# Anhang II*



* J. Gerstmann, *Erzeugung und Charakterisierung von kurzlebigen Radikalen stabilisiert durch N-Heterocyclische Carbene*, Dissertation, Regensburg, **2021**.

# Projekt A

## Wasserstoffatom, Methylradikal und Methan

(u)M06-2X/6-311+G** SCRF=(PCM,Solvent=Tetrahydrofuran)

### Wasserstoffatom H•

1

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| H | 0.0000000000 | 0.0000000000 | 0.0000000000 |

Thermochemie

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.010654
Sum of electronic and zero-point Energies= -0.498155
Sum of electronic and thermal Energies= -0.496738
Sum of electronic and thermal Enthalpies= -0.495794
Sum of electronic and thermal Free Energies= -0.508809

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 0.889 | 2.981 | 27.392 |

### Methylradikal $CH_3$•

4

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 0.0000930000 | 0.0002070000 | -0.0000460000 |
| H | -0.8704400000 | 0.6376330000 | 0.0000910000 |
| H | 0.9881010000 | 0.4334120000 | 0.0000910000 |
| H | -0.1182200000 | -1.0722880000 | 0.0000910000 |

Thermochemie

Zero-point correction= 0.029643 (Hartree/Particle)
Thermal correction to Energy= 0.032762
Thermal correction to Enthalpy= 0.033706
Thermal correction to Gibbs Free Energy= 0.009818
Sum of electronic and zero-point Energies= -39.791832
Sum of electronic and thermal Energies= -39.788713
Sum of electronic and thermal Enthalpies= -39.787769
Sum of electronic and thermal Free Energies= -39.811656

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 20.558 | 7.554 | 50.276 |

### Methan $CH_4$

5

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 0.0002210000 | 0.0001500000 | -0.0002620000 |
| H | 0.6591930000 | -0.7358250000 | -0.4580440000 |
| H | -0.8524140000 | 0.1821660000 | -0.6529650000 |
| H | -0.3534070000 | -0.3771090000 | 0.9584300000 |
| H | 0.5453020000 | 0.9298680000 | 0.1541520000 |

Thermochemie

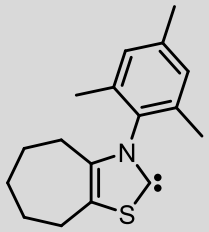
Zero-point correction= 0.044782 (Hartree/Particle)
Thermal correction to Energy= 0.047652
Thermal correction to Enthalpy= 0.048596
Thermal correction to Gibbs Free Energy= 0.025123
Sum of electronic and zero-point Energies= -40.452162
Sum of electronic and thermal Energies= -40.449292
Sum of electronic and thermal Enthalpies= -40.448348
Sum of electronic and thermal Free Energies= -40.471821

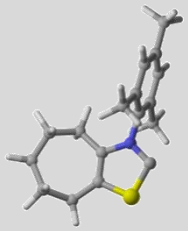
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 29.902 | 6.485 | 49.404 |

## NHC-Katalysatoren

M06-2X/6-311+G** SCRF=(PCM,Solvent=Tetrahydrofuran)

**A**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| N | -0.1053180000 | -0.8803770000 | 0.1846540000 |
| C | -0.3654470000 | -2.0984340000 | 0.6894180000 |
| S | -2.0741290000 | -2.2629740000 | 0.6029350000 |
| C | -2.3594470000 | -0.6976910000 | -0.1100570000 |
| C | -1.1722190000 | -0.0728850000 | -0.2665800000 |
| C | 1.2630280000 | -0.4258610000 | 0.1087100000 |
| C | 1.8255650000 | 0.1997710000 | 1.2214020000 |
| C | 3.1470910000 | 0.6309760000 | 1.1238090000 |
| C | 3.8905480000 | 0.4536660000 | -0.0433100000 |
| C | 3.2871820000 | -0.1749570000 | -1.1318930000 |
| C | 1.9677540000 | -0.6227030000 | -1.0774510000 |
| C | 1.0207160000 | 0.3886940000 | 2.4786280000 |
| H | 3.6070030000 | 1.1153600000 | 1.9800040000 |
| C | 5.3079790000 | 0.9582080000 | -0.1304000000 |
| H | 3.8551060000 | -0.3245450000 | -2.0450460000 |
| C | 1.3109660000 | -1.2973970000 | -2.2516140000 |
| C | -3.7223150000 | -0.1822640000 | -0.4699580000 |
| C | -4.0493170000 | 1.1802730000 | 0.1538580000 |
| H | -4.4704530000 | -0.9132920000 | -0.1556580000 |
| H | -3.8009540000 | -0.1073670000 | -1.5615970000 |
| C | -3.2760990000 | 2.3590660000 | -0.4437250000 |
| H | -3.8737670000 | 1.1310830000 | 1.2339250000 |
| H | -5.1180150000 | 1.3650550000 | 0.0131780000 |
| H | -3.7169280000 | 3.2843650000 | -0.0616100000 |
| C | -0.9511940000 | 1.2969320000 | -0.8408520000 |
| H | 0.1097840000 | 1.5452560000 | -0.7758180000 |
| C | -1.7734520000 | 2.3953180000 | -0.1521740000 |
| H | -1.2032870000 | 1.2791800000 | -1.9087120000 |
| H | -1.3837450000 | 3.3596520000 | -0.4897300000 |
| H | -3.4280260000 | 2.3711570000 | -1.5303340000 |
| H | -1.6058270000 | 2.3477610000 | 0.9293010000 |

