(Ergebnisse[j][i]))
    f.write(string+'\n')

f.close()

```

# Berechnungen zur photoaktivierten Synthese von enantiomerenreinen $\gamma$ -Cyclobutanaminosäuren und 3-(Aminomethyl)-5-phenylpentansäuren

#B3LYP/6-311+G\*\* 69-lin-<sup>t</sup>Bu

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

xyz-matrix

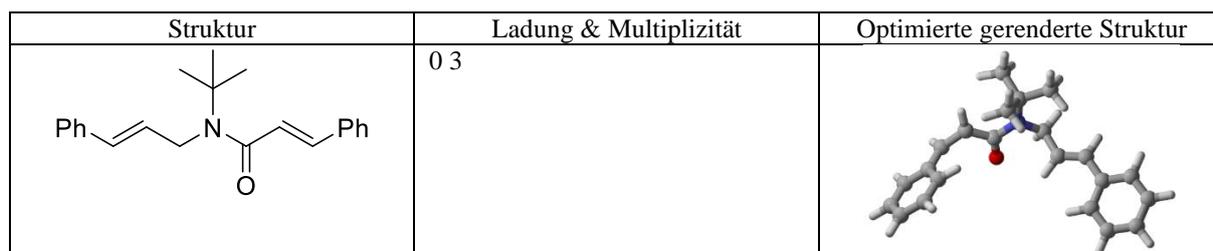
6	-3.611896000	0.390215000	0.667884000
6	-2.319144000	0.102421000	0.859879000
6	-1.326527000	1.048454000	1.480485000
7	-0.074516000	1.201265000	0.701516000
6	0.849856000	0.201744000	0.961136000
6	0.059755000	2.301859000	-0.324070000
6	2.219267000	0.248415000	0.370054000
8	0.551385000	-0.730393000	1.710166000
6	3.055888000	-0.784200000	0.562172000
6	-1.265389000	3.081075000	-0.466390000
6	1.122988000	3.332405000	0.117415000
6	0.354411000	1.710807000	-1.721011000
6	-4.651585000	-0.495137000	0.119692000
6	-5.906700000	0.045936000	-0.200610000
6	-6.920166000	-0.745057000	-0.736414000
6	-6.701646000	-2.102309000	-0.959993000
6	-5.462246000	-2.659044000	-0.637386000
6	-4.452212000	-1.868741000	-0.101896000
6	4.435087000	-0.915537000	0.086778000
6	5.125829000	-2.108073000	0.359591000
6	6.437606000	-2.295888000	-0.066856000
6	7.090330000	-1.290674000	-0.776347000
6	6.420132000	-0.096961000	-1.054598000
6	5.111278000	0.088884000	-0.629016000
1	-3.961058000	1.388006000	0.932469000
1	-1.916886000	-0.872864000	0.604634000
1	-1.775022000	2.025330000	1.644374000
1	-1.034393000	0.651281000	2.454523000
1	2.541122000	1.110121000	-0.190450000
1	2.667171000	-1.620325000	1.136442000
1	-1.145919000	3.798949000	-1.280731000
1	-2.101161000	2.427762000	-0.717251000
1	-1.515223000	3.651720000	0.430181000
1	1.157467000	4.160196000	-0.596701000
1	2.128053000	2.921176000	0.194693000
1	0.859291000	3.740786000	1.096294000
1	-0.466046000	1.056958000	-2.026677000
1	0.434786000	2.519019000	-2.453246000
1	1.273837000	1.130533000	-1.764523000
1	-6.085539000	1.102723000	-0.028735000
1	-7.879862000	-0.301126000	-0.977092000
1	-7.488100000	-2.722821000	-1.374336000
1	-5.286153000	-3.717082000	-0.797752000
1	-3.503701000	-2.324536000	0.156668000
1	4.621151000	-2.892825000	0.913040000
1	6.949079000	-3.225530000	0.155812000
1	8.112223000	-1.431921000	-1.109489000
1	6.923550000	0.690548000	-1.604332000
1	4.612373000	1.024661000	-0.852741000

Zero-point correction=  
(Hartree/Particle)

0.414712

Thermal correction to Energy=	0.437996		
Thermal correction to Enthalpy=	0.438940		
Thermal correction to Gibbs Free Energy=	0.357909		
Sum of electronic and zero-point Energies=	-983.197296		
Sum of electronic and thermal Energies=	-983.174011		
Sum of electronic and thermal Enthalpies=	-983.173067		
Sum of electronic and thermal Free Energies=	-983.254098		
	E (Thermal)	CV	S
Total	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
	274.847	89.685	170.544

#UB3LYP/6-311+G**	71-lin-'Bu
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xyz-matrix

6	3.245781000	0.418777000	-0.643149000
6	1.928139000	0.413350000	-0.877402000
6	1.141443000	1.627552000	-1.294194000
7	-0.075929000	1.860356000	-0.483031000
6	-1.167609000	1.116055000	-0.918517000
6	-0.035357000	2.754204000	0.730792000
6	-2.502479000	1.280811000	-0.333621000
8	-1.037486000	0.306912000	-1.846927000
6	-3.624205000	0.489355000	-0.838077000
6	1.402753000	3.247312000	0.997330000
6	-0.896647000	4.017486000	0.506858000
6	-0.460625000	1.974993000	1.995474000
6	4.095339000	-0.728612000	-0.287293000
6	5.426479000	-0.497144000	0.093492000
6	6.269868000	-1.546481000	0.450495000
6	5.799717000	-2.857330000	0.430275000
6	4.480577000	-3.106236000	0.045521000
6	3.640377000	-2.058323000	-0.311158000
6	-4.116021000	-0.702754000	-0.259860000
6	-5.238959000	-1.366433000	-0.831395000
6	-5.742900000	-2.528707000	-0.275715000
6	-5.153687000	-3.082236000	0.867991000
6	-4.045726000	-2.451753000	1.445764000
6	-3.532107000	-1.287867000	0.898807000
1	3.775394000	1.368574000	-0.713130000
1	1.350165000	-0.503397000	-0.815101000
1	1.767842000	2.516214000	-1.276943000
1	0.802112000	1.482216000	-2.321830000
1	-2.709898000	2.045194000	0.403626000
1	-4.118780000	0.854795000	-1.736971000
1	1.396217000	3.814450000	1.930536000
1	2.104712000	2.421196000	1.112693000
1	1.766324000	3.917724000	0.216284000
1	-0.807302000	4.686799000	1.367258000
1	-1.955143000	3.804365000	0.364200000
1	-0.545590000	4.554608000	-0.377837000
1	0.207696000	1.124296000	2.148971000
1	-0.390787000	2.625500000	2.871444000
1	-1.480444000	1.596581000	1.948105000
1	5.801478000	0.521397000	0.110193000
1	7.293648000	-1.339506000	0.742098000
1	6.453030000	-3.677898000	0.704242000
1	4.108245000	-4.124408000	0.016870000
1	2.625326000	-2.275951000	-0.621943000
1	-5.698338000	-0.944883000	-1.719122000
1	-6.598834000	-3.014922000	-0.730861000

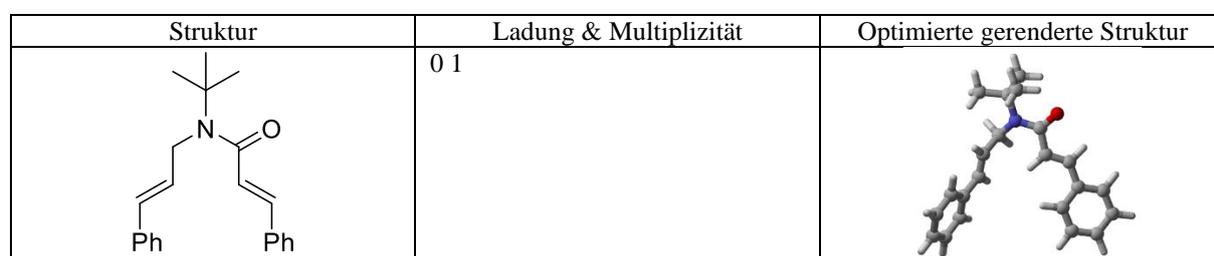
1	-5.550752000	-3.993047000	1.300761000
1	-3.582130000	-2.879549000	2.328113000
1	-2.667715000	-0.814262000	1.350466000

Zero-point correction= 0.410800  
(Hartree/Particle)

Thermal correction to Energy=	0.434332
Thermal correction to Enthalpy=	0.435276
Thermal correction to Gibbs Free Energy=	0.353818
Sum of electronic and zero-point Energies=	-983.117589
Sum of electronic and thermal Energies=	-983.094058
Sum of electronic and thermal Enthalpies=	-983.093114
Sum of electronic and thermal Free Energies=	-983.174572

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	272.547	91.406	171.443

#B3LYP/6-311+G**	69-NAC-Bu
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xyz-matrix

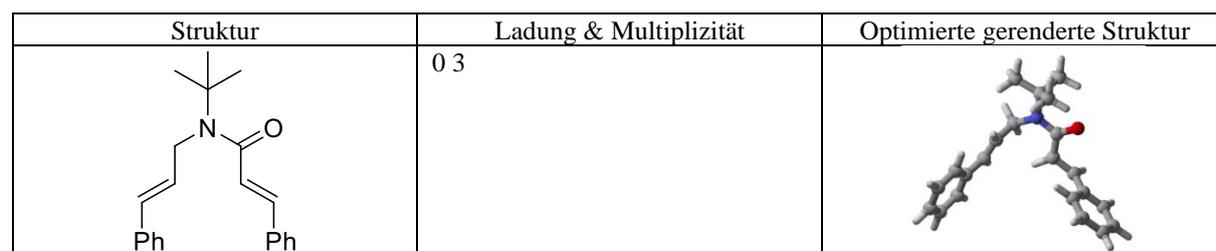
6	-1.993483000	-0.553999000	-0.884271000
6	-1.768977000	0.699558000	-0.472368000
6	-0.781160000	1.630022000	-1.131840000
7	0.012048000	2.456690000	-0.199606000
6	1.279840000	2.027556000	0.158590000
6	-0.383597000	3.894869000	0.047622000
6	1.550138000	0.562009000	0.045816000
8	2.145391000	2.789537000	0.580826000
6	2.808859000	0.104999000	0.136827000
6	-1.887310000	4.100338000	-0.224343000
6	-0.149890000	4.248899000	1.531020000
6	0.420556000	4.828534000	-0.877684000
6	-2.953458000	-1.524543000	-0.335897000
6	-3.093819000	-2.768791000	-0.970341000
6	-3.987563000	-3.725756000	-0.495565000
6	-4.761094000	-3.459399000	0.631268000
6	-4.630974000	-2.228030000	1.277124000
6	-3.740180000	-1.273779000	0.801351000
6	3.254113000	-1.290238000	0.103114000
6	4.633203000	-1.556809000	0.091120000
6	5.114942000	-2.862556000	0.055386000
6	4.224370000	-3.933347000	0.036787000
6	2.849372000	-3.686796000	0.055979000
6	2.369643000	-2.383841000	0.089413000
1	-1.414082000	-0.922305000	-1.730640000
1	-2.318380000	1.112350000	0.368088000
1	-0.107702000	1.059878000	-1.774674000
1	-1.311363000	2.305305000	-1.805228000
1	0.715113000	-0.117346000	-0.060459000
1	3.590214000	0.852088000	0.250788000
1	-2.149093000	5.114521000	0.083682000
1	-2.155759000	4.011472000	-1.278749000
1	-2.507960000	3.412282000	0.354133000
1	-0.497346000	5.269332000	1.714686000
1	0.899976000	4.184141000	1.802446000
1	-0.722343000	3.575597000	2.175448000
1	0.242911000	4.576737000	-1.927971000
1	0.110098000	5.866648000	-0.725471000
1	1.487122000	4.748571000	-0.673053000

1	-2.494906000	-2.983742000	-1.849670000
1	-4.078343000	-4.678143000	-1.005894000
1	-5.456998000	-4.201371000	1.005728000
1	-5.226402000	-2.013484000	2.157674000
1	-3.652542000	-0.328046000	1.323291000
1	5.330065000	-0.725443000	0.108829000
1	6.183998000	-3.042860000	0.045015000
1	4.594718000	-4.951937000	0.012096000
1	2.150780000	-4.516128000	0.050153000
1	1.299570000	-2.214640000	0.115732000

Zero-point correction= 0.414419  
(Hartree/Particle)  
Thermal correction to Energy= 0.437767  
Thermal correction to Enthalpy= 0.438712  
Thermal correction to Gibbs Free Energy= 0.357551  
Sum of electronic and zero-point Energies= -983.201184  
Sum of electronic and thermal Energies= -983.177836  
Sum of electronic and thermal Enthalpies= -983.176892  
Sum of electronic and thermal Free Energies= -983.258053

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	274.703	89.810	170.817

#UB3LYP/6-311+G**	71-NAC-Bu
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xyz-matrix

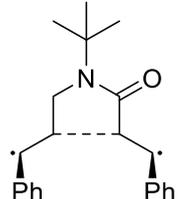
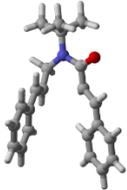
6	-2.430898000	0.094596000	-1.015828000
6	-1.784159000	1.105571000	-0.423277000
6	-0.791508000	1.996572000	-1.128293000
7	0.429455000	2.287977000	-0.357991000
6	1.513035000	1.423085000	-0.420942000
6	0.556288000	3.565669000	0.444391000
6	1.344417000	0.131569000	-1.106234000
8	2.605827000	1.688800000	0.088840000
6	2.495924000	-0.734958000	-1.350635000
6	-0.766724000	4.354544000	0.448266000
6	0.891708000	3.222050000	1.911167000
6	1.642279000	4.468759000	-0.175568000
6	-3.439451000	-0.798072000	-0.424778000
6	-3.875985000	-1.908679000	-1.163688000
6	-4.819703000	-2.793585000	-0.648359000
6	-5.352694000	-2.583730000	0.620979000
6	-4.934981000	-1.479495000	1.366771000
6	-3.994028000	-0.596793000	0.850643000
6	2.930969000	-1.780318000	-0.504245000
6	4.059633000	-2.571738000	-0.860777000
6	4.494417000	-3.604317000	-0.049048000
6	3.828466000	-3.893808000	1.148512000
6	2.717437000	-3.128588000	1.521675000
6	2.273224000	-2.092028000	0.718542000
1	-2.195183000	-0.118788000	-2.058335000
1	-1.965257000	1.339567000	0.622215000
1	-0.519176000	1.564442000	-2.093701000
1	-1.269515000	2.945593000	-1.367549000
1	0.362661000	-0.216615000	-1.408113000
1	3.061252000	-0.559541000	-2.265119000
1	-0.643242000	5.205142000	1.121605000
1	-1.022409000	4.760284000	-0.533337000

1	-1.609956000	3.766297000	0.818102000
1	0.979132000	4.144936000	2.491493000
1	1.828947000	2.676036000	1.988071000
1	0.093029000	2.619408000	2.353744000
1	1.390822000	4.706970000	-1.213417000
1	1.701488000	5.408852000	0.381109000
1	2.616773000	3.986067000	-0.151621000
1	-3.464778000	-2.080034000	-2.153333000
1	-5.137934000	-3.645571000	-1.238666000
1	-6.088851000	-3.268786000	1.025713000
1	-5.350060000	-1.304310000	2.353148000
1	-3.694174000	0.260290000	1.442355000
1	4.581734000	-2.350860000	-1.785849000
1	5.357965000	-4.191440000	-0.342119000
1	4.172025000	-4.703053000	1.782335000
1	2.200446000	-3.346745000	2.449855000
1	1.415458000	-1.502221000	1.020999000

Zero-point correction= 0.410393  
(Hartree/Particle)  
Thermal correction to Energy= 0.433978  
Thermal correction to Enthalpy= 0.434922  
Thermal correction to Gibbs Free Energy= 0.352383  
Sum of electronic and zero-point Energies= -983.121114  
Sum of electronic and thermal Energies= -983.097529  
Sum of electronic and thermal Enthalpies= -983.096585  
Sum of electronic and thermal Free Energies= -983.179124

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.325	91.581	173.719

#UB3LYP/6-311+G**	73-Bu-cis
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Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3  $\nu_{imag} = -171.5 \text{ cm}^{-1}$	

xyz-matrix

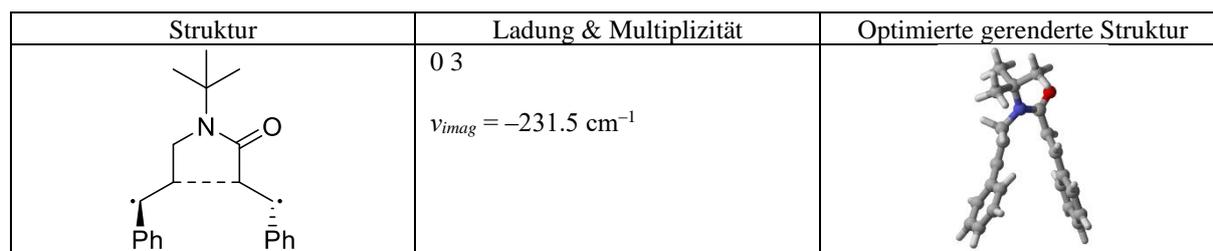
1	-2.691259000	1.026965000	1.923653000
1	-4.800448000	0.131722000	2.065473000
1	-2.012506000	-0.522342000	2.358134000
1	2.039818000	1.339891000	1.668125000
1	0.074861000	0.517029000	2.050231000
1	-4.507967000	1.658963000	1.201151000
6	-2.061479000	0.221906000	1.551055000
1	4.127515000	2.543303000	1.229470000
6	-0.665386000	0.762624000	1.295676000
6	2.063514000	2.085531000	0.882711000
6	-4.866324000	0.631838000	1.095726000
1	-5.923262000	0.687066000	0.826135000
6	3.248797000	2.764458000	0.633860000
1	3.872158000	-2.339994000	2.423303000
6	-0.370135000	1.676492000	0.341541000
6	0.907293000	2.345856000	0.120995000
1	-4.762418000	-2.072946000	0.776278000
1	1.547284000	-1.880239000	1.808023000
1	-1.153450000	1.935969000	-0.367700000
7	-2.681791000	-0.342759000	0.343918000
6	-4.131452000	-0.141008000	-0.012758000
6	3.317950000	3.722729000	-0.380143000
6	3.584381000	-2.342861000	1.377234000
1	4.245860000	4.249689000	-0.570746000
1	-0.548500000	-1.838180000	1.167783000

6	0.998798000	3.309349000	-0.901334000
6	2.273801000	-2.080425000	1.030542000
6	-4.815459000	-1.515204000	-0.163304000
6	2.185527000	3.991035000	-1.147710000
6	-4.237532000	0.667299000	-1.321251000
1	-4.347931000	-2.105078000	-0.949552000
1	5.571807000	-2.830477000	0.678282000
1	0.122550000	3.520176000	-1.505769000
6	-0.569354000	-1.501989000	0.137387000
6	4.547149000	-2.620719000	0.395606000
6	-1.864862000	-1.127478000	-0.442501000
1	2.227926000	4.729216000	-1.940809000
1	-5.870452000	-1.376817000	-0.415841000
6	1.854018000	-2.083396000	-0.347024000
6	0.549012000	-1.827067000	-0.751442000
6	4.167592000	-2.632493000	-0.962123000
8	-2.166332000	-1.510482000	-1.579126000
6	2.867864000	-2.374708000	-1.327856000
1	0.309367000	-1.864533000	-1.808054000
1	4.908399000	-2.848558000	-1.724166000
1	2.581575000	-2.386071000	-2.373947000
1	-3.766070000	1.647698000	-1.204595000
1	-5.289381000	0.828653000	-1.575630000
1	-3.754560000	0.141457000	-2.142971000

Zero-point correction= 0.409760  
(Hartree/Particle)  
Thermal correction to Energy= 0.432699  
Thermal correction to Enthalpy= 0.433643  
Thermal correction to Gibbs Free Energy= 0.354275  
Sum of electronic and zero-point Energies= -983.111250  
Sum of electronic and thermal Energies= -983.088311  
Sum of electronic and thermal Enthalpies= -983.087366  
Sum of electronic and thermal Free Energies= -983.166735

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	271.523	89.973	167.045

#UB3LYP/6-311+G**	73-Bu-trans
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xyz-matrix

6	-0.580357000	1.305856000	-1.552886000
6	0.703071000	0.899540000	-1.355873000
6	0.940554000	-1.517598000	-0.840848000
6	0.040167000	-1.692414000	0.312526000
6	1.577897000	1.111771000	-0.144830000
7	2.586230000	0.046991000	0.010184000
6	2.350176000	-1.133339000	-0.666072000
8	3.237141000	-1.876106000	-1.094949000
6	3.953499000	0.405671000	0.516364000
6	3.829377000	1.533688000	1.561097000
6	4.585334000	-0.802605000	1.235190000
6	4.843575000	0.865782000	-0.653242000
6	-1.596898000	1.840839000	-0.646387000
6	-2.618875000	2.628364000	-1.216332000
6	-3.616981000	3.200097000	-0.437113000
6	-3.636972000	2.985989000	0.940797000
6	-2.653630000	2.184869000	1.521495000
6	-1.650994000	1.617790000	0.743335000

6	-1.315630000	-2.004772000	0.243111000
6	-2.066793000	-2.239070000	1.447115000
6	-3.398728000	-2.584621000	1.406102000
6	-4.065788000	-2.716953000	0.174425000
6	-3.361354000	-2.490200000	-1.018741000
6	-2.026679000	-2.141890000	-0.998462000
1	-0.912760000	1.268695000	-2.588023000
1	1.262367000	0.665555000	-2.257330000
1	0.757272000	-2.103718000	-1.735807000
1	0.495772000	-1.636473000	1.297652000
1	0.997759000	1.247070000	0.767464000
1	2.109195000	2.053716000	-0.316753000
1	4.810333000	1.704732000	2.009640000
1	3.501115000	2.483250000	1.134743000
1	3.139501000	1.255878000	2.362587000
1	4.768020000	-1.631500000	0.556496000
1	3.934486000	-1.148845000	2.043257000
1	5.536221000	-0.494280000	1.677824000
1	4.405175000	1.728480000	-1.164630000
1	5.831113000	1.162717000	-0.287961000
1	4.967392000	0.057891000	-1.375352000
1	-2.614145000	2.798196000	-2.288076000
1	-4.382880000	3.808611000	-0.904964000
1	-4.417007000	3.424782000	1.552364000
1	-2.676569000	1.987730000	2.587582000
1	-0.932184000	0.961975000	1.213527000
1	-1.556621000	-2.149365000	2.400698000
1	-3.937926000	-2.760316000	2.330614000
1	-5.113074000	-2.993017000	0.147034000
1	-3.873512000	-2.589901000	-1.969712000
1	-1.503607000	-1.962729000	-1.929191000

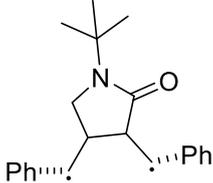
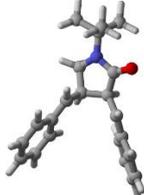
Zero-point correction=  
(Hartree/Particle)

0.410000

Thermal correction to Energy=	0.432921
Thermal correction to Enthalpy=	0.433865
Thermal correction to Gibbs Free Energy=	0.354551
Sum of electronic and zero-point Energies=	-983.101880
Sum of electronic and thermal Energies=	-983.078960
Sum of electronic and thermal Enthalpies=	-983.078016
Sum of electronic and thermal Free Energies=	-983.157330

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	271.662	89.758	166.931

#UB3LYP/6-311+G**	72-Bu-cis
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Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3	

xyz-matrix

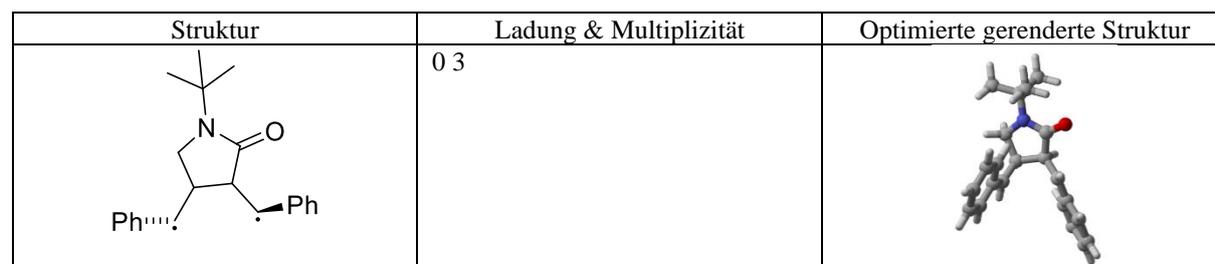
1	-3.627731000	-2.971352000	-2.363242000
1	-5.246074000	-3.530195000	-0.563604000
6	-3.370639000	-2.780766000	-1.326740000
6	-4.283968000	-3.097400000	-0.315608000
1	-1.449190000	-1.994556000	-1.822154000
6	-2.138445000	-2.226628000	-1.018564000
6	-3.941930000	-2.851168000	1.020103000
1	-4.643160000	-3.095100000	1.810676000
6	-1.763754000	-1.966898000	0.330762000
6	-2.714103000	-2.300379000	1.339317000
1	0.598354000	-1.719933000	-1.086380000

1	-2.455491000	-2.115824000	2.376532000
6	-0.519082000	-1.409533000	0.699643000
1	4.500191000	-2.164904000	-0.009165000
6	0.562684000	-1.013707000	-0.243785000
1	-2.039711000	1.257283000	-1.678310000
1	-0.117932000	0.431705000	-1.758284000
1	-0.323094000	-1.268406000	1.756835000
1	-4.072221000	2.611713000	-1.669349000
1	2.187891000	0.193709000	-2.254180000
8	2.335854000	-1.870198000	1.211813000
6	1.970905000	-1.066107000	0.370523000
6	0.508831000	0.427819000	-0.866458000
1	4.173333000	-0.635471000	2.055275000
6	4.869261000	-1.297745000	-0.557186000
6	-2.157856000	2.022479000	-0.921405000
1	4.654700000	-1.436009000	-1.621231000
6	1.993507000	0.623815000	-1.261202000
6	-3.313464000	2.786079000	-0.914209000
7	2.734843000	-0.088719000	-0.214952000
1	5.954986000	-1.248523000	-0.436561000
6	4.218239000	-0.002919000	-0.033337000
6	4.536555000	0.200095000	1.459866000
6	0.063880000	1.479865000	0.098312000
1	5.618348000	0.286469000	1.595585000
6	-1.140609000	2.216976000	0.056979000
1	2.261925000	1.679001000	-1.292040000
6	-3.515655000	3.771217000	0.058401000
1	-4.423220000	4.363415000	0.057058000
6	4.769244000	1.197573000	-0.819042000
1	0.745481000	1.696088000	0.917222000
1	4.073124000	1.120131000	1.826920000
6	-1.377808000	3.223603000	1.040056000
6	-2.535559000	3.979683000	1.036866000
1	-0.623956000	3.392473000	1.802031000
1	-2.684332000	4.737972000	1.797893000
1	4.586759000	1.111695000	-1.893055000
1	5.850493000	1.242915000	-0.671662000
1	4.348379000	2.142593000	-0.466410000

Zero-point correction= 0.412924  
(Hartree/Particle)  
Thermal correction to Energy= 0.435433  
Thermal correction to Enthalpy= 0.436377  
Thermal correction to Gibbs Free Energy= 0.357934  
Sum of electronic and zero-point Energies= -983.160575  
Sum of electronic and thermal Energies= -983.138066  
Sum of electronic and thermal Enthalpies= -983.137121  
Sum of electronic and thermal Free Energies= -983.215565

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	273.238	89.098	165.097

#UB3LYP/6-311+G**	72-'Bu-trans
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xyz-matrix

1	4.983071000	-2.155232000	1.887572000
6	4.622721000	-1.683789000	0.979520000
1	2.571280000	-1.962172000	1.503258000
1	6.602981000	-1.282627000	0.219145000
6	3.258602000	-1.573578000	0.760666000

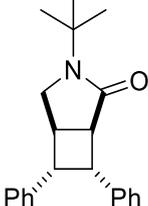
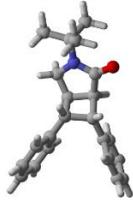
6	5.537570000	-1.193962000	0.041551000
1	0.524577000	-2.284843000	0.600633000
1	0.341977000	-0.848995000	2.336703000
1	-3.533487000	-3.252252000	0.941162000
1	-1.894400000	-1.244245000	2.350340000
6	2.749271000	-0.964299000	-0.421228000
6	5.063546000	-0.589802000	-1.129835000
6	0.270213000	-1.290418000	0.208564000
6	-0.094310000	-0.384334000	1.451262000
1	1.294653000	1.185951000	2.081073000
1	5.766067000	-0.209452000	-1.863376000
6	-1.640104000	-0.537180000	1.551670000
6	1.368953000	-0.827975000	-0.690183000
6	3.704244000	-0.475895000	-1.359430000
6	-3.761127000	-2.839895000	-0.046439000
6	-1.057455000	-1.499451000	-0.528066000
1	-4.807945000	-3.062157000	-0.271206000
6	0.441688000	1.020372000	1.430297000
7	-2.086666000	-1.042528000	0.250211000
8	-1.155766000	-2.025436000	-1.625232000
1	-3.135900000	-3.337809000	-0.787968000
1	-2.116359000	0.414579000	1.787721000
6	-3.526139000	-1.317393000	-0.068873000
1	1.078500000	-0.361654000	-1.624859000
1	3.344684000	-0.008471000	-2.269899000
1	-3.258446000	-1.184620000	-2.233089000
6	-4.428261000	-0.645093000	0.978872000
1	1.517483000	3.420417000	1.603863000
6	0.039646000	2.143649000	0.666879000
6	-3.871721000	-0.736990000	-1.453526000
1	-4.924445000	-0.932410000	-1.676453000
6	0.718112000	3.382160000	0.871256000
1	-1.532215000	1.218342000	-0.516415000
6	-0.996882000	2.134575000	-0.309194000
1	-3.721281000	0.346085000	-1.464938000
6	0.382257000	4.519740000	0.160381000
1	0.919512000	5.444420000	0.340790000
6	-1.323627000	3.281319000	-1.016964000
6	-0.644341000	4.482302000	-0.791349000
1	-2.113763000	3.241543000	-1.759135000
1	-0.906420000	5.373233000	-1.349969000
1	-5.469994000	-0.849981000	0.722462000
1	-4.298402000	0.439690000	0.991677000
1	-4.256059000	-1.030548000	1.986303000

Zero-point correction=	0.413485
(Hartree/Particle)	
Thermal correction to Energy=	0.435949
Thermal correction to Enthalpy=	0.436893
Thermal correction to Gibbs Free Energy=	0.359210
Sum of electronic and zero-point Energies=	-983.154171
Sum of electronic and thermal Energies=	-983.131707
Sum of electronic and thermal Enthalpies=	-983.130763
Sum of electronic and thermal Free Energies=	-983.208447

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	273.562	88.980	163.498

#B3LYP/6-311+G\*\*

70-Bu-cis

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

xyz-matrix

6	-0.216676000	0.662055000	0.186028000
6	0.616360000	0.259086000	-1.070251000
6	0.761072000	-1.161375000	-0.491326000
6	-0.363669000	-0.890984000	0.545844000
6	2.031886000	0.831546000	-1.163530000
7	2.812656000	-0.010533000	-0.243223000
6	2.165710000	-1.172524000	0.106332000
8	2.626012000	-2.081174000	0.780650000
6	4.251560000	0.240045000	0.085449000
6	4.664363000	1.636756000	-0.407146000
6	4.445811000	0.183685000	1.612742000
6	5.121749000	-0.822559000	-0.613633000
6	-1.414519000	1.564077000	0.067931000
6	-1.675003000	2.498325000	1.079713000
6	-2.778708000	3.346086000	1.016535000
6	-3.648609000	3.277757000	-0.069726000
6	-3.403261000	2.355866000	-1.085759000
6	-2.299927000	1.508065000	-1.016258000
6	-1.709545000	-1.529304000	0.297333000
6	-2.640849000	-1.560673000	1.344646000
6	-3.905110000	-2.115867000	1.171633000
6	-4.268980000	-2.658569000	-0.060223000
6	-3.354721000	-2.639581000	-1.109940000
6	-2.089509000	-2.079565000	-0.931917000
1	0.458675000	1.096016000	0.928489000
1	0.066544000	0.347394000	-2.006440000
1	0.646709000	-2.035103000	-1.133831000
1	-0.067963000	-1.104584000	1.575141000
1	2.060769000	1.881722000	-0.864148000
1	2.425113000	0.763209000	-2.185805000
1	5.716748000	1.794175000	-0.161231000
1	4.559827000	1.744669000	-1.489248000
1	4.089932000	2.428017000	0.080766000
1	5.490868000	0.393013000	1.858162000
1	4.183185000	-0.796494000	2.006578000
1	3.824429000	0.937961000	2.104023000
1	4.995669000	-0.771273000	-1.699292000
1	6.178002000	-0.650795000	-0.388019000
1	4.853647000	-1.823650000	-0.276093000
1	-0.999948000	2.563272000	1.927636000
1	-2.955674000	4.061202000	1.812444000
1	-4.507654000	3.936863000	-0.125332000
1	-4.074619000	2.293374000	-1.935162000
1	-2.136281000	0.794105000	-1.814376000
1	-2.366502000	-1.147951000	2.310132000
1	-4.604533000	-2.130262000	2.000270000
1	-5.251358000	-3.096182000	-0.197316000
1	-3.621960000	-3.065027000	-2.071187000
1	-1.396854000	-2.084642000	-1.765652000

Zero-point correction=  
(Hartree/Particle)

0.418140

Thermal correction to Energy=

0.439494

Thermal correction to Enthalpy=

0.440438

Thermal correction to Gibbs Free Energy=

0.366495

Sum of electronic and zero-point Energies=

-983.208379

Sum of electronic and thermal Energies=

-983.187026

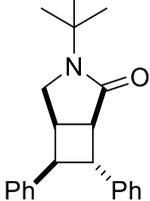
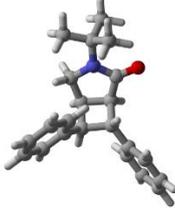
Sum of electronic and thermal Enthalpies=

-983.186082

Sum of electronic and thermal Free Energies= -983.260025

Total E (Thermal) CV S  
 kcal/Mol cal/Mol-Kelvin cal/Mol-Kelvin  
 275.786 85.424 155.626

#B3LYP/6-311+G\*\* 70-Bu-trans

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

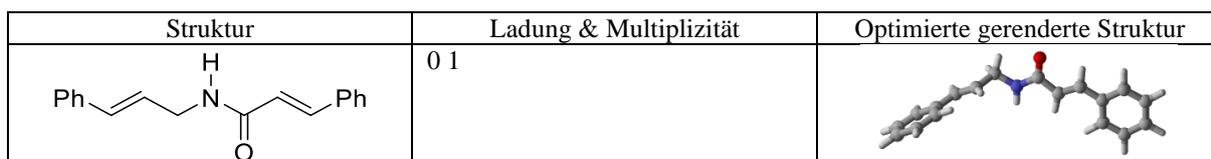
xyz-matrix

6	-0.728938000	0.763936000	-0.893663000
6	0.262868000	-0.192369000	-1.660269000
6	-0.229531000	-1.379321000	-0.804794000
6	-1.139906000	-0.426605000	0.049689000
6	1.774276000	-0.094690000	-1.400820000
7	2.043026000	-1.037435000	-0.302805000
6	0.987586000	-1.880431000	-0.045734000
8	0.999706000	-2.853273000	0.693516000
6	3.422932000	-1.291203000	0.219692000
6	4.347771000	-0.125078000	-0.167919000
6	3.384627000	-1.385614000	1.756681000
6	3.961100000	-2.599996000	-0.390885000
6	-0.240873000	2.064132000	-0.308007000
6	-0.567108000	3.271955000	-0.940043000
6	-0.112738000	4.493020000	-0.446559000
6	0.679680000	4.532037000	0.699101000
6	1.011275000	3.340903000	1.342038000
6	0.557355000	2.121263000	0.842601000
6	-2.609958000	-0.739420000	0.159248000
6	-3.246424000	-0.713727000	1.404899000
6	-4.609100000	-0.984266000	1.523109000
6	-5.362118000	-1.289281000	0.392145000
6	-4.741542000	-1.322034000	-0.856632000
6	-3.380961000	-1.049671000	-0.969666000
1	-1.561881000	0.988042000	-1.563023000
1	0.059043000	-0.232813000	-2.730359000
1	-0.747681000	-2.204786000	-1.290502000
1	-0.735519000	-0.309911000	1.056366000
1	2.077975000	0.918862000	-1.133481000
1	2.333184000	-0.384258000	-2.298733000
1	5.341218000	-0.317828000	0.243208000
1	4.455552000	-0.018060000	-1.249452000
1	3.996093000	0.824075000	0.243735000
1	4.396526000	-1.553081000	2.136299000
1	2.745960000	-2.202294000	2.086989000
1	3.013054000	-0.451237000	2.186985000
1	3.998460000	-2.531905000	-1.482415000
1	4.975255000	-2.795087000	-0.031019000
1	3.327080000	-3.442614000	-0.113949000
1	-1.192352000	3.253671000	-1.827260000
1	-0.383962000	5.413158000	-0.952387000
1	1.030715000	5.480455000	1.089790000
1	1.623460000	3.359895000	2.237142000
1	0.829502000	1.207572000	1.358429000
1	-2.666515000	-0.483249000	2.292491000
1	-5.079700000	-0.959639000	2.499776000
1	-6.421209000	-1.503159000	0.481164000
1	-5.318010000	-1.563145000	-1.743079000
1	-2.916698000	-1.085674000	-1.950463000

Zero-point correction= 0.418328  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.439706  
 Thermal correction to Enthalpy= 0.440651  
 Thermal correction to Gibbs Free Energy= 0.365797  
 Sum of electronic and zero-point Energies= -983.209660  
 Sum of electronic and thermal Energies= -983.188281  
 Sum of electronic and thermal Enthalpies= -983.187337  
 Sum of electronic and thermal Free Energies= -983.262191

Total E (Thermal) CV S  
 KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin  
 275.920 85.333 157.543

#B3LYP/6-311+G\*\* 69-lin-H



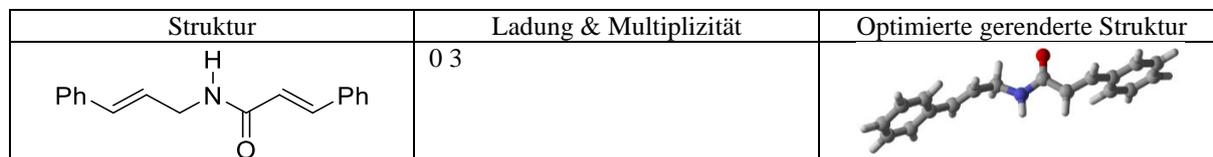
xyz-matrix

6	-3.598643000	0.753141000	-0.615480000
6	-2.449972000	0.954232000	0.042154000
6	-1.321668000	1.794087000	-0.484323000
7	-0.087532000	1.025891000	-0.616621000
6	1.087686000	1.377908000	-0.001588000
6	2.215723000	0.443146000	-0.263828000
8	1.190485000	2.378055000	0.698112000
6	3.426836000	0.676176000	0.262338000
6	-4.759661000	-0.036381000	-0.177809000
6	-5.824870000	-0.225794000	-1.072172000
6	-6.944372000	-0.973336000	-0.715368000
6	-7.025173000	-1.547338000	0.550914000
6	-5.977435000	-1.363121000	1.455644000
6	-4.861150000	-0.616779000	1.098225000
6	4.644299000	-0.123081000	0.110993000
6	5.827184000	0.335688000	0.713506000
6	7.016985000	-0.378229000	0.600659000
6	7.047815000	-1.571170000	-0.117508000
6	5.879722000	-2.044101000	-0.720468000
6	4.693576000	-1.330620000	-0.608120000
1	-3.709298000	1.218264000	-1.594282000
1	-2.276061000	0.500810000	1.014787000
1	-1.595375000	2.238980000	-1.447672000
1	-1.087706000	2.611104000	0.202913000
1	2.023101000	-0.420115000	-0.893982000
1	3.515344000	1.571383000	0.873315000
1	-5.769825000	0.218727000	-2.060776000
1	-7.752691000	-1.105580000	-1.425913000
1	-7.895395000	-2.128259000	0.834359000
1	-6.034995000	-1.799954000	2.446516000
1	-4.065943000	-0.477575000	1.821249000
1	5.806234000	1.264146000	1.274202000
1	7.917787000	-0.003517000	1.073355000
1	7.971741000	-2.131041000	-0.207507000
1	5.897239000	-2.973552000	-1.278616000
1	3.798030000	-1.717004000	-1.080635000
1	-0.114650000	0.180917000	-1.166476000

Zero-point correction= 0.302573  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.320687  
 Thermal correction to Enthalpy= 0.321631  
 Thermal correction to Gibbs Free Energy= 0.250949  
 Sum of electronic and zero-point Energies= -826.039754  
 Sum of electronic and thermal Energies= -826.021640  
 Sum of electronic and thermal Enthalpies= -826.020696  
 Sum of electronic and thermal Free Energies= -826.091378

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	201.234	68.519	148.763

#UB3LYP/6-311+G**	71-lin-H
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xyz-matrix

6	-3.456144000	-0.846783000	-0.354129000
6	-2.348230000	-0.153694000	-0.645347000
6	-1.024207000	-0.790757000	-0.956828000
7	0.013462000	-0.373586000	-0.019853000
6	1.202142000	0.200255000	-0.420214000
6	2.101827000	0.570162000	0.680060000
8	1.481926000	0.385694000	-1.601561000
6	3.395828000	1.202881000	0.452020000
6	-4.794760000	-0.319141000	-0.050320000
6	-5.799802000	-1.214343000	0.348309000
6	-7.082748000	-0.769745000	0.657853000
6	-7.390946000	0.585553000	0.571125000
6	-6.404737000	1.489229000	0.169853000
6	-5.125025000	1.044087000	-0.138584000
6	4.632080000	0.523920000	0.350840000
6	5.837923000	1.253756000	0.149928000
6	7.057317000	0.607152000	0.055892000
6	7.130079000	-0.787792000	0.156355000
6	5.958028000	-1.527716000	0.350885000
6	4.731577000	-0.892443000	0.446092000
1	-3.381262000	-1.933258000	-0.332770000
1	-2.357561000	0.933190000	-0.664161000
1	-1.119216000	-1.882898000	-0.956952000
1	-0.666715000	-0.490961000	-1.945360000
1	1.758133000	0.413772000	1.703486000
1	3.405199000	2.287544000	0.351945000
1	-5.567848000	-2.272380000	0.416853000
1	-7.840483000	-1.482150000	0.964455000
1	-8.388735000	0.936460000	0.808532000
1	-6.637800000	2.545503000	0.093010000
1	-4.379184000	1.762267000	-0.458533000
1	5.787568000	2.334396000	0.068880000
1	7.961862000	1.185035000	-0.098626000
1	8.086872000	-1.291158000	0.080943000
1	6.009291000	-2.608623000	0.423329000
1	3.828730000	-1.475879000	0.587319000