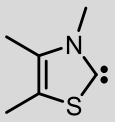
| | | | |
|---|---|---|---|
| H | 0.4492980000 | -0.7215700000 | -2.6023500000 |
| H | 0.9437220000 | -2.2878140000 | -1.9717430000 |
| H | 2.0134390000 | -1.4032070000 | -3.0778000000 |
| H | 0.7423490000 | -0.5781350000 | 2.9052620000 |
| H | 0.0911760000 | 0.9265870000 | 2.2719090000 |
| H | 1.5888230000 | 0.9495670000 | 3.2201970000 |
| H | 5.3209120000 | 2.0236570000 | -0.3765750000 |
| H | 5.8668620000 | 0.4303220000 | -0.9039900000 |
| H | 5.8277690000 | 0.8328800000 | 0.8207890000 |

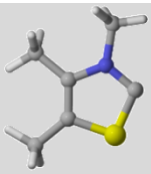
Thermochemie

Zero-point correction= 0.341970 (Hartree/Particle)
Thermal correction to Energy= 0.360599
Thermal correction to Enthalpy= 0.361543
Thermal correction to Gibbs Free Energy= 0.294317
Sum of electronic and zero-point Energies= -1112.898178
Sum of electronic and thermal Energies= -1112.879550
Sum of electronic and thermal Enthalpies= -1112.878606
Sum of electronic and thermal Free Energies= -1112.945832

| | E (Thermal) | CV | S |
|---|---|---|---|
| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 226.279 | 71.338 | 141.489 |

**B**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 0.5799120000 | -1.6523680000 | 0.0021540000 |
| N | 1.1196200000 | -0.4280230000 | 0.0015980000 |
| C | 0.2729460000 | 0.7003630000 | -0.0013010000 |
| C | -1.0305880000 | 0.3448070000 | -0.0023610000 |
| S | -1.1232900000 | -1.4001220000 | 0.0003200000 |
| C | 0.8619600000 | 2.0746690000 | 0.0021580000 |
| H | 0.0732970000 | 2.8233630000 | -0.0370660000 |
| H | 1.5152830000 | 2.2280890000 | -0.8598080000 |
| H | 1.4505060000 | 2.2510080000 | 0.9058070000 |
| C | -2.2546920000 | 1.2045190000 | -0.0008990000 |
| H | -2.8606380000 | 1.0156130000 | 0.8877320000 |
| H | -2.8743070000 | 1.0002650000 | -0.8765070000 |
| H | -1.9913920000 | 2.2620040000 | -0.0115890000 |
| C | 2.5744300000 | -0.2571940000 | -0.0023470000 |
| H | 3.0189450000 | -1.2473420000 | 0.0283240000 |
| H | 2.8909380000 | 0.2608640000 | -0.9083890000 |
| H | 2.8888590000 | 0.3154880000 | 0.8707650000 |

Thermochemie

Zero-point correction= 0.139162 (Hartree/Particle)
Thermal correction to Energy= 0.148282
Thermal correction to Enthalpy= 0.149226
Thermal correction to Gibbs Free Energy= 0.103734
Sum of electronic and zero-point Energies= -686.755867
Sum of electronic and thermal Energies= -686.746746
Sum of electronic and thermal Enthalpies= -686.745802
Sum of electronic and thermal Free Energies= -686.791294

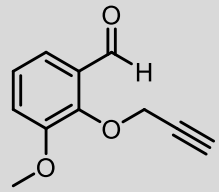
| | E (Thermal) | CV | S |
|---|---|---|---|

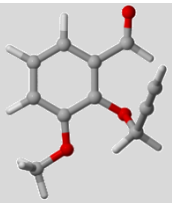
| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 93.048 | 31.803 | 95.746 |