1	-0.169707000	-0.478796000	0.966372000

Zero-point correction=  
(Hartree/Particle)

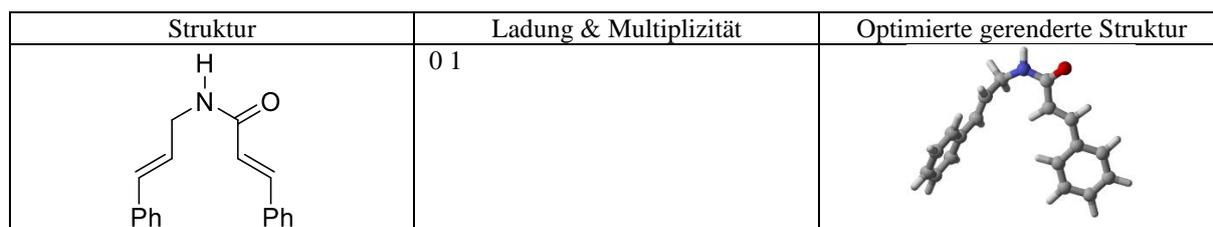
0.298589

Thermal correction to Energy=	0.317043
Thermal correction to Enthalpy=	0.317987
Thermal correction to Gibbs Free Energy=	0.245356
Sum of electronic and zero-point Energies=	-825.958978
Sum of electronic and thermal Energies=	-825.940523
Sum of electronic and thermal Enthalpies=	-825.939579
Sum of electronic and thermal Free Energies=	-826.012210

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	198.948	70.265	152.864

#B3LYP/6-311+G\*\*

69-NAC-H



xyz-matrix

6	-2.175549000	0.701964000	-0.874978000
6	-1.813067000	1.901818000	-0.406730000
6	-0.843031000	2.816931000	-1.108678000
7	0.168369000	3.410644000	-0.233729000
6	1.328017000	2.853594000	0.255158000
6	1.554562000	1.411106000	-0.024217000
8	2.119580000	3.540501000	0.891423000
6	2.716464000	0.836915000	0.325365000
6	-3.133581000	-0.244718000	-0.284087000
6	-3.445050000	-1.418833000	-0.987281000
6	-4.345783000	-2.350054000	-0.476153000
6	-4.954576000	-2.127511000	0.756278000
6	-4.652852000	-0.966264000	1.470945000
6	-3.755227000	-0.037445000	0.959109000
6	3.111501000	-0.561263000	0.145459000
6	4.437091000	-0.927990000	0.431012000
6	4.871402000	-2.240796000	0.270226000
6	3.984014000	-3.218586000	-0.173305000
6	2.659403000	-2.873301000	-0.452340000
6	2.227706000	-1.562773000	-0.294787000
1	-1.727567000	0.366597000	-1.810243000
1	-2.227610000	2.290518000	0.519782000
1	-0.369683000	2.297729000	-1.947933000
1	-1.391972000	3.658888000	-1.544024000
1	0.763146000	0.843909000	-0.496580000
1	3.453319000	1.486419000	0.791499000
1	-2.975570000	-1.599364000	-1.949121000
1	-4.570309000	-3.248343000	-1.040355000
1	-5.654993000	-2.849946000	1.159418000
1	-5.118869000	-0.786745000	2.433465000
1	-3.532605000	0.853092000	1.535195000
1	5.129836000	-0.169361000	0.779625000
1	5.900077000	-2.499888000	0.494011000
1	4.316951000	-4.242959000	-0.296104000
1	1.961609000	-3.632378000	-0.787896000
1	1.192760000	-1.317615000	-0.502425000
1	0.087594000	4.394170000	-0.019571000

Zero-point correction=  
(Hartree/Particle)

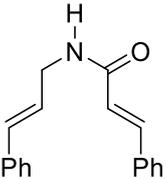
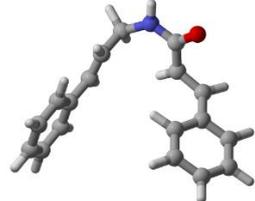
0.302655

Thermal correction to Energy=	0.320665
Thermal correction to Enthalpy=	0.321609
Thermal correction to Gibbs Free Energy=	0.252185
Sum of electronic and zero-point Energies=	-826.032923
Sum of electronic and thermal Energies=	-826.014914
Sum of electronic and thermal Enthalpies=	-826.013969
Sum of electronic and thermal Free Energies=	-826.083394

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	201.220	68.518	146.116

#BU3LYP/6-311+G\*\*

71-NAC-H

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3	

xyz-matrix

6	-2.026644000	1.279308000	-0.661352000
6	-1.445695000	2.165129000	0.156331000
6	-0.575604000	3.301056000	-0.316884000
7	0.705752000	3.409309000	0.378296000
6	1.780945000	2.542109000	0.329257000
6	1.793841000	1.527076000	-0.726298000
8	2.710783000	2.659092000	1.127497000
6	2.875754000	0.551114000	-0.825993000
6	-2.903427000	0.156010000	-0.297466000
6	-3.350876000	-0.706721000	-1.310101000
6	-4.174520000	-1.792191000	-1.022580000
6	-4.571048000	-2.038242000	0.289413000
6	-4.138412000	-1.187249000	1.308725000
6	-3.317550000	-0.103901000	1.020200000
6	2.808882000	-0.785176000	-0.371114000
6	3.934802000	-1.647153000	-0.505277000
6	3.885439000	-2.959591000	-0.071328000
6	2.718871000	-3.471062000	0.511541000
6	1.598809000	-2.643849000	0.653864000
6	1.635281000	-1.327853000	0.225070000
1	-1.840003000	1.377899000	-1.730320000
1	-1.583695000	2.105125000	1.233133000
1	-0.417869000	3.232221000	-1.397796000
1	-1.089432000	4.253409000	-0.148261000
1	1.022964000	1.543821000	-1.492729000
1	3.808715000	0.889703000	-1.273601000
1	-3.044305000	-0.523016000	-2.334841000
1	-4.505032000	-2.444581000	-1.823011000
1	-5.212552000	-2.881534000	0.518279000
1	-4.446062000	-1.368961000	2.332529000
1	-2.999477000	0.546107000	1.826948000
1	4.842394000	-1.255646000	-0.952365000
1	4.757102000	-3.595344000	-0.181705000
1	2.683855000	-4.500133000	0.849783000
1	0.692889000	-3.035251000	1.103630000
1	0.761029000	-0.697060000	0.340098000
1	0.769861000	4.062470000	1.146137000

Zero-point correction=  
(Hartree/Particle)

0.298633

Thermal correction to Energy=

0.317006

Thermal correction to Enthalpy=

0.317950

Thermal correction to Gibbs Free Energy=

0.246072

Sum of electronic and zero-point Energies=

-825.952917

Sum of electronic and thermal Energies=

-825.934545

Sum of electronic and thermal Enthalpies=

-825.933600

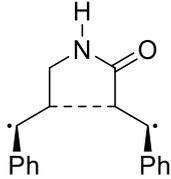
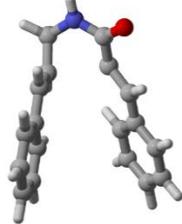
Sum of electronic and thermal Free Energies=

-826.005478

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	198.924	70.280	151.279

#UB3LYP/6-311+G\*\*

73-H-cis

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3  $\nu_{imag} = -284.2 \text{ cm}^{-1}$	

xyz-matrix

1	2.941323000	-2.126598000	2.460453000
1	4.741622000	-2.281778000	0.755257000
6	2.689343000	-2.086291000	1.405996000
6	3.708410000	-2.175723000	0.446871000
1	0.598581000	-1.900291000	1.785651000
6	1.367934000	-1.954787000	1.025530000
6	3.376061000	-2.134477000	-0.921779000
1	-1.474049000	-2.035563000	1.065284000
1	4.160728000	-2.205974000	-1.666935000
6	0.996200000	-1.907206000	-0.363255000
1	-1.140732000	0.316908000	1.978652000
1	0.787343000	1.257655000	1.676171000
1	-3.255336000	-0.675057000	2.301420000
6	2.065931000	-2.006825000	-1.320151000
1	2.828028000	2.561529000	1.313255000
6	-1.494616000	-1.639006000	0.056164000
6	-0.318425000	-1.771264000	-0.801274000
6	-1.863863000	0.531512000	1.199901000
1	1.816077000	-1.976916000	-2.375153000
6	0.799807000	2.012205000	0.899381000
6	-3.259688000	-0.039078000	1.407755000
6	1.958100000	2.748571000	0.693690000
6	-2.813432000	-1.439381000	-0.561708000
8	-3.081510000	-1.804912000	-1.705153000
1	-0.515109000	-1.761292000	-1.867707000
7	-3.714968000	-0.782401000	0.237595000
1	-3.980484000	0.761939000	1.600451000
6	-1.590529000	1.498797000	0.279258000
6	-0.345287000	2.227623000	0.104530000
6	2.011673000	3.722260000	-0.306760000
1	2.918679000	4.294968000	-0.462608000
1	-2.374534000	1.747849000	-0.433731000
6	-0.269221000	3.210258000	-0.903431000
6	0.890397000	3.948676000	-1.105160000
1	-1.136348000	3.388073000	-1.531107000
1	0.921912000	4.699363000	-1.886879000
1	-4.633590000	-0.623898000	-0.147779000

Zero-point correction=  
(Hartree/Particle)

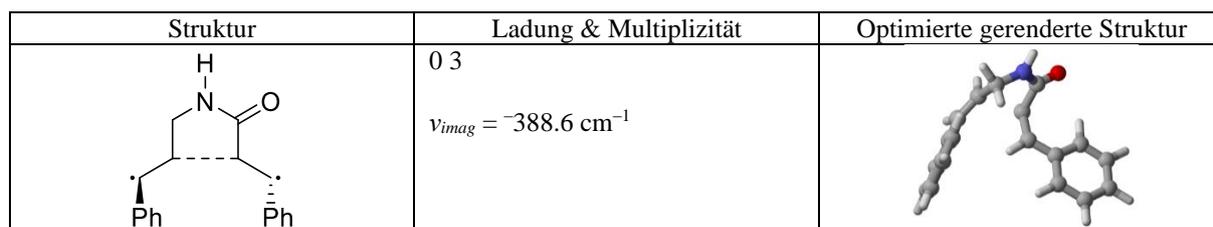
0.297998

Thermal correction to Energy=	0.315607
Thermal correction to Enthalpy=	0.316551
Thermal correction to Gibbs Free Energy=	0.248926
Sum of electronic and zero-point Energies=	-825.938015
Sum of electronic and thermal Energies=	-825.920406
Sum of electronic and thermal Enthalpies=	-825.919462
Sum of electronic and thermal Free Energies=	-825.987087

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	198.046	68.654	142.330

#UB3LYP/6-311+G\*\*

73-H-trans



xyz-matrix

1	-0.962135000	2.963750000	-1.158834000
8	2.551190000	2.946395000	-0.029121000
1	1.150722000	1.570290000	-1.896935000
1	-2.272039000	1.319190000	-2.131023000
1	3.544959000	0.694624000	-0.589501000
6	1.432077000	2.460589000	0.064934000
6	-1.211145000	2.113727000	-0.529842000
6	0.928002000	1.376361000	-0.847083000
6	-2.115835000	1.225546000	-1.059109000
1	-3.042761000	-0.877695000	-2.363252000
1	5.475729000	-0.780864000	-0.208737000
7	0.506920000	2.851336000	0.985511000
1	-1.526511000	3.043999000	1.391299000
6	3.385663000	-0.342759000	-0.320329000
6	-0.848785000	2.319958000	0.924866000
6	4.471321000	-1.174877000	-0.098017000
6	-3.265654000	-0.936227000	-1.302994000
6	-2.828935000	0.106656000	-0.456232000
6	0.910134000	-0.025529000	-0.402883000
6	2.055754000	-0.831231000	-0.178870000
1	-0.924876000	1.385430000	1.488133000
1	-4.268775000	-2.822652000	-1.482146000
1	-0.059173000	-0.505512000	-0.287463000
6	-3.956525000	-2.033778000	-0.806947000
6	4.286254000	-2.512231000	0.269318000
6	-3.162563000	0.010654000	0.911624000
1	5.141843000	-3.155094000	0.441332000
1	-2.913111000	0.815140000	1.589748000
6	1.892955000	-2.195776000	0.197357000
6	2.986838000	-3.014252000	0.414972000
6	-4.251856000	-2.120160000	0.554425000
6	-3.858563000	-1.087453000	1.405418000
1	0.888311000	-2.589860000	0.311163000
1	2.836153000	-4.049885000	0.699938000
1	-4.794710000	-2.973433000	0.944265000
1	-4.107255000	-1.131150000	2.460042000
1	0.780841000	3.527891000	1.682713000

Zero-point correction=  
(Hartree/Particle)

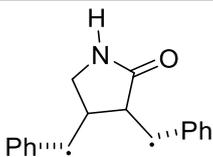
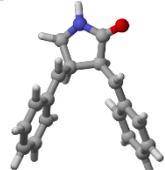
0.298915

Thermal correction to Energy=	0.316050
Thermal correction to Enthalpy=	0.316994
Thermal correction to Gibbs Free Energy=	0.250884
Sum of electronic and zero-point Energies=	-825.935093
Sum of electronic and thermal Energies=	-825.917958
Sum of electronic and thermal Enthalpies=	-825.917014
Sum of electronic and thermal Free Energies=	-825.983124

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	198.324	67.738	139.140

#UB3LYP/6-311+G\*\*

72-H-cis

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3	

xyz-matrix

6	0.873918000	1.653695000	-0.091879000
6	-0.272278000	1.626681000	0.867568000
6	-1.611408000	1.083838000	0.227133000
6	-1.514916000	-0.064625000	-0.714962000
6	-0.696553000	3.066960000	1.272552000
7	-1.659614000	3.418136000	0.238707000
6	-2.234255000	2.349088000	-0.390733000
8	-3.084273000	2.398293000	-1.256396000
6	2.031959000	0.845378000	-0.056825000
6	3.046115000	1.035767000	-1.042212000
6	4.201469000	0.276042000	-1.046981000
6	4.404512000	-0.711453000	-0.074804000
6	3.424482000	-0.924222000	0.900575000
6	2.263098000	-0.169619000	0.915845000
6	-1.484858000	-1.426491000	-0.339407000
6	-1.381033000	-2.433363000	-1.342605000
6	-1.348184000	-3.776875000	-1.015639000
6	-1.417092000	-4.183464000	0.322773000
6	-1.522208000	-3.217184000	1.328670000
6	-1.554917000	-1.868373000	1.012665000
1	0.799094000	2.371623000	-0.904940000
1	-0.021208000	1.045986000	1.754526000
1	-2.275893000	0.825412000	1.064445000
1	-1.473364000	0.170313000	-1.772766000
1	0.149549000	3.756990000	1.278181000
1	-1.153459000	3.072686000	2.270956000
1	2.896637000	1.797759000	-1.800116000
1	4.953463000	0.446486000	-1.809665000
1	5.309540000	-1.307477000	-0.080294000
1	3.570477000	-1.693269000	1.651271000
1	1.517188000	-0.371187000	1.674463000
1	-1.329320000	-2.126519000	-2.381776000
1	-1.269509000	-4.519442000	-1.802117000
1	-1.391881000	-5.236672000	0.576910000
1	-1.580463000	-3.525368000	2.367097000
1	-1.641623000	-1.142031000	1.812580000
1	-2.014842000	4.350733000	0.091040000

Zero-point correction=  
(Hartree/Particle)

0.301302

Thermal correction to Energy=

0.318400

Thermal correction to Enthalpy=

0.319345

Thermal correction to Gibbs Free Energy=

0.252750

Sum of electronic and zero-point Energies=

-825.980808

Sum of electronic and thermal Energies=

-825.963710

Sum of electronic and thermal Enthalpies=

-825.962766

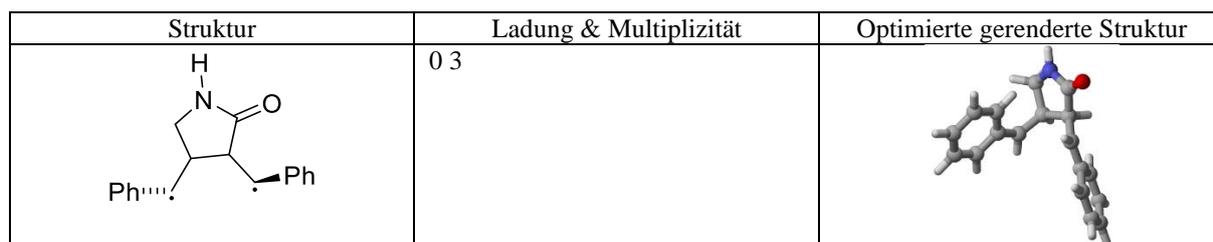
Sum of electronic and thermal Free Energies=

-826.029360

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	199.799	67.710	140.160

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72-H-trans



xyz-matrix

1	-4.378078000	-3.125303000	1.289557000
1	-4.101500000	-0.717400000	1.835255000
6	-3.657625000	-2.522827000	0.748810000
1	-2.978002000	-4.147058000	-0.497147000
6	-3.501496000	-1.166994000	1.051532000
6	-2.868972000	-3.095170000	-0.256697000
1	2.208394000	-1.279175000	2.200950000
1	4.302023000	-2.474640000	1.696149000
6	-2.582238000	-0.386146000	0.367378000
1	0.550016000	0.350598000	1.676873000
6	-1.947731000	-2.326915000	-0.944763000
6	2.761369000	-1.045216000	1.297581000
1	-2.479675000	0.655964000	0.637291000
6	3.937594000	-1.715182000	1.013059000
1	-1.338895000	-2.780386000	-1.719945000
6	-1.769234000	-0.939886000	-0.662128000
6	1.045677000	0.622897000	0.751950000
8	-0.404255000	2.953463000	1.876260000
6	2.250407000	-0.039757000	0.426761000
6	4.660831000	-1.417543000	-0.148869000
6	-0.562274000	2.567039000	0.734850000
1	5.582777000	-1.942814000	-0.369281000
6	-0.803991000	-0.218924000	-1.407680000
6	0.404377000	1.688991000	-0.072245000
7	-1.627831000	2.854232000	-0.066630000
1	-0.224060000	-0.809474000	-2.109822000
6	3.005169000	0.242341000	-0.747018000
1	-2.563874000	1.753773000	-1.604672000
6	-0.428182000	1.235275000	-1.348904000
6	4.183401000	-0.433947000	-1.021293000
6	-1.615978000	2.252129000	-1.389887000
1	1.177158000	2.383006000	-0.429777000
1	2.658751000	1.001187000	-1.439302000
1	0.194539000	1.416166000	-2.225611000
1	4.740050000	-0.196619000	-1.921537000
1	-1.446787000	3.007901000	-2.164715000
1	-2.340613000	3.495950000	0.247437000

Zero-point correction=  
(Hartree/Particle)

0.301712

Thermal correction to Energy=

0.318797

Thermal correction to Enthalpy=

0.319741

Thermal correction to Gibbs Free Energy=

0.253218

Sum of electronic and zero-point Energies=

-825.975247

Sum of electronic and thermal Energies=

-825.958162

Sum of electronic and thermal Enthalpies=

-825.957218

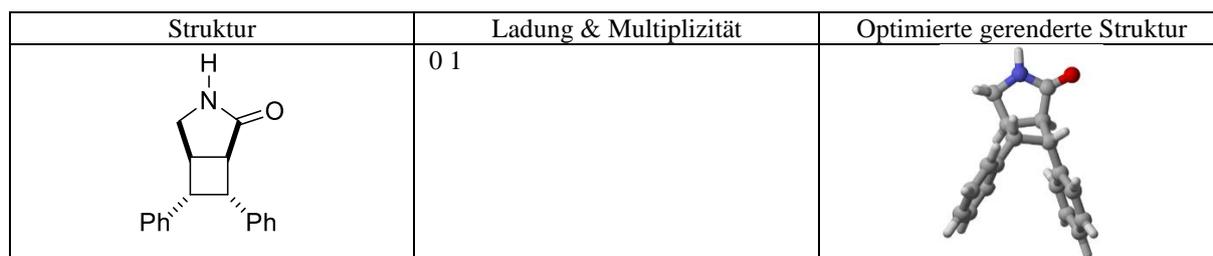
Sum of electronic and thermal Free Energies=

-826.023741

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	200.048	67.600	140.009

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70-H-cis



xyz-matrix

6	0.662406000	-0.901471000	-0.270374000
6	1.609851000	-0.710227000	0.953936000
6	2.059599000	0.645687000	0.356840000
6	0.854152000	0.647520000	-0.622747000
6	2.855536000	-1.609300000	1.003177000
7	3.761957000	-0.935235000	0.078632000
6	3.403438000	0.330845000	-0.304085000
8	4.045040000	1.060364000	-1.035300000
6	-0.702257000	-1.514052000	-0.111254000
6	-1.205867000	-2.343830000	-1.122259000
6	-2.469460000	-2.921976000	-1.021757000
6	-3.258409000	-2.682296000	0.101426000
6	-2.772092000	-1.860780000	1.116742000
6	-1.509142000	-1.282243000	1.010138000
6	-0.298493000	1.568544000	-0.300800000
6	-1.253971000	1.820290000	-1.295242000
6	-2.349985000	2.642490000	-1.052196000
6	-2.514964000	3.238555000	0.197587000
6	-1.573432000	3.002147000	1.195358000
6	-0.478202000	2.174452000	0.947614000
1	1.197756000	-1.466758000	-1.038364000
1	1.087032000	-0.663208000	1.907961000
1	2.180364000	1.517120000	1.001155000
1	1.137292000	0.802068000	-1.665919000
1	2.637088000	-2.630381000	0.674415000
1	3.283369000	-1.659568000	2.011433000
1	-0.596227000	-2.541071000	-1.998767000
1	-2.834191000	-3.562397000	-1.817325000
1	-4.241083000	-3.132456000	0.185991000
1	-3.378534000	-1.666324000	1.994497000
1	-1.158176000	-0.639476000	1.808326000
1	-1.131762000	1.368445000	-2.274349000
1	-3.072299000	2.823428000	-1.840562000
1	-3.364535000	3.884496000	0.388173000
1	-1.685732000	3.465388000	2.169597000
1	0.241766000	2.013560000	1.741743000
1	4.651613000	-1.315261000	-0.208656000

Zero-point correction=

0.306479

(Hartree/Particle)

Thermal correction to Energy= 0.322408

Thermal correction to Enthalpy= 0.323352

Thermal correction to Gibbs Free Energy= 0.261146