## *O*-propargylierte Aldehyde: H-Substituent

(u)M06-2X/6-311+G**

**19a**





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XYZ-Matrix in Ångström

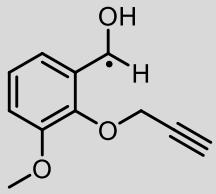
| | | | |
|---|---|---|---|
| C | 1.7411400000 | -1.4601850000 | 0.5069920000 |
| C | 0.7548560000 | -2.4328960000 | 0.6992940000 |
| C | -0.5492670000 | -2.1959600000 | 0.3149290000 |
| C | -0.8878240000 | -0.9716760000 | -0.2715770000 |
| C | 0.0881700000 | -0.0019620000 | -0.4740440000 |
| C | 1.4168590000 | -0.2425390000 | -0.0782930000 |
| H | 2.7580380000 | -1.6674610000 | 0.8124680000 |
| H | 1.0279950000 | -3.3766260000 | 1.1550520000 |
| H | -1.3312470000 | -2.9319140000 | 0.4561940000 |
| C | -2.2985200000 | -0.7136270000 | -0.6741260000 |
| O | -0.2281420000 | 1.1755220000 | -1.0972500000 |
| O | 2.2937310000 | 0.7657330000 | -0.3136130000 |
| C | 3.6520840000 | 0.5397650000 | 0.0096600000 |
| H | 3.7795430000 | 0.3692240000 | 1.0830510000 |
| H | 4.1842840000 | 1.4425020000 | -0.2805400000 |
| H | 4.0496490000 | -0.3136490000 | -0.5476870000 |
| O | -3.1868320000 | -1.5029560000 | -0.4723220000 |
| H | -2.4901650000 | 0.2492050000 | -1.1719410000 |
| C | -0.2701930000 | 2.3147520000 | -0.2362620000 |
| H | 0.6812270000 | 2.4228260000 | 0.2903860000 |
| C | -1.3799670000 | 2.2279800000 | 0.7184680000 |
| H | -0.4052640000 | 3.1723580000 | -0.8952370000 |
| C | -2.2965270000 | 2.1200620000 | 1.4846440000 |
| H | -3.1089730000 | 2.0248520000 | 2.1656240000 |

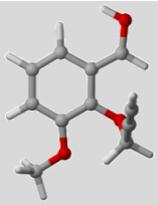
Thermochemie

Zero-point correction= 0.186239 (Hartree/Particle)
Thermal correction to Energy= 0.199438
Thermal correction to Enthalpy= 0.200382
Thermal correction to Gibbs Free Energy= 0.145744
Sum of electronic and zero-point Energies= -650.482556
Sum of electronic and thermal Energies= -650.469357
Sum of electronic and thermal Enthalpies= -650.468413
Sum of electronic and thermal Free Energies= -650.523050

| | E (Thermal) | CV | S |
|---|---|---|---|
| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 125.149 | 48.624 | 114.994 |

**25a**



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XYZ-Matrix in Ångström

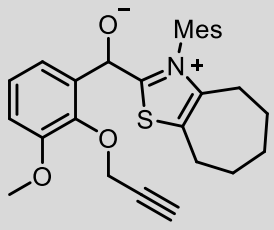
| | | | |
|---|---|---|---|
| C | 1.6078690000 | -1.5938870000 | 0.5464810000 |
| C | 0.5330430000 | -2.4619510000 | 0.7560160000 |
| C | -0.7442100000 | -2.1320730000 | 0.3585300000 |
| C | -1.0063060000 | -0.8834540000 | -0.2656710000 |
| C | 0.0897550000 | -0.0113260000 | -0.4753400000 |
| C | 1.3799230000 | -0.3672240000 | -0.0820740000 |
| H | 2.6006920000 | -1.8826000000 | 0.8598410000 |
| H | 0.7149570000 | -3.4184400000 | 1.2313950000 |
| H | -1.5381430000 | -2.8542680000 | 0.5150190000 |
| C | -2.2891970000 | -0.4820450000 | -0.6826340000 |
| O | -0.1359210000 | 1.1716450000 | -1.1320280000 |
| O | 2.3525450000 | 0.5446710000 | -0.3531580000 |
| C | 3.6866810000 | 0.1909340000 | -0.0484600000 |
| H | 3.8190970000 | 0.0303290000 | 1.0258100000 |
| H | 4.2999000000 | 1.0310350000 | -0.3669310000 |
| H | 3.9878490000 | -0.7083920000 | -0.5937620000 |
| O | -3.4080560000 | -1.2052010000 | -0.4746380000 |
| H | -2.4644970000 | 0.4400540000 | -1.2122180000 |
| C | 0.0132670000 | 2.3479970000 | -0.3399950000 |
| H | 1.0216890000 | 2.3971400000 | 0.0763850000 |
| C | -0.9813920000 | 2.4270700000 | 0.7357060000 |
| H | -0.1204680000 | 3.1804570000 | -1.0314040000 |
| C | -1.7972500000 | 2.4860230000 | 1.6130640000 |
| H | -2.5219700000 | 2.5359030000 | 2.3902970000 |
| H | -3.2207500000 | -1.9605220000 | 0.0904230000 |