Sum of electronic and zero-point Energies= -826.029154

Sum of electronic and thermal Energies= -826.013225

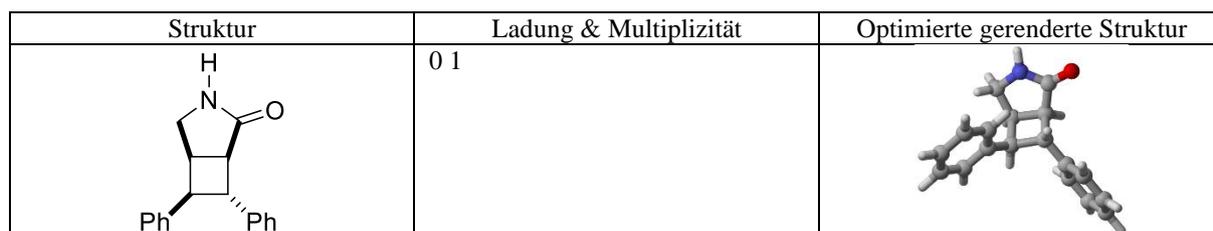
Sum of electronic and thermal Enthalpies= -826.012281

Sum of electronic and thermal Free Energies= -826.074487

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	202.314	63.991	130.925

#B3LYP/6-311+G\*\*

70-H-trans



xyz-matrix

6	-0.433122000	-0.143440000	-0.821977000
6	-0.595643000	1.314351000	-1.401012000
6	0.566001000	1.795340000	-0.494367000
6	0.677428000	0.375011000	0.165361000
6	-1.825210000	2.162033000	-1.009091000
7	-1.371206000	2.907798000	0.160880000
6	-0.032707000	2.837405000	0.441589000
8	0.545795000	3.463010000	1.310115000
6	-1.627152000	-0.891064000	-0.285161000
6	-2.165942000	-1.952482000	-1.025052000
6	-3.281501000	-2.655653000	-0.575682000
6	-3.883661000	-2.311110000	0.632767000
6	-3.360317000	-1.258996000	1.382168000
6	-2.245677000	-0.556261000	0.927472000
6	2.010077000	-0.327842000	0.134284000
6	2.529021000	-0.907414000	1.297053000
6	3.754224000	-1.572812000	1.284904000
6	4.486145000	-1.668603000	0.104121000
6	3.983666000	-1.093168000	-1.062942000
6	2.759121000	-0.431103000	-1.046203000
1	0.033164000	-0.763269000	-1.590124000
1	-0.428943000	1.355202000	-2.477206000
1	1.477704000	2.167209000	-0.959474000
1	0.325155000	0.401595000	1.197626000
1	-2.695861000	1.544696000	-0.772181000
1	-2.103033000	2.842996000	-1.821190000
1	-1.698127000	-2.236303000	-1.962548000
1	-3.674394000	-3.476598000	-1.165362000
1	-4.748286000	-2.859284000	0.989422000
1	-3.818695000	-0.984510000	2.325933000
1	-1.858156000	0.259240000	1.527840000
1	1.969010000	-0.831971000	-2.223254000
1	4.136577000	-2.012437000	2.199457000
1	5.440553000	-2.182653000	0.091870000
1	4.548243000	-1.157869000	-1.986659000
1	2.389107000	0.014089000	-1.964761000
1	-1.950447000	3.576049000	0.647624000

Zero-point correction=  
(Hartree/Particle)

0.306689

Thermal correction to Energy=

0.322650

Thermal correction to Enthalpy=

0.323595

Thermal correction to Gibbs Free Energy=

0.260729

Sum of electronic and zero-point Energies=

-826.030579

Sum of electronic and thermal Energies=

-826.014618

Sum of electronic and thermal Enthalpies=

-826.013674

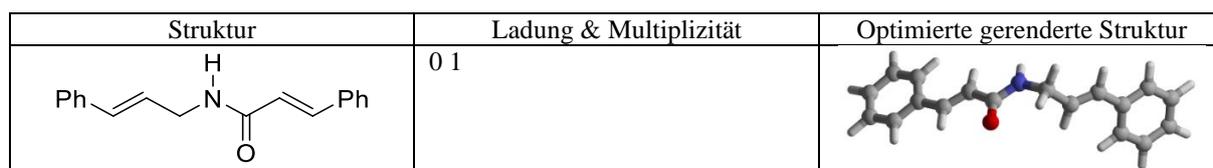
Sum of electronic and thermal Free Energies=

-826.076540

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	202.466	63.880	132.312

#B3LYP-D3/6-311+G\*\*

69-lin-H



xyz-matrix

6	-3.560948000	-0.887855000	0.563596000
6	-2.389347000	-1.084752000	-0.052184000
6	-1.350635000	-2.064619000	0.416415000
7	-0.080671000	-1.411123000	0.722786000
6	0.998340000	-1.452467000	-0.125606000
6	2.159280000	-0.635780000	0.321491000
8	0.999936000	-2.119293000	-1.153424000
6	3.275278000	-0.580495000	-0.419499000
6	-4.632592000	0.041495000	0.176196000
6	-5.730972000	0.205951000	1.034753000
6	-6.768259000	1.081180000	0.721883000
6	-6.731479000	1.811243000	-0.463657000
6	-5.649437000	1.654106000	-1.332817000
6	-4.615299000	0.780354000	-1.019427000
6	4.503479000	0.164523000	-0.138022000
6	5.535560000	0.144264000	-1.090579000
6	6.724232000	0.837665000	-0.879001000
6	6.907120000	1.565067000	0.294861000
6	5.892396000	1.592606000	1.255015000
6	4.706470000	0.901953000	1.042380000
1	-3.765606000	-1.471331000	1.460712000
1	-2.118668000	-0.519937000	-0.940420000
1	-1.700803000	-2.606774000	1.300152000
1	-1.133026000	-2.796228000	-0.365129000
1	2.068629000	-0.091276000	1.256615000
1	3.263656000	-1.156439000	-1.342074000
1	-5.768701000	-0.359643000	1.960364000
1	-7.604631000	1.190920000	1.403183000
1	-7.537502000	2.491905000	-0.712871000
1	-5.616025000	2.212533000	-2.261775000
1	-3.792347000	0.665055000	-1.714863000
1	5.398042000	-0.422471000	-2.005370000
1	7.506409000	0.808530000	-1.629053000
1	7.831606000	2.105162000	0.464478000
1	6.030597000	2.154215000	2.172144000
1	3.934292000	0.931817000	1.802020000
1	-0.069845000	-0.750461000	1.484995000

Zero-point correction=  
(Hartree/Particle)

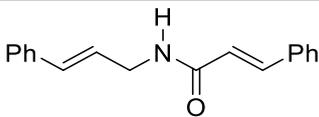
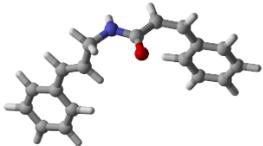
0.303064

Thermal correction to Energy=	0.321048
Thermal correction to Enthalpy=	0.321992
Thermal correction to Gibbs Free Energy=	0.251757
Sum of electronic and zero-point Energies=	-826.067187
Sum of electronic and thermal Energies=	-826.049203
Sum of electronic and thermal Enthalpies=	-826.048259
Sum of electronic and thermal Free Energies=	-826.118493

	E (Thermal) kCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	201.461	68.286	147.822

#UB3LYP-D3/6-311+G\*\*

71-lin-H

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3	

xyz-matrix

6	-3.106954000	1.235744000	-0.031517000
6	-1.858006000	1.392121000	0.421917000
6	-1.091101000	2.683295000	0.341259000
7	0.135586000	2.548865000	-0.444486000
6	1.298519000	2.072363000	0.128417000
6	2.390936000	1.805785000	-0.813164000
8	1.407385000	1.899421000	1.340034000
6	3.675485000	1.280302000	-0.367365000
6	-3.926060000	0.014755000	0.000678000
6	-5.220008000	0.051503000	-0.542127000
6	-6.036375000	-1.077111000	-0.542383000
6	-5.574176000	-2.272527000	0.002642000
6	-4.289444000	-2.326113000	0.548344000
6	-3.476352000	-1.199372000	0.548298000
6	3.978877000	-0.094210000	-0.239455000
6	5.267551000	-0.511993000	0.197928000
6	5.577266000	-1.854434000	0.325610000
6	4.623087000	-2.834872000	0.025070000
6	3.347705000	-2.448505000	-0.403855000
6	3.024923000	-1.108600000	-0.534258000
1	-3.597336000	2.100796000	-0.477165000
1	-1.313764000	0.569177000	0.876432000
1	-1.702174000	3.474228000	-0.101489000
1	-0.786939000	3.005326000	1.339820000
1	2.236299000	2.021921000	-1.870603000
1	4.442801000	2.002466000	-0.093050000
1	-5.588817000	0.978980000	-0.968635000
1	-7.032396000	-1.021496000	-0.967338000
1	-6.205847000	-3.153478000	0.005650000
1	-3.922064000	-3.251776000	0.977464000
1	-2.484812000	-1.264364000	0.980462000
1	6.010146000	0.242344000	0.435541000
1	6.565119000	-2.148457000	0.662812000
1	4.869361000	-3.885277000	0.127333000
1	2.603959000	-3.204265000	-0.631614000
1	2.030299000	-0.819767000	-0.855439000
1	0.032742000	2.467433000	-1.445290000

Zero-point correction=  
(Hartree/Particle)

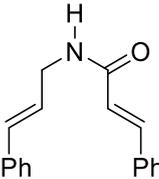
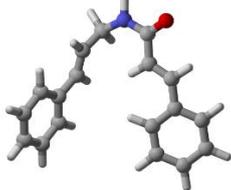
0.298992

Thermal correction to Energy=	0.317307
Thermal correction to Enthalpy=	0.318251
Thermal correction to Gibbs Free Energy=	0.246473
Sum of electronic and zero-point Energies=	-825.986909
Sum of electronic and thermal Energies=	-825.968594
Sum of electronic and thermal Enthalpies=	-825.967650
Sum of electronic and thermal Free Energies=	-826.039428

	E (Thermal) kCal/Mol	CV cal/Mol-Kelvin	S cal/Mol-Kelvin
Total	199.113	70.064	151.070

#B3LYP-D3/6-311+G\*\*

69-NAC-H

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

xyz-matrix

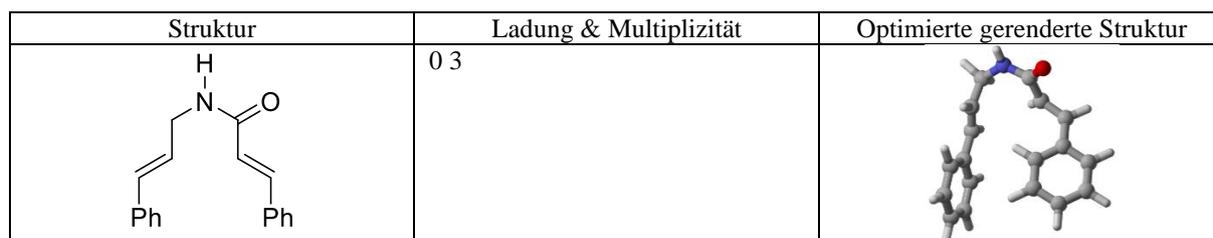
6	1.952665000	0.923230000	0.901615000
6	1.659805000	2.122564000	0.386515000
6	0.720383000	3.099555000	1.043320000
7	-0.339387000	3.588671000	0.158088000
6	-1.453063000	2.918652000	-0.298118000
6	-1.531771000	1.468061000	0.012456000
8	-2.313294000	3.512178000	-0.938705000
6	-2.589736000	0.739162000	-0.372067000
6	2.819556000	-0.115868000	0.329611000
6	2.830376000	-1.388183000	0.923118000
6	3.610109000	-2.419290000	0.404823000
6	4.402039000	-2.197140000	-0.719248000
6	4.408950000	-0.934499000	-1.316481000
6	3.630647000	0.093509000	-0.798608000
6	-2.760092000	-0.701672000	-0.170342000
6	-4.041293000	-1.262722000	-0.294236000
6	-4.250990000	-2.624359000	-0.092600000
6	-3.178253000	-3.456303000	0.222000000
6	-1.893997000	-2.916910000	0.328426000
6	-1.685473000	-1.557342000	0.133738000
1	1.477333000	0.649473000	1.843444000
1	2.070393000	2.441419000	-0.567501000
1	0.292598000	2.660995000	1.951549000
1	1.277931000	3.985539000	1.363122000
1	-0.707388000	1.004128000	0.533907000
1	-3.398912000	1.265108000	-0.873010000
1	2.216373000	-1.569054000	1.799878000
1	3.599892000	-3.393913000	0.879823000
1	5.011760000	-2.995941000	-1.125554000
1	5.027737000	-0.751802000	-2.187935000
1	3.658441000	1.068023000	-1.271686000
1	-4.878242000	-0.618845000	-0.543356000
1	-5.249692000	-3.035758000	-0.186018000
1	-3.337026000	-4.518142000	0.372189000
1	-1.051802000	-3.562381000	0.551771000
1	-0.677949000	-1.161327000	0.190822000
1	-0.348550000	4.571687000	-0.071951000

Zero-point correction= 0.303249  
(Hartree/Particle)

Thermal correction to Energy=	0.321131
Thermal correction to Enthalpy=	0.322076
Thermal correction to Gibbs Free Energy=	0.252770
Sum of electronic and zero-point Energies=	-826.063045
Sum of electronic and thermal Energies=	-826.045162
Sum of electronic and thermal Enthalpies=	-826.044218
Sum of electronic and thermal Free Energies=	-826.113524

#UB3LYP-D3/6-311+G\*\*

71-NAC-H



xyz-matrix

6	-0.627640000	2.111960000	-0.678245000
6	0.321337000	2.571092000	0.145322000
6	1.648030000	3.114438000	-0.315409000
7	2.792739000	2.454618000	0.317702000
6	3.061154000	1.095657000	0.305837000
6	2.453298000	0.296744000	-0.759196000
8	3.821579000	0.599473000	1.136185000
6	2.498239000	-1.162542000	-0.738740000
6	-1.905348000	1.487370000	-0.307390000
6	-2.675573000	0.877794000	-1.309569000
6	-3.863533000	0.218270000	-1.005391000
6	-4.309600000	0.156871000	0.312666000
6	-3.558650000	0.765041000	1.321264000
6	-2.373639000	1.423588000	1.016075000
6	1.421437000	-1.977674000	-0.322126000
6	1.532828000	-3.397374000	-0.336288000
6	0.471205000	-4.197539000	0.047943000
6	-0.740717000	-3.625161000	0.458706000
6	-0.872732000	-2.231741000	0.485960000
6	0.184206000	-1.421353000	0.109579000
1	-0.431550000	2.148601000	-1.749128000
1	0.193838000	2.524024000	1.223903000
1	1.727903000	3.052611000	-1.405811000
1	1.731436000	4.176304000	-0.063980000
1	1.994441000	0.802416000	-1.605313000
1	3.421837000	-1.643635000	-1.054231000
1	-2.328437000	0.909125000	-2.337159000
1	-4.436209000	-0.251887000	-1.796713000
1	-5.232568000	-0.357420000	0.554756000
1	-3.899780000	0.724514000	2.349680000
1	-1.808068000	1.888381000	1.814911000
1	2.467220000	-3.847945000	-0.654004000
1	0.578624000	-5.276650000	0.030163000
1	-1.569518000	-4.258528000	0.753325000
1	-1.806497000	-1.776405000	0.797670000
1	0.072652000	-0.345973000	0.135738000
1	3.217063000	2.921705000	1.106809000

Zero-point correction=  
(Hartree/Particle)

0.299266

Thermal correction to Energy=

0.317391

Thermal correction to Enthalpy=

0.318335

Thermal correction to Gibbs Free Energy=

0.249252

Sum of electronic and zero-point Energies=

-825.986423

Sum of electronic and thermal Energies=

-825.968299

Sum of electronic and thermal Enthalpies=

-825.967355

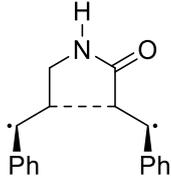
Sum of electronic and thermal Free Energies=

-826.036438

	E (Thermal)	CV	S
	kCal/Mol	cal/Mol-Kelvin	cal/Mol-kelvin
Total	199.166	69.983	145.398

#UB3LYP-D3/6-311+G\*\*

73-H-cis

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3  $\nu_{imag} = -167.2 \text{ cm}^{-1}$	

xyz-matrix

1	-2.198115000	-2.375961000	-2.425919000
1	-4.105963000	-2.250665000	-0.839095000
6	-2.016095000	-2.152973000	-1.379900000
6	-3.094512000	-2.083551000	-0.488267000
1	0.094523000	-1.998162000	-1.651586000
6	-0.722761000	-1.936193000	-0.944272000
6	-2.852254000	-1.798790000	0.869637000
1	2.145701000	-1.804257000	-0.843683000
1	-3.684890000	-1.736648000	1.561467000
6	-0.443048000	-1.651791000	0.436055000
1	1.138271000	0.377977000	-2.123680000
1	-0.947715000	0.880659000	-2.049292000
1	3.442962000	-0.048764000	-2.299169000
6	-1.570410000	-1.596429000	1.325013000
1	-3.335889000	1.175703000	-1.597515000
6	2.037497000	-1.276233000	0.096202000
6	0.840924000	-1.415369000	0.920394000
6	1.738869000	0.819269000	-1.335934000
1	-1.391494000	-1.372442000	2.370932000
6	-1.254866000	1.351514000	-1.124612000
6	3.242636000	0.659704000	-1.487244000
6	-2.609025000	1.523306000	-0.872583000
6	3.202152000	-0.573339000	0.650171000
8	3.522603000	-0.650001000	1.834745000
1	0.978193000	-1.234836000	1.981210000
7	3.879501000	0.217239000	-0.247548000
1	3.706924000	1.606824000	-1.782097000
6	1.141690000	1.569820000	-0.377787000
6	-0.286954000	1.771109000	-0.191072000
6	-3.037882000	2.128955000	0.309265000
1	-4.096536000	2.258311000	0.502962000
1	1.778212000	1.999825000	0.393346000
6	-0.738191000	2.385723000	0.993430000
6	-2.093984000	2.562467000	1.241167000
1	-0.009631000	2.711781000	1.728621000
1	-2.416175000	3.033275000	2.163218000
1	4.661568000	0.733528000	0.127176000

Zero-point correction=  
(Hartree/Particle)

0.298635

Thermal correction to Energy=

0.316041

Thermal correction to Enthalpy=

0.316985

Thermal correction to Gibbs Free Energy=

0.250674

Sum of electronic and zero-point Energies=

-825.975895

Sum of electronic and thermal Energies=

-825.958489

Sum of electronic and thermal Enthalpies=

-825.957545

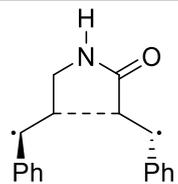
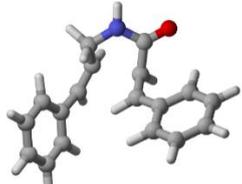
Sum of electronic and thermal Free Energies=

-826.023857

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	198.319	68.485	139.564

#UB3LYP-D3/6-311+G\*\*

73-H-trans

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3  $\nu_{imag} = -385.2 \text{ cm}^{-1}$	

xyz-matrix

1	-0.998924000	3.100483000	-1.058805000
8	2.560962000	2.920705000	-0.052865000
1	1.085543000	1.634728000	-1.922011000
1	-2.329241000	1.485858000	-2.088137000
1	3.450736000	0.660786000	-0.603325000
6	1.432573000	2.461034000	0.058680000
6	-1.227423000	2.211954000	-0.476570000
6	0.868959000	1.427791000	-0.874156000
6	-2.136244000	1.343004000	-1.027917000
1	-2.839817000	-0.833983000	-2.368369000
1	5.328833000	-0.871572000	-0.182790000
7	0.546283000	2.832366000	1.024641000
1	-1.473243000	3.022265000	1.508643000
6	3.255534000	-0.369408000	-0.330493000
6	-0.818416000	2.323570000	0.976953000
6	4.310988000	-1.233441000	-0.086196000
6	-3.070041000	-0.920364000	-1.311623000
6	-2.758893000	0.156773000	-0.454022000
6	0.794805000	0.022571000	-0.450088000
6	1.909181000	-0.817169000	-0.207321000
1	-0.887407000	1.354158000	1.478867000
1	-3.849588000	-2.908608000	-1.505087000
1	-0.191638000	-0.422046000	-0.345073000
6	-3.636016000	-2.091615000	-0.824965000
6	4.078511000	-2.562583000	0.285498000
6	-3.095662000	0.021469000	0.908544000
1	4.910999000	-3.230378000	0.474961000
1	-2.945259000	0.850880000	1.586346000
6	1.697021000	-2.174013000	0.173053000
6	2.761755000	-3.024140000	0.412718000
6	-3.930483000	-2.217459000	0.533885000
6	-3.667583000	-1.150105000	1.392812000
1	0.678534000	-2.535416000	0.273027000
1	2.575229000	-4.053018000	0.700919000
1	-4.374370000	-3.129658000	0.915424000
1	-3.920843000	-1.226360000	2.444417000
1	0.857375000	3.462468000	1.748655000

Zero-point correction=  
(Hartree/Particle)

0.299441

Thermal correction to Energy=

0.316422

Thermal correction to Enthalpy=

0.317366

Thermal correction to Gibbs Free Energy=

0.251879

Sum of electronic and zero-point Energies=

-825.971139

Sum of electronic and thermal Energies=

-825.954158

Sum of electronic and thermal Enthalpies=

-825.953213

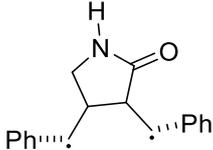
Sum of electronic and thermal Free Energies=

-826.018700

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	198.558	67.486	137.829

#UB3LYP-D3/6-311+G\*\*

72-H-cis

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3	

xyz-matrix

6	1.100098000	-1.598486000	0.142411000
6	1.679507000	-0.493155000	0.967079000
6	1.843713000	0.847924000	0.147584000
6	0.743956000	1.202808000	-0.787868000
6	3.152380000	-0.791061000	1.346613000
7	3.883115000	-0.280078000	0.194256000
6	3.210378000	0.664266000	-0.529868000
8	3.624331000	1.249767000	-1.509616000
6	-0.257497000	-1.982041000	0.087840000
6	-0.657073000	-3.030314000	-0.792857000
6	-1.979275000	-3.424081000	-0.891815000
6	-2.966089000	-2.794890000	-0.121931000
6	-2.601377000	-1.764700000	0.751809000
6	-1.280497000	-1.364956000	0.862550000
6	-0.493589000	1.754001000	-0.392119000
6	-1.529486000	1.937582000	-1.351839000
6	-2.768544000	2.432696000	-0.987287000
6	-3.032231000	2.777384000	0.344545000
6	-2.027220000	2.622583000	1.305653000
6	-0.784440000	2.122728000	0.952362000
1	1.788223000	-2.102905000	-0.530903000
1	1.078792000	-0.316001000	1.860018000
1	1.996145000	1.654169000	0.881034000
1	0.898659000	0.978049000	-1.836971000
1	3.332379000	-1.858512000	1.489200000
1	3.433727000	-0.265565000	2.268226000
1	0.099496000	-3.519640000	-1.397639000
1	-2.252631000	-4.222691000	-1.572794000
1	-4.002436000	-3.100712000	-0.205224000
1	-3.359869000	-1.263762000	1.343085000
1	-1.035311000	-0.550623000	1.530547000
1	-1.335804000	1.666310000	-2.384032000
1	-3.541455000	2.552178000	-1.738538000
1	-4.004235000	3.164151000	0.627499000
1	-2.221653000	2.895551000	2.337329000
1	-0.024058000	2.009759000	1.716372000
1	4.857301000	-0.467087000	0.012768000

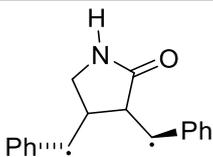
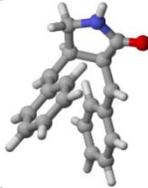
Zero-point correction= 0.301869  
(Hartree/Particle)

Thermal correction to Energy=	0.318753
Thermal correction to Enthalpy=	0.319697
Thermal correction to Gibbs Free Energy=	0.254750
Sum of electronic and zero-point Energies=	-826.017094
Sum of electronic and thermal Energies=	-826.000210
Sum of electronic and thermal Enthalpies=	-825.999266
Sum of electronic and thermal Free Energies=	-826.064213

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	200.020	67.476	136.693

#UB3LYP-D3/6-311+G\*\*

72-H-trans

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3	

xyz-matrix

6	-0.571852000	-0.195230000	-1.509622000
6	-0.713883000	1.290704000	-1.354143000
6	-0.142399000	1.894946000	-0.003151000
6	0.675796000	0.988908000	0.857527000
6	-2.187736000	1.821576000	-1.419539000
7	-2.418338000	2.434434000	-0.122238000
6	-1.363631000	2.446752000	0.739278000
8	-1.387486000	2.831731000	1.892264000
6	-1.176001000	-1.215201000	-0.737316000
6	-0.879634000	-2.576086000	-1.040184000
6	-1.428212000	-3.615745000	-0.310854000
6	-2.297675000	-3.351791000	0.754444000
6	-2.605465000	-2.025368000	1.074916000
6	-2.062665000	-0.975999000	0.350643000
6	1.940940000	0.474044000	0.502689000
6	2.598035000	-0.448797000	1.365567000
6	3.829969000	-0.986863000	1.038112000
6	4.466260000	-0.629068000	-0.157267000
6	3.846000000	0.281895000	-1.019784000
6	2.610449000	0.823596000	-0.704010000
1	0.123913000	-0.523493000	-2.274242000
1	-0.162078000	1.741543000	-2.178742000
1	0.454451000	2.779302000	-0.266914000
1	0.253755000	0.709738000	1.815761000
1	-2.891886000	1.005249000	-1.597529000
1	-2.301800000	2.552975000	-2.225353000
1	-0.201655000	-2.790839000	-1.859510000
1	-1.179466000	-4.640312000	-0.564819000
1	-2.725142000	-4.166395000	1.327251000
1	-3.272126000	-1.811368000	1.903172000
1	-2.314919000	0.035946000	0.634499000
1	2.110040000	-0.732763000	2.291758000
1	4.305317000	-1.690551000	1.712682000
1	5.431508000	-1.051442000	-0.410960000
1	4.336301000	0.567835000	-1.944160000
1	2.150676000	1.528348000	-1.386866000
1	-3.318415000	2.777711000	0.177695000

Zero-point correction=  
(Hartree/Particle)

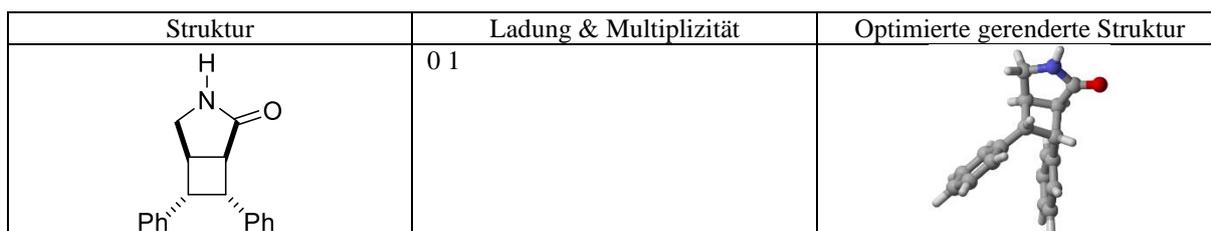
0.302100

Thermal correction to Energy=	0.319071
Thermal correction to Enthalpy=	0.320015
Thermal correction to Gibbs Free Energy=	0.254552
Sum of electronic and zero-point Energies=	-826.012774
Sum of electronic and thermal Energies=	-825.995803
Sum of electronic and thermal Enthalpies=	-825.994859
Sum of electronic and thermal Free Energies=	-826.060322

Total	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
	200.220	67.459	137.778

#B3LYP-D3/6-311+G\*\*

70-H-cis-trans



xyz-matrix

6	0.716717000	-0.879675000	-0.244212000
6	1.637625000	-0.607783000	0.984623000
6	2.084935000	0.713396000	0.314246000
6	0.883424000	0.653200000	-0.662459000
6	2.887747000	-1.491302000	1.100608000
7	3.787967000	-0.878975000	0.128090000
6	3.422129000	0.356814000	-0.336335000
8	4.051008000	1.036270000	-1.124252000
6	-0.649594000	-1.478599000	-0.077953000
6	-1.142079000	-2.358144000	-1.050104000
6	-2.423597000	-2.896967000	-0.953186000
6	-3.240184000	-2.563686000	0.125788000
6	-2.763297000	-1.690371000	1.102306000
6	-1.482561000	-1.153550000	1.000133000
6	-0.307001000	1.523857000	-0.348805000
6	-1.338188000	1.606279000	-1.294230000
6	-2.496097000	2.332133000	-1.035750000
6	-2.648127000	2.998339000	0.180537000
6	-1.630371000	2.929975000	1.127916000
6	-0.472363000	2.197308000	0.865045000
1	1.273400000	-1.477050000	-0.971549000
1	1.095877000	-0.509138000	1.923439000
1	2.213394000	1.620235000	0.905573000
1	1.154994000	0.782809000	-1.712067000
1	2.674371000	-2.534094000	0.845308000
1	3.316517000	-1.464073000	2.109059000
1	-0.512811000	-2.621994000	-1.894587000
1	-2.782020000	-3.577079000	-1.718058000
1	-4.238006000	-2.980159000	0.205404000
1	-3.392653000	-1.419877000	1.942900000
1	-1.141364000	-0.459479000	1.757883000
1	-1.232009000	1.084837000	-2.239878000
1	-3.280329000	2.378790000	-1.783129000
1	-3.548323000	3.567059000	0.384167000
1	-1.734008000	3.447398000	2.075439000
1	0.300885000	2.155044000	1.622950000
1	4.673545000	-1.277910000	-0.144484000

Zero-point correction=  
(Hartree/Particle)

0.306947

Thermal correction to Energy=

0.322760

Thermal correction to Enthalpy=

0.323705

Thermal correction to Gibbs Free Energy=

0.262215

Sum of electronic and zero-point Energies=

-826.067512

Sum of electronic and thermal Energies=

-826.051699

Sum of electronic and thermal Enthalpies=

-826.050755

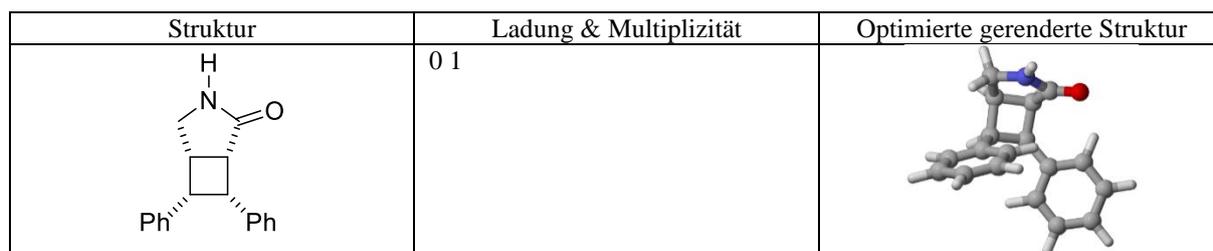
Sum of electronic and thermal Free Energies=

-826.112244

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	202.535	63.810	129.415

#B3LYP-D3/6-311+G\*\*

70H-cis-cis



xyz-matrix

6	-0.826627000	0.291158000	-1.458585000
6	-1.316625000	1.776094000	-1.233006000
6	0.101787000	2.170100000	-0.740802000
6	0.648986000	0.820780000	-1.309019000
6	-2.290978000	2.060281000	-0.079968000
7	-1.397499000	2.275633000	1.049491000
6	-0.065310000	2.356486000	0.770193000
8	0.811365000	2.579563000	1.586819000
6	-1.368259000	-0.749088000	-0.507758000
6	-0.923345000	-0.897735000	0.812601000
6	-1.502082000	-1.840982000	1.658795000
6	-2.537484000	-2.657111000	1.206081000
6	-2.987362000	-2.525941000	-0.106356000
6	-2.404446000	-1.582707000	-0.950304000
6	1.736662000	-0.009193000	-0.674152000
6	2.696010000	0.543239000	0.178761000
6	3.723163000	-0.248810000	0.693265000
6	3.807831000	-1.599282000	0.362958000
6	2.856346000	-2.157593000	-0.491073000
6	1.832055000	-1.367657000	-1.004194000
1	-1.037010000	-0.048146000	-2.474479000
1	-1.636653000	2.241353000	-2.164524000
1	0.571962000	3.070723000	-1.140067000
1	0.985270000	1.049986000	-2.326684000
1	-2.962216000	1.216643000	0.103670000
1	-2.896742000	2.952071000	-0.275008000
1	-0.110007000	-0.291381000	1.186614000
1	-1.134883000	-1.941841000	2.674059000
1	-2.983112000	-3.392629000	1.866325000
1	-3.786571000	-3.159187000	-0.475533000
1	-2.758231000	-1.491975000	-1.972918000
1	2.622754000	1.582242000	0.470920000
1	4.453570000	0.194125000	1.361417000
1	4.603795000	-2.213250000	0.769491000
1	2.908180000	-3.208915000	-0.752187000
1	1.087977000	-1.814105000	-1.655037000
1	-1.718426000	2.396112000	1.998340000

Zero-point correction=  
(Hartree/Particle)

0.307520

Thermal correction to Energy=

0.323071

Thermal correction to Enthalpy=

0.324015

Thermal correction to Gibbs Free Energy=

0.263655

Sum of electronic and zero-point Energies=

-826.064082

Sum of electronic and thermal Energies=

-826.048531

Sum of electronic and thermal Enthalpies=

-826.047587

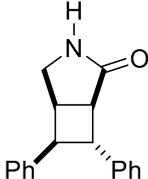
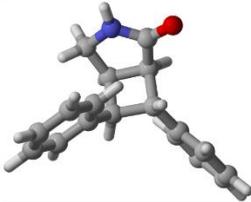
Sum of electronic and thermal Free Energies=

-826.107947

	E (Thermal)	CV	S
	kCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	202.730	63.504	127.039

#B3LYP-D3/6-311+G\*\*

70-H-(R)-(R)

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

xyz-matrix

6	-0.292797000	-0.286814000	-0.749183000
6	-0.417642000	1.132348000	-1.432825000
6	0.489264000	1.727440000	-0.330064000
6	0.730226000	0.313030000	0.287976000
6	-1.758415000	1.883647000	-1.354058000
7	-1.655824000	2.610959000	-0.094291000
6	-0.435977000	2.592410000	0.520038000
8	-0.158491000	3.136259000	1.572968000
6	-1.550583000	-0.942743000	-0.241546000
6	-2.135568000	-1.973646000	-0.988968000
6	-3.325955000	-2.573644000	-0.583882000
6	-3.957140000	-2.153050000	0.585584000
6	-3.386324000	-1.130464000	1.341467000
6	-2.196860000	-0.530663000	0.931315000
6	2.130038000	-0.235023000	0.201309000
6	2.719135000	-0.851267000	1.309540000
6	4.007126000	-1.381231000	1.235566000
6	4.729967000	-1.301283000	0.047694000
6	4.155258000	-0.687155000	-1.065651000
6	2.868935000	-0.160988000	-0.987396000
1	0.211437000	-0.981196000	-1.422959000
1	-0.016565000	1.135793000	-2.445874000
1	1.381823000	2.287357000	-0.608457000
1	0.391850000	0.250244000	1.322584000
1	-2.610771000	1.198505000	-1.344690000
1	-1.878703000	2.574109000	-2.195995000
1	-1.647754000	-2.312302000	-1.897654000
1	-3.755911000	-3.372902000	-1.177461000
1	-4.880916000	-2.620527000	0.907096000
1	-3.866347000	-0.797602000	2.255129000
1	-1.778603000	0.268187000	1.531209000
1	2.165007000	-0.912409000	2.240325000
1	4.445240000	-1.853131000	2.108073000
1	5.732389000	-1.709822000	-0.011127000
1	4.711132000	-0.616718000	-1.994181000
1	2.436963000	0.316253000	-1.861687000
1	-2.417702000	3.133955000	0.310467000

Zero-point correction=  
(Hartree/Particle)

0.307078

Thermal correction to Energy=

0.322939

Thermal correction to Enthalpy=

0.323883

Thermal correction to Gibbs Free Energy=

0.261304

Sum of electronic and zero-point Energies=

-826.068072

Sum of electronic and thermal Energies=

-826.052212

Sum of electronic and thermal Enthalpies=

-826.051267

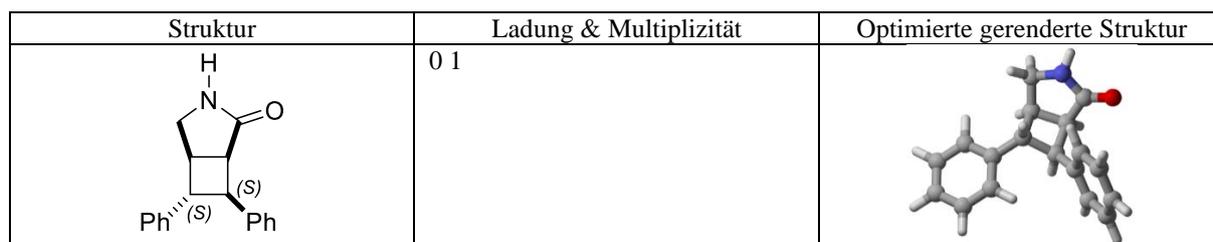
Sum of electronic and thermal Free Energies=

-826.113846

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	202.647	63.701	131.707

#B3LYP-D3/6-311+G\*\*

70-H-(S)-(S)



xyz-matrix

6	-0.743168000	0.598310000	0.132851000
6	-0.619105000	2.014160000	-0.504002000
6	0.735081000	1.583428000	-1.126571000
6	0.388362000	0.085979000	-0.816805000
6	-0.312933000	3.173147000	0.455754000
7	1.121952000	3.021848000	0.678571000
6	1.786195000	2.248052000	-0.242257000
8	2.991967000	2.128390000	-0.324749000
6	-2.064126000	-0.124301000	0.120094000
6	-3.275840000	0.571069000	0.179771000
6	-4.492130000	-0.111331000	0.191217000
6	-4.513778000	-1.503700000	0.141732000
6	-3.310899000	-2.207589000	0.083680000
6	-2.097430000	-1.523744000	0.073226000
6	1.416327000	-0.892687000	-0.319174000
6	2.044552000	-0.738400000	0.922568000
6	2.978729000	-1.667692000	1.370251000
6	3.304058000	-2.772739000	0.584137000
6	2.688876000	-2.938367000	-0.654784000
6	1.754070000	-2.004763000	-1.098736000
1	-0.366493000	0.636151000	1.161087000
1	-1.414452000	2.241264000	-1.212603000
1	0.953604000	1.809428000	-2.170507000
1	-0.081872000	-0.324671000	-1.714348000
1	-0.870886000	3.086340000	1.393205000
1	-0.543827000	4.146589000	0.006462000
1	-3.273445000	1.655421000	0.217244000
1	-5.421736000	0.445467000	0.236094000
1	-5.458371000	-2.035673000	0.147123000
1	-3.317451000	-3.291370000	0.045145000
1	-1.166287000	-2.078325000	0.029307000
1	1.815583000	0.119399000	1.544220000
1	3.458502000	-1.526085000	2.332254000
1	4.032129000	-3.496023000	0.933740000
1	2.934894000	-3.792764000	-1.275669000
1	1.277256000	-2.141012000	-2.064493000
1	1.652417000	3.632818000	1.282027000

Zero-point correction=  
(Hartree/Particle)

0.306990

Thermal correction to Energy=

0.322818

Thermal correction to Enthalpy=

0.323763

Thermal correction to Gibbs Free Energy=

0.261849

Sum of electronic and zero-point Energies=

-826.068258

Sum of electronic and thermal Energies=

-826.052429

Sum of electronic and thermal Enthalpies=

-826.051485

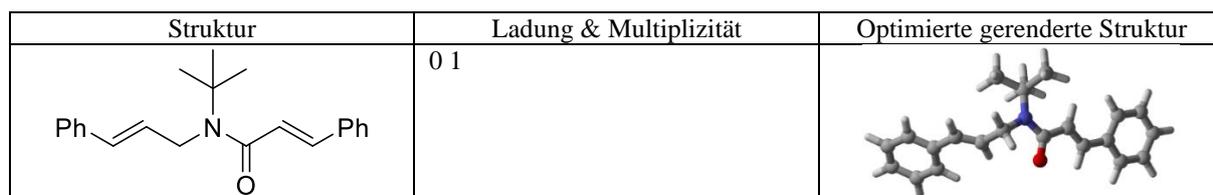
Sum of electronic and thermal Free Energies=

-826.113399

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	202.572	63.709	130.309

#B3LYP-D3/6-311+G\*\*

69-lin-'Bu



xyz-matrix

6	3.585682000	0.420238000	-0.681476000
6	2.305032000	0.132278000	-0.937736000
6	1.325501000	1.102978000	-1.536990000
7	0.075156000	1.228349000	-0.753054000
6	-0.838815000	0.223304000	-1.024894000
6	-0.032934000	2.256438000	0.346493000
6	-2.208777000	0.266329000	-0.439890000
8	-0.533028000	-0.700142000	-1.781668000
6	-3.026754000	-0.788913000	-0.574302000
6	1.310890000	2.991430000	0.542078000
6	-1.073668000	3.335875000	-0.021043000
6	-0.344502000	1.573518000	1.695974000
6	4.605238000	-0.480268000	-0.122798000
6	5.837636000	0.054702000	0.284349000
6	6.828828000	-0.752504000	0.837740000
6	6.610343000	-2.119558000	0.992042000
6	5.393509000	-2.669667000	0.582578000
6	4.405857000	-1.863389000	0.029404000
6	-4.401450000	-0.908901000	-0.084413000
6	-5.099006000	-2.103947000	-0.326720000
6	-6.408048000	-2.276895000	0.114818000
6	-7.049825000	-1.255080000	0.810792000
6	-6.371167000	-0.059627000	1.061181000
6	-5.065556000	0.111806000	0.620101000
1	3.934567000	1.431972000	-0.887112000
1	1.893964000	-0.851880000	-0.738270000
1	1.775192000	2.084854000	-1.664940000
1	1.037950000	0.743844000	-2.526777000
1	-2.547404000	1.152480000	0.070086000
1	-2.629124000	-1.649432000	-1.105157000
1	1.204983000	3.663528000	1.396166000
1	2.125817000	2.300988000	0.757882000
1	1.581705000	3.605535000	-0.318604000
1	-1.091121000	4.113061000	0.748125000
1	-2.085978000	2.948266000	-0.121908000
1	-0.803204000	3.801575000	-0.971913000
1	0.448414000	0.861942000	1.938845000
1	-0.385706000	2.325131000	2.488960000
1	-1.289049000	1.033409000	1.700291000
1	6.016567000	1.119056000	0.168071000
1	7.771114000	-0.313433000	1.146427000
1	7.379619000	-2.752351000	1.419778000
1	5.218274000	-3.734637000	0.688555000
1	3.475839000	-2.313351000	-0.297378000
1	-4.603750000	-2.902336000	-0.869166000
1	-6.925809000	-3.208204000	-0.085093000
1	-8.069081000	-1.385364000	1.156166000
1	-6.865090000	0.739649000	1.602423000
1	-4.558641000	1.047507000	0.825546000

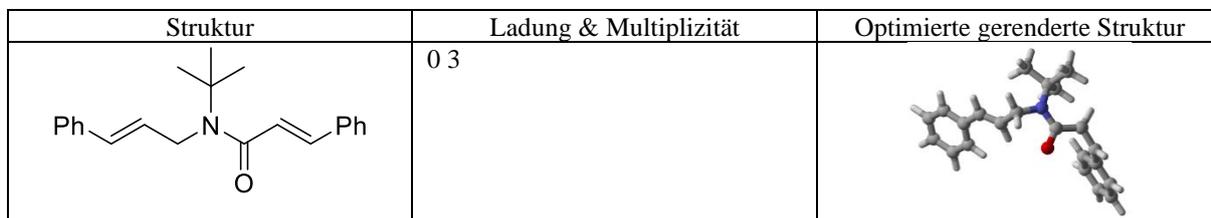
Zero-point correction=  
(Hartree/Particle)

0.415620

Thermal correction to Energy=	0.438659
Thermal correction to Enthalpy=	0.439603
Thermal correction to Gibbs Free Energy=	0.359568
Sum of electronic and zero-point Energies=	-983.245002
Sum of electronic and thermal Energies=	-983.221963
Sum of electronic and thermal Enthalpies=	-983.221019
Sum of electronic and thermal Free Energies=	-983.301054

Total E (Thermal) CV S  
 kcal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin  
 275.263 89.210 168.447

#UB3LYP-D3/6-311+G\*\* 71-lin-Bu



xyz-matrix

6	-3.084259000	0.512642000	0.665744000
6	-1.782122000	0.556297000	0.968100000
6	-1.041665000	1.813384000	1.333995000
7	0.175401000	2.019849000	0.516797000
6	1.262476000	1.280778000	0.970495000
6	0.100300000	2.763930000	-0.791898000
6	2.582977000	1.381690000	0.343063000
8	1.140451000	0.523897000	1.943026000
6	3.661315000	0.495438000	0.775277000
6	-1.342181000	3.235993000	-1.070549000
6	0.974821000	4.034688000	-0.740195000
6	0.486641000	1.837641000	-1.965565000
6	-3.880135000	-0.674319000	0.319410000
6	-5.210615000	-0.504446000	-0.094877000
6	-6.004133000	-1.594377000	-0.445280000
6	-5.482791000	-2.884639000	-0.386830000
6	-4.162360000	-3.071862000	0.028675000
6	-3.372187000	-1.983828000	0.379058000
6	3.916431000	-0.779896000	0.223404000
6	5.011382000	-1.562928000	0.687047000
6	5.273132000	-2.812056000	0.152471000
6	4.459523000	-3.336113000	-0.860351000
6	3.372807000	-2.587913000	-1.328164000
6	3.100306000	-1.336758000	-0.801428000
1	-3.640215000	1.449855000	0.662010000
1	-1.173337000	-0.341915000	0.983581000
1	-1.686575000	2.685291000	1.258119000
1	-0.712786000	1.739352000	2.371955000
1	2.802581000	2.124955000	-0.411464000
1	4.292636000	0.836451000	1.593758000
1	-1.356007000	3.717689000	-2.050441000
1	-2.046632000	2.404873000	-1.096817000
1	-1.685089000	3.974236000	-0.343352000
1	0.871002000	4.595545000	-1.673093000
1	2.033772000	3.827747000	-0.596211000
1	0.648707000	4.674557000	0.083356000
1	-0.182059000	0.973675000	-1.989780000
1	0.387320000	2.375182000	-2.912316000
1	1.510025000	1.471639000	-1.901343000
1	-5.625925000	0.497384000	-0.142581000
1	-7.028831000	-1.434852000	-0.762254000
1	-6.096806000	-3.736428000	-0.656263000
1	-3.749745000	-4.073204000	0.084905000
1	-2.354721000	-2.154324000	0.710444000
1	5.642788000	-1.165188000	1.474523000
1	6.112567000	-3.390046000	0.523188000
1	4.666890000	-4.315711000	-1.274948000
1	2.734767000	-2.993120000	-2.106042000
1	2.246285000	-0.773829000	-1.160346000

Zero-point correction=  
 (Hartree/Particle)

0.411675

Thermal correction to Energy=

0.434954

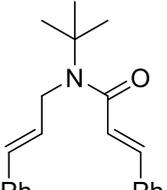
Thermal correction to Enthalpy=

0.435898

Thermal correction to Gibbs Free Energy= 0.354848  
 Sum of electronic and zero-point Energies= -983.166047  
 Sum of electronic and thermal Energies= -983.142769  
 Sum of electronic and thermal Enthalpies= -983.141824  
 Sum of electronic and thermal Free Energies= -983.222874

Total E (Thermal) CV S  
 kcal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin  
 272.937 90.934 170.584

#B3LYP-D3/6-311+G\*\* 69-NAC-'Bu

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

xyz-matrix

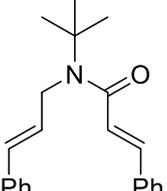
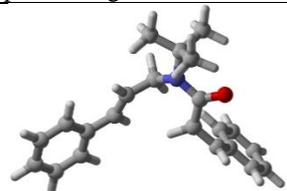
6	-0.325956000	-1.873352000	0.893153000
6	0.955067000	-1.678491000	0.559045000
6	1.802026000	-0.582272000	1.146792000
7	2.505004000	0.248669000	0.143660000
6	1.949877000	1.482907000	-0.165852000
6	3.967393000	-0.005598000	-0.100584000
6	0.460785000	1.551589000	-0.101238000
8	2.615660000	2.454633000	-0.507117000
6	-0.175265000	2.731973000	-0.115561000
6	4.246436000	-1.521434000	-0.046302000
6	4.362901000	0.458789000	-1.517301000
6	4.804853000	0.722191000	0.965698000
6	-1.245046000	-2.896050000	0.374400000
6	-2.604843000	-2.818680000	0.714879000
6	-3.523399000	-3.748570000	0.233643000
6	-3.099268000	-4.782089000	-0.598250000
6	-1.748458000	-4.877517000	-0.940577000
6	-0.832990000	-3.949486000	-0.459427000
6	-1.624805000	2.944379000	-0.101981000
6	-2.115637000	4.258036000	-0.027726000
6	-3.483944000	4.516018000	-0.004213000
6	-4.393043000	3.462026000	-0.058543000
6	-3.921980000	2.148791000	-0.138438000
6	-2.557402000	1.891927000	-0.160508000
1	-0.768872000	-1.191796000	1.619006000
1	1.438831000	-2.305688000	-0.182385000
1	1.188835000	0.058353000	1.783985000
1	2.554688000	-1.007429000	1.813686000
1	-0.092672000	0.623134000	-0.086796000
1	0.443638000	3.625632000	-0.139673000
1	5.301929000	-1.687581000	-0.270970000
1	4.054462000	-1.967822000	0.930473000
1	3.658095000	-2.055167000	-0.796500000
1	5.377257000	0.111943000	-1.731042000
1	4.332998000	1.539360000	-1.617511000
1	3.689594000	0.021170000	-2.259428000
1	4.551550000	0.368296000	1.970038000
1	5.871073000	0.538774000	0.804547000
1	4.621280000	1.795586000	0.914383000
1	-2.943208000	-2.016723000	1.363620000
1	-4.568574000	-3.666366000	0.510291000
1	-3.809985000	-5.509460000	-0.973452000
1	-1.408642000	-5.683142000	-1.581958000
1	0.212005000	-4.049032000	-0.728673000
1	-1.411537000	5.082520000	0.012865000
1	-3.838864000	5.538774000	0.054392000
1	-5.459097000	3.658279000	-0.042757000

1 -4.624093000 1.323904000 -0.188765000  
 1 -2.214817000 0.866215000 -0.232715000

Zero-point correction= 0.415075  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.438238  
 Thermal correction to Enthalpy= 0.439182  
 Thermal correction to Gibbs Free Energy= 0.359062  
 Sum of electronic and zero-point Energies= -983.249686  
 Sum of electronic and thermal Energies= -983.226523  
 Sum of electronic and thermal Enthalpies= -983.225578  
 Sum of electronic and thermal Free Energies= -983.305698

Total E (Thermal) CV S  
 KCal/Mol Cal/Mol-kelvin Cal/Mol-kelvin  
 274.998 89.429 168.626

#UB3LYP-D3/6-311+G\*\* 71-NAC-Bu

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 3	

xyz-matrix

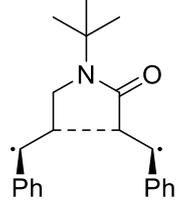
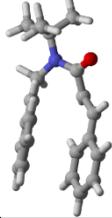
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 6 -1.815623000 0.649625000 -0.596391000  
 6 -0.490778000 1.192076000 -1.060001000  
 7 0.215725000 2.010913000 -0.055461000  
 6 1.244646000 1.410961000 0.659544000  
 6 0.146048000 3.511904000 -0.149179000  
 6 1.145271000 -0.040176000 0.881855000  
 8 2.190412000 2.035687000 1.143568000  
 6 2.284939000 -0.795512000 1.392463000  
 6 -1.215810000 3.946574000 -0.727353000  
 6 0.242045000 4.134958000 1.258162000  
 6 1.277739000 4.023867000 -1.058663000  
 6 -3.432708000 -1.256730000 -0.290471000  
 6 -3.529896000 -2.656824000 -0.269448000  
 6 -4.703727000 -3.292614000 0.127658000  
 6 -5.811361000 -2.538753000 0.508576000  
 6 -5.734320000 -1.144479000 0.484085000  
 6 -4.562786000 -0.511400000 0.086748000  
 6 3.186809000 -1.523454000 0.584285000  
 6 4.272352000 -2.235332000 1.170062000  
 6 5.159598000 -2.954733000 0.389303000  
 6 5.008665000 -2.998048000 -1.002833000  
 6 3.951535000 -2.303879000 -1.603167000  
 6 3.057027000 -1.580868000 -0.832489000  
 1 -1.434177000 -1.329577000 -1.121570000  
 1 -2.492155000 1.371335000 -0.150601000  
 1 0.154554000 0.368820000 -1.374899000  
 1 -0.628866000 1.800856000 -1.956048000  
 1 0.180514000 -0.531650000 0.789025000  
 1 2.460607000 -0.775231000 2.466454000  
 1 -1.254818000 5.037690000 -0.726972000  
 1 -1.377366000 3.623663000 -1.756913000  
 1 -2.043574000 3.585524000 -0.112802000  
 1 0.061442000 5.210488000 1.183134000  
 1 1.216555000 3.975399000 1.709817000  
 1 -0.522214000 3.705439000 1.911693000  
 1 1.187192000 3.598141000 -2.062994000  
 1 1.229914000 5.113015000 -1.148880000  
 1 2.247940000 3.748149000 -0.645989000  
 1 -2.671225000 -3.252000000 -0.563482000

1	-4.752337000	-4.375704000	0.138467000
1	-6.727727000	-3.029301000	0.816195000
1	-6.594958000	-0.549878000	0.769839000
1	-4.530139000	0.571500000	0.059498000
1	4.397821000	-2.203559000	2.247152000
1	5.979208000	-3.487177000	0.859317000
1	5.706486000	-3.562157000	-1.610497000
1	3.833131000	-2.329925000	-2.681020000
1	2.246149000	-1.040724000	-1.308615000

Zero-point correction= 0.410921  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.434404  
 Thermal correction to Enthalpy= 0.435348  
 Thermal correction to Gibbs Free Energy= 0.353092  
 Sum of electronic and zero-point Energies= -983.169631  
 Sum of electronic and thermal Energies= -983.146148  
 Sum of electronic and thermal Enthalpies= -983.145203  
 Sum of electronic and thermal Free Energies= -983.227460

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	272.593	91.182	173.123

#UB3LYP-D3/6-311+G**	73-Bu-cis
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Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
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xyz-matrix

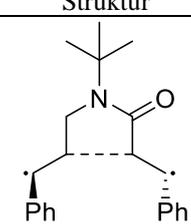
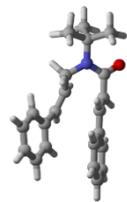
1	-2.688534000	0.646241000	2.189058000
1	-4.937531000	-0.104467000	2.019502000
1	-2.082722000	-0.981514000	2.269260000
1	1.999282000	0.883939000	2.035962000
1	-0.004045000	0.135609000	2.258666000
1	-4.390853000	1.565887000	1.741641000
6	-2.104957000	-0.086109000	1.634874000
1	4.268296000	1.632351000	1.504851000
6	-0.689549000	0.431024000	1.470475000
6	2.168855000	1.443516000	1.125286000
6	-4.858041000	0.694288000	1.277252000
1	-5.870913000	0.990094000	0.995798000
6	3.456651000	1.867314000	0.825813000
1	3.500088000	-2.099239000	2.411020000
6	-0.263835000	1.234278000	0.479167000
6	1.099255000	1.710824000	0.252262000
1	-5.127191000	-1.703902000	0.024125000
1	1.180372000	-2.105613000	1.621512000
1	-0.976237000	1.500450000	-0.297698000
7	-2.786948000	-0.372130000	0.362382000
6	-4.122700000	0.225146000	0.009647000
6	3.712473000	2.579722000	-0.346901000
6	3.292022000	-1.940373000	1.358068000
1	4.719896000	2.906261000	-0.578629000
1	-0.895654000	-2.324914000	0.773605000
6	1.374231000	2.430956000	-0.923710000
6	1.983284000	-1.940758000	0.914312000
6	-5.000666000	-0.855069000	-0.653632000
6	2.662985000	2.862811000	-1.219981000
6	-3.928507000	1.429970000	-0.929691000
1	-4.565935000	-1.210667000	-1.584342000
1	5.375407000	-1.732547000	0.822759000
1	0.564834000	2.639561000	-1.615857000

6	-0.838243000	-1.730688000	-0.131080000
6	4.352395000	-1.735641000	0.465684000
6	-2.033105000	-1.016724000	-0.598771000
1	2.849385000	3.413542000	-2.135276000
1	-5.988532000	-0.438845000	-0.868586000
6	1.671086000	-1.745484000	-0.473650000
6	0.367200000	-1.732280000	-0.966543000
6	4.077353000	-1.538849000	-0.900413000
8	-2.299718000	-1.004640000	-1.804615000
6	2.781219000	-1.550125000	-1.363262000
1	0.206280000	-1.626139000	-2.034003000
1	4.894402000	-1.373500000	-1.593956000
1	2.576397000	-1.391309000	-2.416401000
1	-3.323876000	2.200595000	-0.442146000
1	-4.897462000	1.871365000	-1.180937000
1	-3.435205000	1.122307000	-1.850932000

Zero-point correction= 0.410812  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.433394  
 Thermal correction to Enthalpy= 0.434338  
 Thermal correction to Gibbs Free Energy= 0.357521  
 Sum of electronic and zero-point Energies= -983.165921  
 Sum of electronic and thermal Energies= -983.143339  
 Sum of electronic and thermal Enthalpies= -983.142394  
 Sum of electronic and thermal Free Energies= -983.219212

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	271.959	89.579	161.677

B3LYP-D3/6-311+G**	71-Bu-trans
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Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
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xyz-matrix

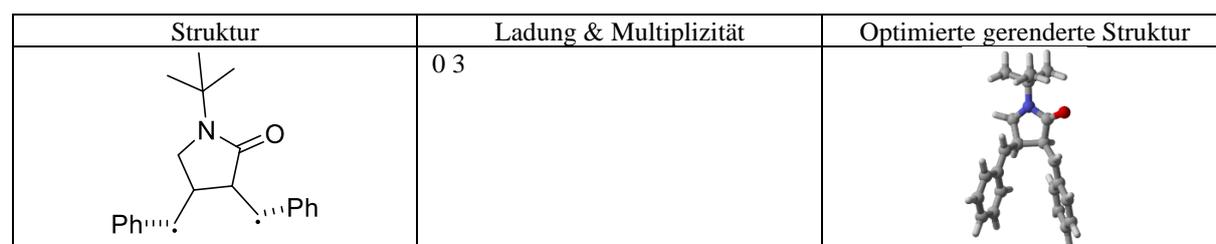
6	-0.468237000	0.862477000	-1.796459000
6	0.842037000	0.581308000	-1.545053000
6	0.868604000	-1.611365000	-0.502375000
6	-0.101421000	-1.299969000	0.553091000
6	1.662476000	1.004766000	-0.353089000
7	2.623141000	-0.044043000	0.027367000
6	2.303901000	-1.328585000	-0.375144000
8	3.136466000	-2.203917000	-0.623452000
6	4.006208000	0.325121000	0.463002000
6	3.965794000	1.673676000	1.209028000
6	4.538968000	-0.726017000	1.455890000
6	4.924613000	0.429150000	-0.766960000
6	-1.466929000	1.517890000	-0.962334000
6	-2.815297000	1.133690000	-1.111865000
6	-3.817427000	1.700416000	-0.335292000
6	-3.507633000	2.691904000	0.595046000
6	-2.184239000	3.115032000	0.731800000
6	-1.177880000	2.540931000	-0.036171000
6	-1.469311000	-1.551905000	0.498393000
6	-2.317771000	-1.160884000	1.590876000
6	-3.671073000	-1.409999000	1.574391000
6	-4.266249000	-2.062541000	0.478940000
6	-3.466534000	-2.449944000	-0.607610000
6	-2.108483000	-2.202198000	-0.613212000
1	-0.858536000	0.462364000	-2.729085000
1	1.421705000	0.162612000	-2.362577000

1	0.638601000	-2.385509000	-1.224052000
1	0.289060000	-0.820254000	1.444889000
1	1.020591000	1.269074000	0.489940000
1	2.216417000	1.905449000	-0.628749000
1	4.947310000	1.861875000	1.648967000
1	3.741967000	2.518483000	0.554893000
1	3.230700000	1.654337000	2.018063000
1	4.653217000	-1.701252000	0.990333000
1	3.857519000	-0.821932000	2.305934000
1	5.512049000	-0.400882000	1.833109000
1	4.544134000	1.177676000	-1.469161000
1	5.934420000	0.727678000	-0.470267000
1	4.976377000	-0.534055000	-1.275662000
1	-3.064886000	0.356244000	-1.824151000
1	-4.841082000	1.364639000	-0.453487000
1	-4.288811000	3.139558000	1.198722000
1	-1.938295000	3.907180000	1.430450000
1	-0.168493000	2.920044000	0.051717000
1	-1.868837000	-0.651156000	2.436586000
1	-4.285173000	-1.096948000	2.411546000
1	-5.331257000	-2.261562000	0.472906000
1	-3.921437000	-2.949778000	-1.456279000
1	-1.515692000	-2.501958000	-1.467904000

Zero-point correction= 0.411221  
(Hartree/Particle)  
Thermal correction to Energy= 0.433664  
Thermal correction to Enthalpy= 0.434608  
Thermal correction to Gibbs Free Energy= 0.357949  
Sum of electronic and zero-point Energies= -983.161616  
Sum of electronic and thermal Energies= -983.139172  
Sum of electronic and thermal Enthalpies= -983.138228  
Sum of electronic and thermal Free Energies= -983.214888

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.128	89.135	161.344

#UB3LYP-D3/6-311+G**	72-Bu-cis
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xyz-matrix

1	-3.585554000	-2.735804000	-2.321943000
1	-5.367916000	-2.853240000	-0.594743000
6	-3.359810000	-2.476442000	-1.293087000
6	-4.365074000	-2.545713000	-0.322281000
1	-1.316971000	-2.031590000	-1.724339000
6	-2.076968000	-2.078703000	-0.953176000
6	-4.061456000	-2.218942000	1.005666000
1	-4.834474000	-2.272515000	1.764398000
6	-1.743729000	-1.731499000	0.387322000
6	-2.782712000	-1.825512000	1.356825000
1	0.736186000	-1.860154000	-0.900293000
1	-2.557573000	-1.567595000	2.386067000
6	-0.460302000	-1.286607000	0.770061000
1	4.577758000	-2.059442000	0.426555000
6	0.659091000	-1.034502000	-0.175772000
1	-2.098837000	0.607773000	-1.504679000
1	-0.011669000	0.176198000	-1.890395000
1	-0.275567000	-1.077188000	1.817480000
1	-4.337196000	1.552718000	-1.285321000
1	2.325391000	-0.150357000	-2.294202000

8	2.378047000	-1.604146000	1.469262000
6	2.038257000	-0.961498000	0.490011000
6	0.612812000	0.298814000	-1.004150000
1	4.160890000	-0.188749000	2.155712000
6	4.960832000	-1.304584000	-0.260068000
6	-2.247568000	1.455890000	-0.850471000
1	4.781179000	-1.637079000	-1.286861000
6	2.098444000	0.438438000	-1.394637000
6	-3.519459000	1.987467000	-0.721209000
7	2.811849000	-0.083549000	-0.223957000
1	6.041036000	-1.217794000	-0.114472000
6	4.282674000	0.055066000	-0.007718000
6	4.537331000	0.533097000	1.433316000
6	0.160862000	1.468667000	-0.187522000
1	5.611055000	0.665778000	1.593023000
6	-1.150970000	1.984051000	-0.111215000
1	2.362109000	1.476232000	-1.592727000
6	-3.760475000	3.066050000	0.136999000
1	-4.759391000	3.474800000	0.235085000
6	4.855157000	1.096167000	-0.981345000
1	0.910729000	1.916579000	0.459147000
1	4.043377000	1.493301000	1.606436000
6	-1.424842000	3.084138000	0.754413000
6	-2.698906000	3.609466000	0.872110000
1	-0.609714000	3.507785000	1.332163000
1	-2.876340000	4.444788000	1.540742000
1	4.705366000	0.811256000	-2.025609000
1	5.930858000	1.177347000	-0.811654000
1	4.418819000	2.085100000	-0.820396000

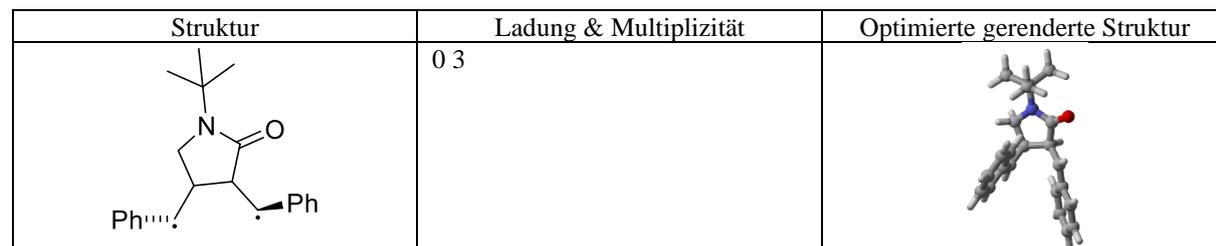
Zero-point correction=  
(Hartree/Particle)

0.414052

Thermal correction to Energy=	0.436206
Thermal correction to Enthalpy=	0.437150
Thermal correction to Gibbs Free Energy=	0.360583
Sum of electronic and zero-point Energies=	-983.213844
Sum of electronic and thermal Energies=	-983.191690
Sum of electronic and thermal Enthalpies=	-983.190746
Sum of electronic and thermal Free Energies=	-983.267313

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	273.723	88.492	161.150

#UB3LYP-D3/6-311+G**	72-Bu-trans
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xyz-matrix

1	4.613744000	-2.319037000	1.931069000
6	4.285255000	-1.878666000	0.995700000
1	2.215897000	-2.142594000	1.453330000
1	6.291076000	-1.499066000	0.292024000
6	2.930199000	-1.777438000	0.725069000
6	5.232540000	-1.419697000	0.073611000
1	0.083301000	-2.511691000	0.389722000
1	0.135668000	-1.255488000	2.273058000
1	-4.218723000	-2.801963000	0.317816000
1	-2.125054000	-0.990966000	2.409071000
6	2.463515000	-1.208773000	-0.494004000
6	4.799879000	-0.860431000	-1.135601000
6	-0.024697000	-1.453532000	0.110342000

6	-0.184432000	-0.625654000	1.442977000
1	1.432691000	0.627297000	2.255475000
1	5.527935000	-0.505200000	-1.856716000
6	-1.725866000	-0.417759000	1.567883000
6	1.093568000	-1.074844000	-0.804367000
6	3.449199000	-0.757567000	-1.417757000
6	-4.325856000	-2.066063000	-0.484165000
6	-1.388575000	-1.362384000	-0.576893000
1	-5.390279000	-1.959588000	-0.710509000
6	0.627479000	0.634314000	1.528682000
7	-2.307329000	-0.873110000	0.305166000
8	-1.596882000	-1.690158000	-1.735128000
1	-3.814746000	-2.436901000	-1.370676000
1	-1.956338000	0.634983000	1.742426000
6	-3.753388000	-0.707356000	-0.041292000
1	0.817329000	-0.677680000	-1.774060000
1	3.121851000	-0.321825000	-2.355679000
1	-3.334585000	0.019321000	-2.050474000
6	-4.534058000	-0.224876000	1.191943000
1	2.111251000	2.813659000	1.789155000
6	0.507035000	1.803474000	0.741317000
6	-3.887013000	0.335961000	-1.165991000
1	-4.939328000	0.459224000	-1.436466000
6	1.377553000	2.903112000	0.994900000
1	-1.104433000	1.150645000	-0.566876000
6	-0.432947000	1.958208000	-0.316303000
1	-3.506088000	1.306408000	-0.835824000
6	1.307116000	4.067862000	0.251473000
1	1.985778000	4.885491000	0.468387000
6	-0.495414000	3.129192000	-1.054171000
6	0.368216000	4.194862000	-0.779791000
1	-1.219418000	3.213410000	-1.857491000
1	0.314945000	5.106898000	-1.362727000
1	-5.588420000	-0.136759000	0.921412000
1	-4.200619000	0.755809000	1.537224000
1	-4.462918000	-0.933030000	2.020824000

Zero-point correction=  
(Hartree/Particle)

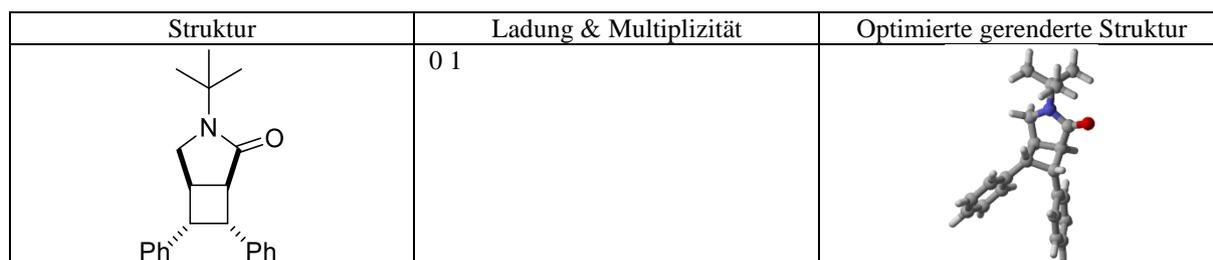
0.414579

Thermal correction to Energy=	0.436743
Thermal correction to Enthalpy=	0.437688
Thermal correction to Gibbs Free Energy=	0.360989
Sum of electronic and zero-point Energies=	-983.209913
Sum of electronic and thermal Energies=	-983.187748
Sum of electronic and thermal Enthalpies=	-983.186804
Sum of electronic and thermal Free Energies=	-983.263503

	E (Thermal)	CV	S
Total	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
	274.061	88.427	161.426

#B3LYP-D3/6-311+G\*\*

70-Bu-cis-trans



xyz-matrix

6	0.177747000	-0.624039000	0.164893000
6	-0.623014000	-0.157114000	-1.089208000
6	-0.792026000	1.225959000	-0.432060000
6	0.326693000	0.907792000	0.592749000
6	-2.028280000	-0.736291000	-1.236661000
7	-2.817407000	0.021801000	-0.255080000
6	-2.193252000	1.170312000	0.167593000
8	-2.666282000	2.022539000	0.903509000
6	-4.244353000	-0.280688000	0.067030000
6	-4.633319000	-1.646449000	-0.520343000
6	-4.420682000	-0.336695000	1.595721000
6	-5.139888000	0.810967000	-0.547795000
6	1.390082000	-1.498936000	0.033795000
6	1.645677000	-2.474604000	1.005410000
6	2.782588000	-3.277722000	0.941415000
6	3.689993000	-3.118810000	-0.104178000
6	3.449079000	-2.152082000	-1.079617000
6	2.312242000	-1.351000000	-1.010043000
6	1.688405000	1.505446000	0.343725000
6	2.667941000	1.364246000	1.336039000
6	3.963218000	1.832200000	1.141939000
6	4.309456000	2.457231000	-0.056309000
6	3.346766000	2.607306000	-1.050686000
6	2.049587000	2.133110000	-0.851946000
1	-0.515960000	-1.092990000	0.868110000
1	-0.049067000	-0.189701000	-2.013814000
1	-0.697337000	2.139930000	-1.018677000
1	0.042763000	1.089505000	1.631480000
1	-2.042499000	-1.806223000	-1.018942000
1	-2.422800000	-0.591192000	-2.250105000
1	-5.680974000	-1.842032000	-0.281917000
1	-4.531156000	-1.673569000	-1.607594000
1	-4.038854000	-2.456655000	-0.091188000
1	-5.455276000	-0.596358000	1.836750000
1	-4.182759000	0.621745000	2.053045000
1	-3.767169000	-1.102288000	2.023646000
1	-5.019333000	0.835976000	-1.634962000
1	-6.190612000	0.604113000	-0.326276000
1	-4.884176000	1.789733000	-0.142637000
1	0.944064000	-2.604854000	1.823668000
1	2.957598000	-4.027193000	1.705469000
1	4.576006000	-3.741254000	-0.158916000
1	4.151512000	-2.016319000	-1.894518000
1	2.155884000	-0.591859000	-1.766162000
1	2.409511000	0.872237000	2.268054000
1	4.703273000	1.709470000	1.924963000
1	5.317592000	2.824967000	-0.210331000
1	3.602257000	3.094513000	-1.985376000
1	1.321657000	2.256535000	-1.645049000

Zero-point correction=  
(Hartree/Particle)

0.419010

Thermal correction to Energy=

0.440149

Thermal correction to Enthalpy=

0.441093

Thermal correction to Gibbs Free Energy=

0.367461

Sum of electronic and zero-point Energies=

-983.263833

Sum of electronic and thermal Energies=

-983.242694

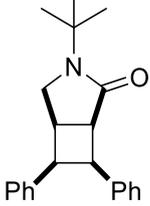
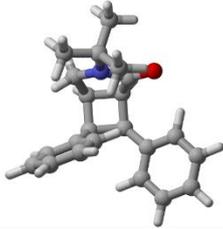
sum of electronic and thermal Enthalpies=

-983.241750

Sum of electronic and thermal Free Energies= -983.315382

Total E (Thermal) CV S  
 kcal/Mol cal/Mol-Kelvin cal/Mol-Kelvin  
 276.198 84.924 154.971

#B3LYP-D3/6-311+G\*\* 70-Bu-cis-cis

Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

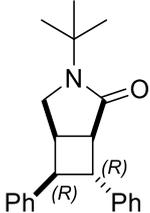
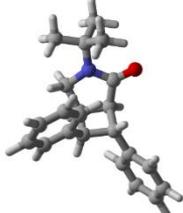
xyz-matrix

6	0.519103000	0.831316000	1.813476000
6	-0.748392000	0.005715000	2.266251000
6	-0.085059000	-1.300408000	1.773952000
6	1.276605000	-0.540811000	1.649183000
6	-2.034569000	0.168350000	1.460069000
7	-1.865772000	-0.743592000	0.323352000
6	-0.873505000	-1.666946000	0.518068000
8	-0.671180000	-2.659675000	-0.168422000
6	-2.900615000	-0.879612000	-0.745467000
6	-3.763920000	0.392019000	-0.784510000
6	-2.222270000	-1.037356000	-2.119097000
6	-3.780474000	-2.102234000	-0.428047000
6	0.322120000	1.761881000	0.641079000
6	0.295473000	1.335093000	-0.692440000
6	0.038759000	2.234284000	-1.725049000
6	-0.201550000	3.579143000	-1.449484000
6	-0.174132000	4.021118000	-0.127856000
6	0.089085000	3.119500000	0.901371000
6	2.300569000	-0.765490000	0.564963000
6	2.373720000	-1.957005000	-0.161926000
6	3.374784000	-2.141019000	-1.117031000
6	4.315708000	-1.142666000	-1.356903000
6	4.252563000	0.047800000	-0.631718000
6	3.254388000	0.231738000	0.319948000
1	0.925228000	1.420718000	2.637818000
1	-0.923353000	0.079132000	3.339122000
1	-0.071148000	-2.174196000	2.427370000
1	1.791051000	-0.708718000	2.602285000
1	-2.168967000	1.197191000	1.123987000
1	-2.914097000	-0.115919000	2.051433000
1	-4.490719000	0.296109000	-1.594073000
1	-4.322251000	0.544681000	0.141833000
1	-3.155420000	1.278127000	-0.980661000
1	-2.992310000	-1.110667000	-2.891999000
1	-1.601512000	-1.929456000	-2.156392000
1	-1.602927000	-0.164788000	-2.336319000
1	-4.266310000	-1.983916000	0.545387000
1	-4.561365000	-2.214526000	-1.185365000
1	-3.176631000	-3.010163000	-0.411806000
1	0.484946000	0.299244000	-0.934392000
1	0.030797000	1.880376000	-2.750129000
1	-0.399813000	4.276206000	-2.255910000
1	-0.351987000	5.065880000	0.102109000
1	0.112657000	3.474272000	1.927428000
1	1.632120000	-2.729126000	-0.006052000
1	3.411722000	-3.068672000	-1.677697000
1	5.089408000	-1.287069000	-2.102825000
1	4.976658000	0.834787000	-0.812143000
1	3.203724000	1.166573000	0.867918000

Zero-point correction= 0.420087  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.440752  
 Thermal correction to Enthalpy= 0.441696  
 Thermal correction to Gibbs Free Energy= 0.370696  
 Sum of electronic and zero-point Energies= -983.262367  
 Sum of electronic and thermal Energies= -983.241702  
 Sum of electronic and thermal Enthalpies= -983.240758  
 Sum of electronic and thermal Free Energies= -983.311759

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-kelvin	Cal/Mol-kelvin
Total	276.576	84.424	149.434

#B3LYP-D3/6-311+G**	70-Bu-(R)-(R)
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Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

xyz-matrix

6	-0.731569000	0.813920000	-0.772650000
6	-0.052388000	-0.346416000	-1.600195000
6	-0.571216000	-1.370496000	-0.572125000
6	-1.344844000	-0.256450000	0.206301000
6	1.473083000	-0.459216000	-1.575875000
7	1.767113000	-1.205457000	-0.345451000
6	0.668868000	-1.843995000	0.171316000
8	0.660064000	-2.639025000	1.099536000
6	3.160534000	-1.498953000	0.106081000
6	4.142091000	-0.548794000	-0.598307000
6	3.275560000	-1.268360000	1.624423000
6	3.500716000	-2.957697000	-0.249594000
6	0.165738000	1.894395000	-0.227952000
6	0.291784000	3.098732000	-0.933633000
6	1.166590000	4.096353000	-0.509114000
6	1.936049000	3.908645000	0.638408000
6	1.817599000	2.718535000	1.353797000
6	0.942149000	1.722829000	0.924249000
6	-2.847813000	-0.341723000	0.208224000
6	-3.567212000	-0.128391000	1.388121000
6	-4.960732000	-0.182227000	1.399280000
6	-5.660008000	-0.453666000	0.225666000
6	-4.955077000	-0.671502000	-0.958618000
6	-3.564219000	-0.615292000	-0.965047000
1	-1.519407000	1.282491000	-1.365039000
1	-0.445361000	-0.420871000	-2.613969000
1	-1.164222000	-2.222857000	-0.901936000
1	-0.999605000	-0.158683000	1.235906000
1	1.947892000	0.522907000	-1.563185000
1	1.842046000	-1.004152000	-2.453570000
1	5.151750000	-0.763437000	-0.241178000
1	4.141520000	-0.679464000	-1.682722000
1	3.919472000	0.495988000	-0.368765000
1	4.299530000	-1.479065000	1.945299000
1	2.595327000	-1.914207000	2.175609000
1	3.051850000	-0.226524000	1.865762000
1	3.423186000	-3.117164000	-1.329288000
1	4.523970000	-3.192736000	0.056028000
1	2.819170000	-3.641654000	0.256920000
1	-0.305498000	3.254801000	-1.826666000
1	1.243976000	5.020615000	-1.071064000
1	2.616210000	4.683383000	0.973763000
1	2.408375000	2.562136000	2.249837000

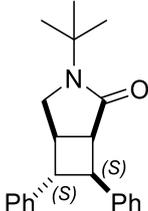
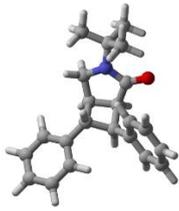
1	0.877104000	0.801690000	1.488012000
1	-3.029906000	0.077482000	2.308012000
1	-5.498079000	-0.015256000	2.326287000
1	-6.743146000	-0.498575000	0.232251000
1	-5.490146000	-0.887403000	-1.876915000
1	-3.030408000	-0.790416000	-1.894056000

Zero-point correction= 0.419620  
(Hartree/Particle)

Thermal correction to Energy=	0.440588
Thermal correction to Enthalpy=	0.441532
Thermal correction to Gibbs Free Energy=	0.368229
Sum of electronic and zero-point Energies=	-983.265675
Sum of electronic and thermal Energies=	-983.244707
Sum of electronic and thermal Enthalpies=	-983.243763
Sum of electronic and thermal Free Energies=	-983.317066

	E (Thermal)	CV	S
	KCal/Mol	cal/Mol-Kelvin	cal/Mol-Kelvin
Total	276.473	84.614	154.281

#B3LYP-D3/6-311+G**	70-Bu-(S)-(S)
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Struktur	Ladung & Multiplizität	Optimierte gerenderte Struktur
	0 1	

xyz-matrix

6	-0.992033000	-0.660321000	0.122897000
6	-0.060070000	-1.497587000	1.048949000
6	0.473688000	-0.183555000	1.661100000
6	-0.714890000	0.601914000	1.003161000
6	1.136299000	-2.166460000	0.373393000
7	2.089488000	-1.063935000	0.181582000
6	1.839291000	0.002342000	1.018159000
8	2.581673000	0.948111000	1.222419000
6	3.398175000	-1.240523000	-0.515746000
6	3.340993000	-2.486585000	-1.413550000
6	3.670154000	-0.013797000	-1.406017000
6	4.512217000	-1.412365000	0.533290000
6	-2.422814000	-1.079107000	-0.088363000
6	-2.794464000	-2.427259000	-0.086551000
6	-4.118038000	-2.804768000	-0.311498000
6	-5.092775000	-1.835930000	-0.542093000
6	-4.733039000	-0.488315000	-0.548072000
6	-3.410161000	-0.114038000	-0.323527000
6	-0.518935000	1.947816000	0.361093000
6	0.279597000	2.112828000	-0.777415000
6	0.439740000	3.365017000	-1.362649000
6	-0.196668000	4.481270000	-0.820267000
6	-0.992135000	4.333303000	0.313757000
6	-1.149429000	3.076637000	0.895998000
1	-0.511299000	-0.539617000	-0.854096000
1	-0.597399000	-2.159434000	1.727118000
1	0.567465000	-0.076200000	2.741761000
1	-1.506550000	0.679514000	1.753120000
1	0.855256000	-2.618174000	-0.579967000
1	1.573125000	-2.951349000	1.004715000
1	4.294293000	-2.584216000	-1.937400000
1	3.184017000	-3.403731000	-0.841258000
1	2.553774000	-2.403562000	-2.167353000
1	4.616211000	-0.150806000	-1.937023000
1	3.727846000	0.897807000	-0.814995000
1	2.876179000	0.097971000	-2.150096000

1	4.312341000	-2.283422000	1.164562000
1	5.475724000	-1.565022000	0.039311000
1	4.579735000	-0.527373000	1.165763000
1	-2.045604000	-3.191796000	0.092151000
1	-4.387151000	-3.855384000	-0.304094000
1	-6.122716000	-2.127416000	-0.713982000
1	-5.484136000	0.273318000	-0.726833000
1	-3.138855000	0.936187000	-0.331469000
1	0.794895000	1.260948000	-1.204952000
1	1.067662000	3.471155000	-2.240372000
1	-0.070936000	5.456823000	-1.276290000
1	-1.490384000	5.194227000	0.745751000
1	-1.771522000	2.969106000	1.779201000

Zero-point correction= 0.419235  
(Hartree/Particle)

Thermal correction to Energy=	0.440278
Thermal correction to Enthalpy=	0.441222
Thermal correction to Gibbs Free Energy=	0.367831
Sum of electronic and zero-point Energies=	-983.265532
Sum of electronic and thermal Energies=	-983.244489
Sum of electronic and thermal Enthalpies=	-983.243545
Sum of electronic and thermal Free Energies=	-983.316937

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	276.279	84.763	154.465

## Zeitaufgelöste Untersuchungen zur Synthese von Arylsulfiden mittels Photoredox-Katalyse mit sichtbarem Licht

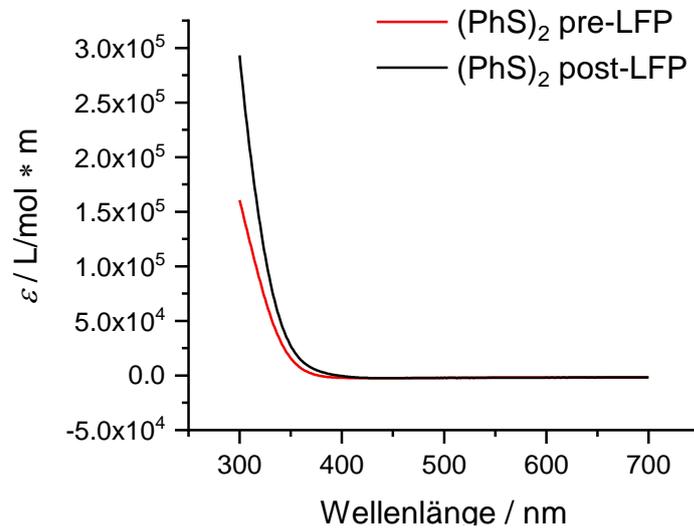


Abbildung A 157: UV-Vis-Spektren von Diphenyldisulfide in Acetonitril, entgast, lösungsmittelkorrigiert, bevor und nach transienten Experimenten.

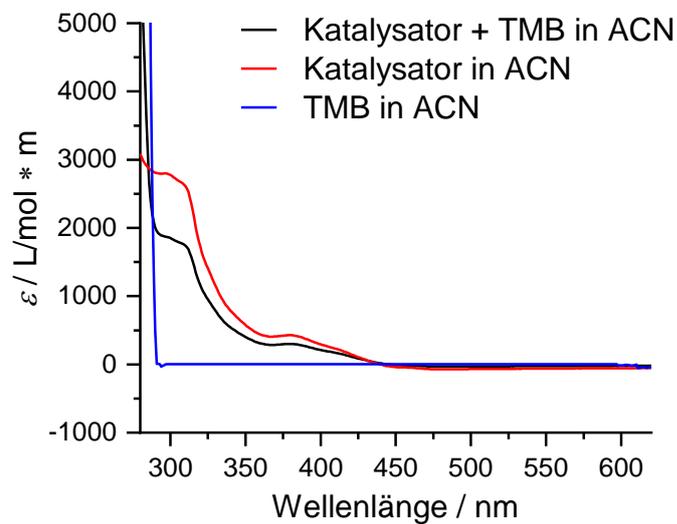


Abbildung A 158: UV-Vis-Spektren des Katalysators (rot), TMB (blau) und des Gemisches aus Katalysator und TMB (schwarz) in Acetonitril, entgast, lösungsmittelkorrigiert.

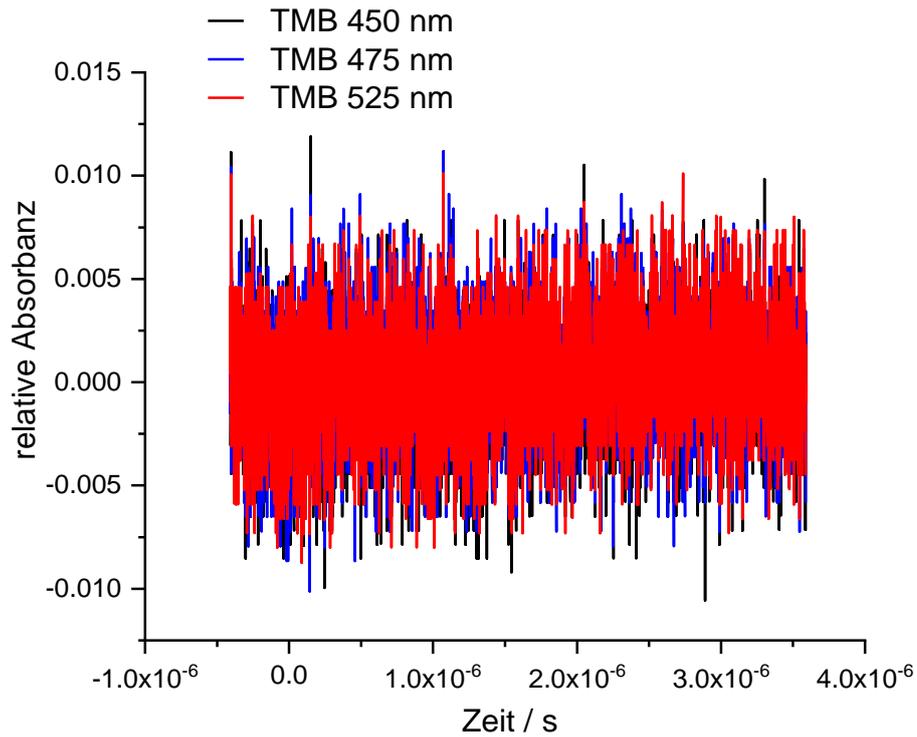


Abbildung A 159: Zeitaufgelöste Absorptionsspektren von TMB bei 450 nm, 475 nm und 525 nm in Acetonitrile, entgast, mit einer zeitlichen Auflösung von 400 ps.

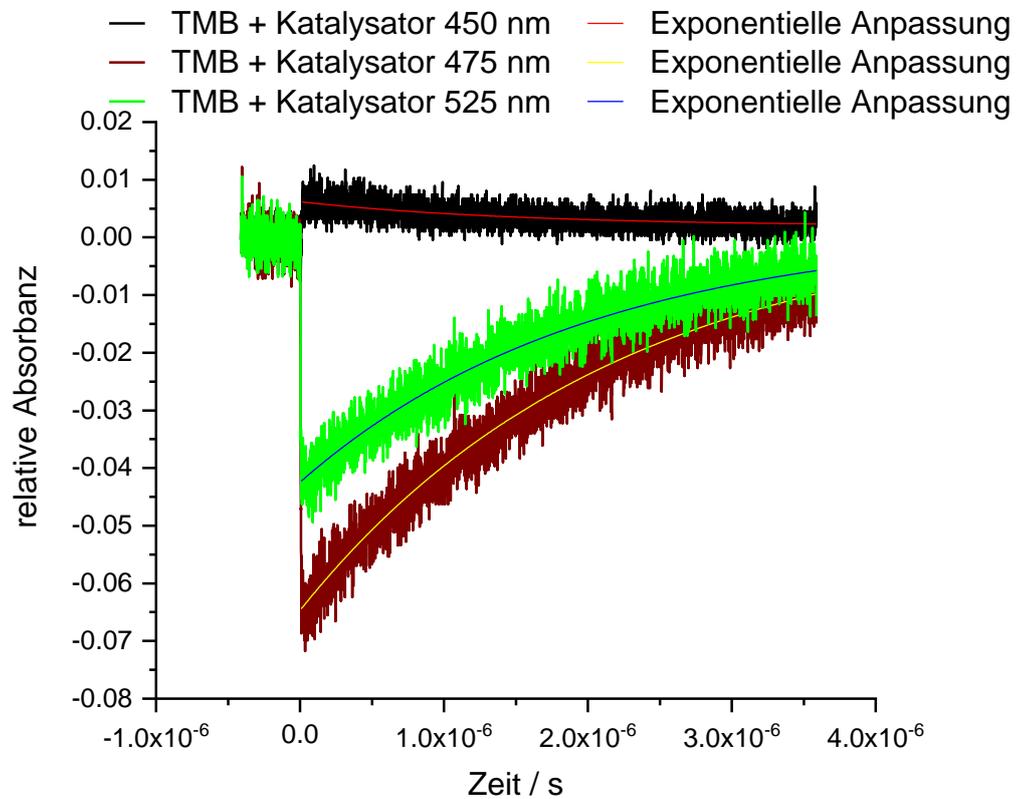


Abbildung A 160: Zeitaufgelöste Absorptionsspektren des Gemisches aus Katalysator und TMB bei 450 nm, 475 nm und 525 nm in Acetonitrile, entgast, mit einer zeitlichen Auflösung von 400 ps.

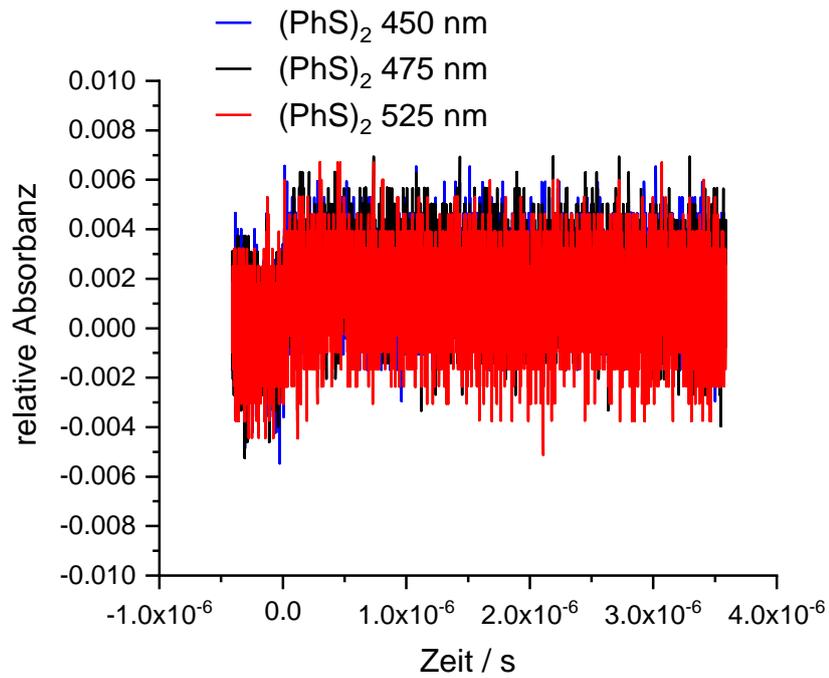


Abbildung A 161: Zeitaufgelöste Absorptionsspektren von Diphenylsulfid bei 450 nm, 475 nm und 525 nm in Acetonitrile, entgast, mit einer zeitlichen Auflösung von 400 ps.

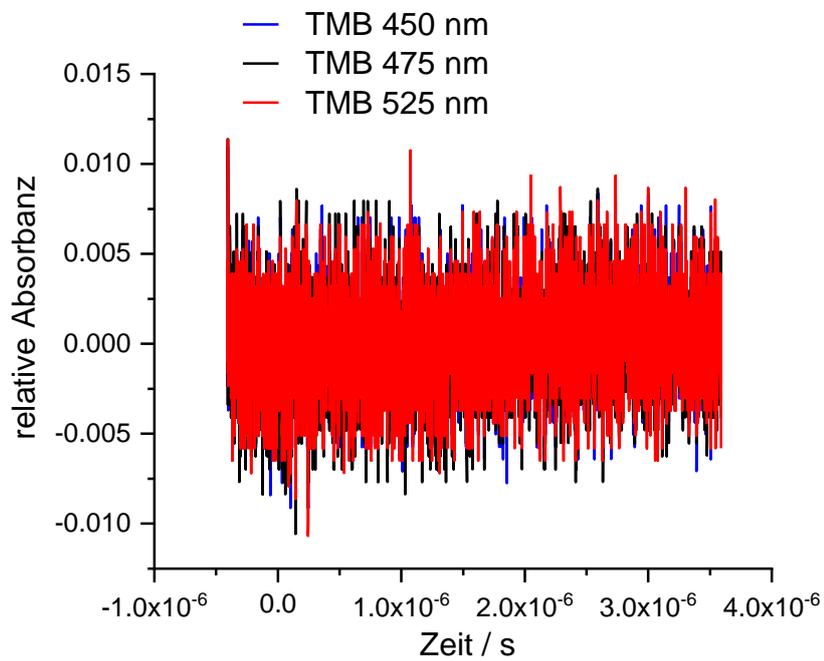


Abbildung A 162: Zeitaufgelöste Absorptionsspektren von TMB bei 450 nm, 475 nm und 525 nm in Acetonitrile, entgast, mit einer zeitlichen Auflösung von 10 ns.

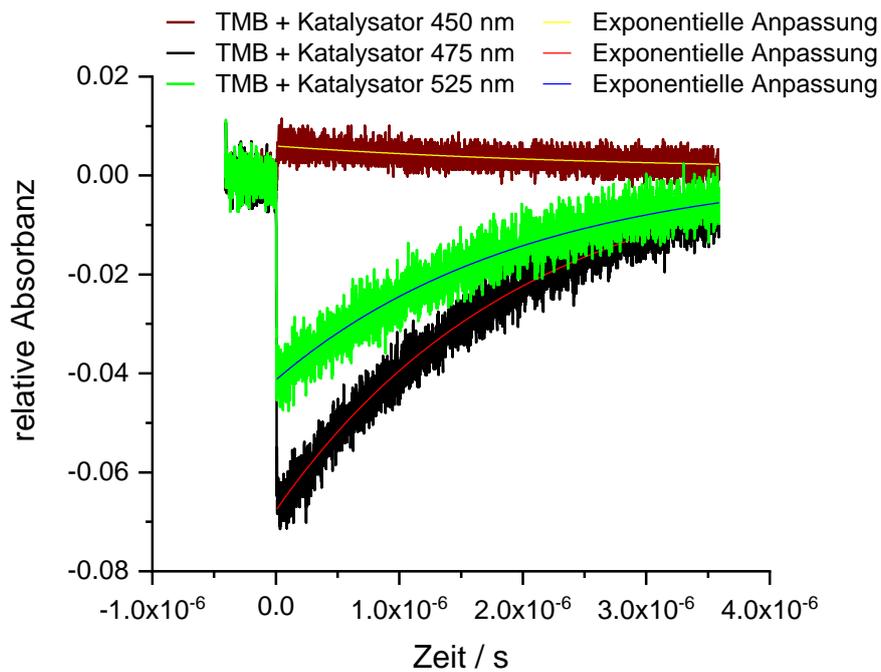


Abbildung A 163: Zeitaufgelöste Absorptionsspektren des Gemisches aus Katalysator und TMB bei 450 nm, 475 nm und 525 nm in Acetonitrile, entgast, mit einer zeitlichen Auflösung von 10 ns.

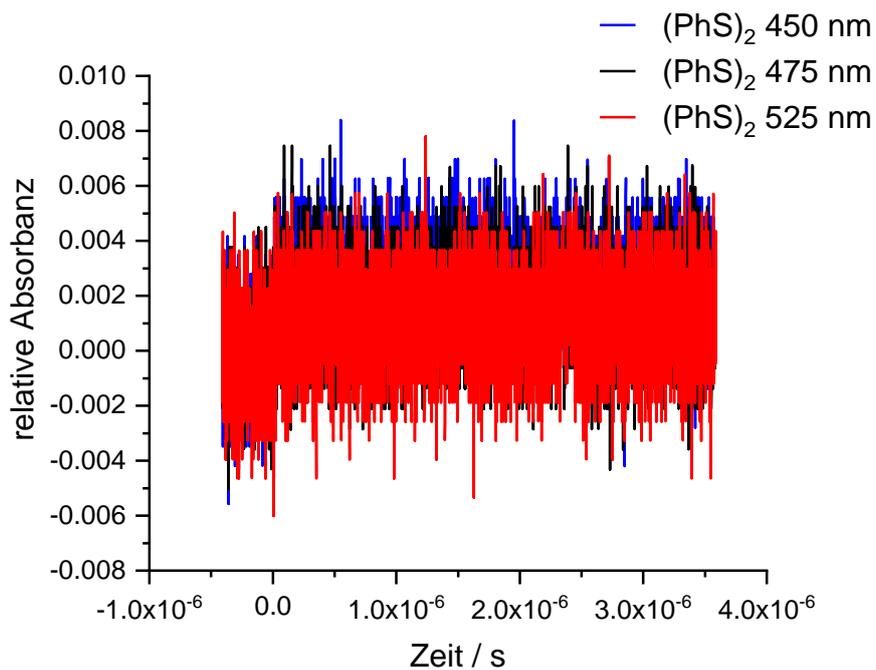


Abbildung A 164: Zeitaufgelöste Absorptionsspektren von Diphenylsulfid bei 450 nm, 475 nm und 525 nm in Acetonitrile, entgast, mit einer zeitlichen Auflösung von 10 ns.

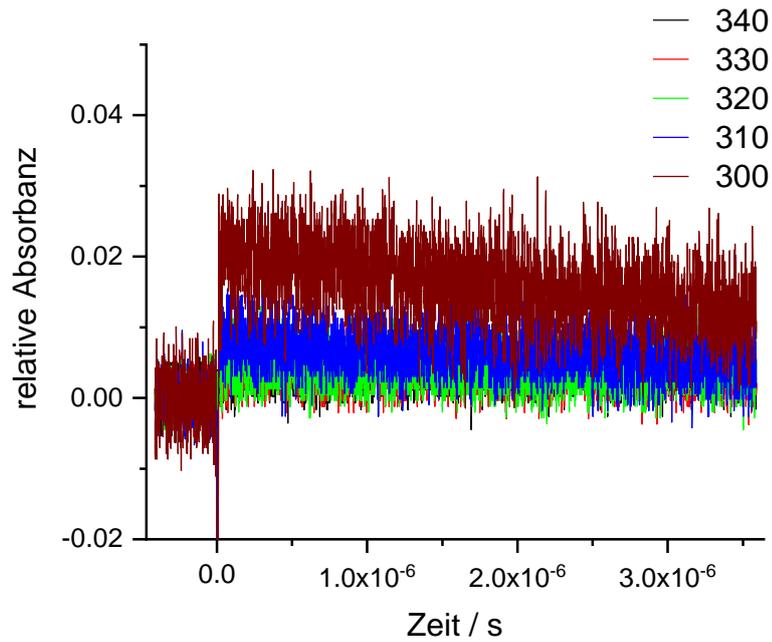


Abbildung A 165: Ausgewählte zeitaufgelöste Absorptionsspektren des Diphenylsulfid in Acetonitril zwischen 300 nm und 340 nm, entgast, mit einer zeitlichen Auflösung von 10 ns.

In Abbildung A 164 ist eine kleine Absorbanz zu erkennen, welche über den beobachteten Zeitraum nicht vollständig abnimmt. Diese könnte die beobachtete irreversible Veränderung des UV-Vis-Spektrums begründen.

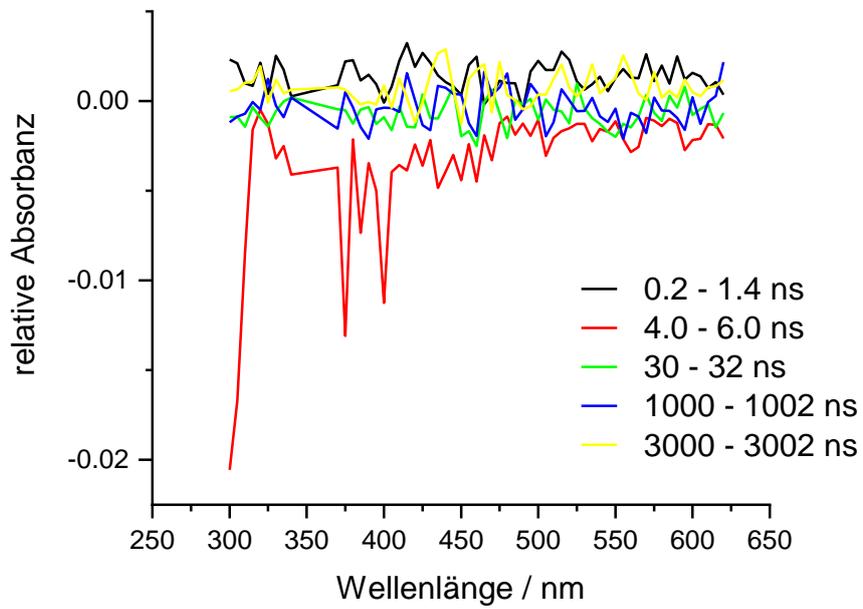


Abbildung A 166: Transiente Absorptionsspektren von TMB über den Spektralbereich in ausgewählten, gemittelten Zeiträumen in Acetonitril, entgast, mit einer zeitlichen Auflösung von 400 ps.

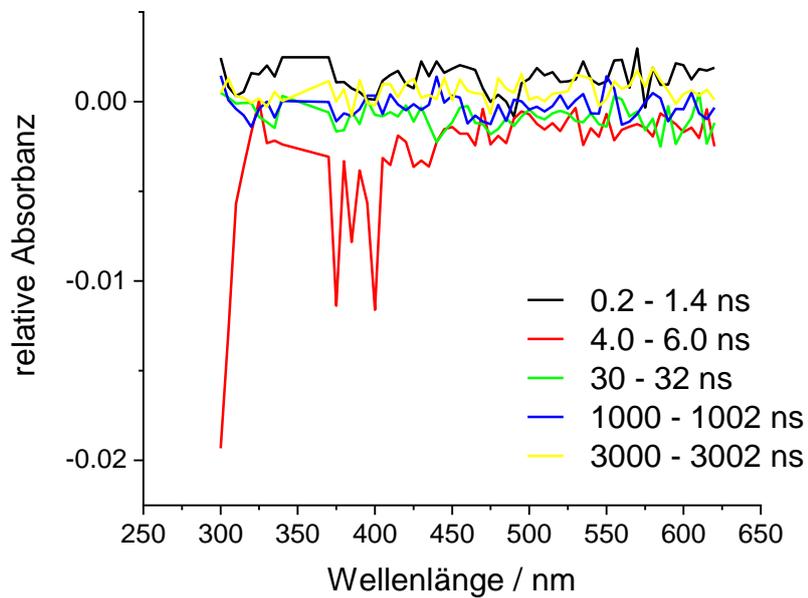


Abbildung A 167: Transiente Absorptionsspektren von TMB über den Spektralbereich in ausgewählten, gemittelten Zeiträumen in Acetonitril, entgast, mit einer zeitlichen Auflösung von 10 ns.

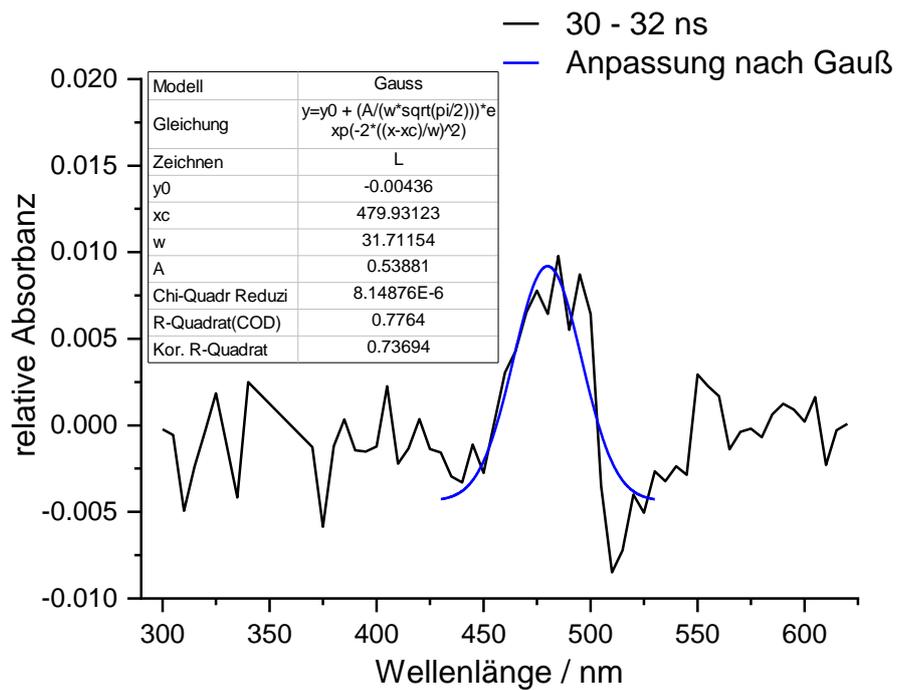


Abbildung A 168: Vergrößerung des Differenzspektrums der transienten Absorptionsspektren von  $(\text{Ir}[\text{dF}(\text{CF}_3)\text{ppy}]_2(\text{dtbpy}))\text{PF}_6$  und des Gemisches aus TMB und  $(\text{Ir}[\text{dF}(\text{CF}_3)\text{ppy}]_2(\text{dtbpy}))\text{PF}_6$  gemittelt über den Zeitbereich 30 – 32 ns, in Acetonitril, entgast, mit einer zeitlichen Auflösung von 400 ps (schwarz), mit einer Anpassung der beobachteten Absorption durch eine Gauß-Funktion (blau).