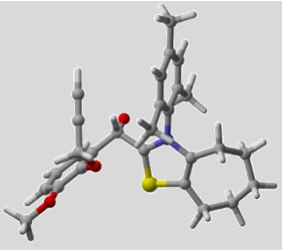
Thermochemie

Zero-point correction= 0.196471 (Hartree/Particle)
Thermal correction to Energy= 0.210220
Thermal correction to Enthalpy= 0.211164
Thermal correction to Gibbs Free Energy= 0.155065
Sum of electronic and zero-point Energies= -651.034709
Sum of electronic and thermal Energies= -651.020960
Sum of electronic and thermal Enthalpies= -651.020016
Sum of electronic and thermal Free Energies= -651.076115

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 131.915 | 51.493 | 118.071 |

**22a**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.9511820000 | -0.9286310000 | 1.0578790000 |
| C | 4.2620250000 | -0.9806650000 | 2.2695580000 |

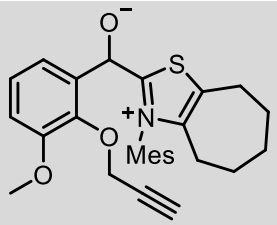
| | | | |
|---|---|---|---|
| C | 2.9353050000 | -0.5871310000 | 2.3485590000 |
| C | 2.2776630000 | -0.1213440000 | 1.2122460000 |
| C | 2.9610160000 | -0.0614330000 | 0.0053380000 |
| C | 4.2989590000 | -0.4757260000 | -0.0852140000 |
| H | 5.9834480000 | -1.2491120000 | 1.0131240000 |
| H | 4.7791460000 | -1.3356640000 | 3.1534530000 |
| H | 2.3620060000 | -0.6121040000 | 3.2679210000 |
| C | 0.8093790000 | 0.3161800000 | 1.3435820000 |
| O | 2.2910610000 | 0.3257850000 | -1.1403320000 |
| O | 4.8653660000 | -0.4032100000 | -1.3246620000 |
| C | 6.1999650000 | -0.8453260000 | -1.4559390000 |
| H | 6.8785790000 | -0.2446240000 | -0.8422310000 |
| H | 6.4564960000 | -0.7230990000 | -2.5061740000 |
| H | 6.2949450000 | -1.8996240000 | -1.1779420000 |
| O | 0.2758790000 | 0.1745010000 | 2.5569020000 |
| C | 2.7145600000 | 1.5618880000 | -1.7086470000 |
| H | 3.8007630000 | 1.6549430000 | -1.6547580000 |
| C | 2.0669540000 | 2.7121870000 | -1.0665690000 |
| H | 2.4292920000 | 1.5229800000 | -2.7620090000 |
| C | 1.5044160000 | 3.6330520000 | -0.5416370000 |
| H | 1.0035010000 | 4.4356440000 | -0.0538030000 |
| N | -1.2780860000 | -0.2774430000 | 0.0388750000 |
| C | -0.0620210000 | -0.5993040000 | 0.4785860000 |
| S | 0.2287020000 | -2.2627980000 | 0.2622080000 |
| C | -1.3584560000 | -2.5139840000 | -0.4091500000 |
| C | -2.0398050000 | -1.3477610000 | -0.4580890000 |
| C | -1.7565420000 | 1.0886720000 | 0.0647340000 |
| C | -2.4813200000 | 1.5224300000 | 1.1772710000 |
| C | -2.9162630000 | 2.8449620000 | 1.1697440000 |
| C | -2.6510460000 | 3.7029460000 | 0.1015990000 |
| C | -1.9405520000 | 3.2154130000 | -0.9921330000 |
| C | -1.4840770000 | 1.8988400000 | -1.0352680000 |
| C | -2.7665590000 | 0.5913690000 | 2.3205410000 |
| H | -3.4714330000 | 3.2155320000 | 2.0260950000 |
| C | -3.1516170000 | 5.1243240000 | 0.1274830000 |
| H | -1.7246090000 | 3.8716210000 | -1.8297500000 |
| C | -0.7478280000 | 1.3586460000 | -2.2307330000 |
| C | -1.8119450000 | -3.8655890000 | -0.8785380000 |
| C | -3.1525390000 | -4.3118110000 | -0.2831730000 |
| H | -1.0428710000 | -4.6006200000 | -0.6299050000 |
| H | -1.8877730000 | -3.8561530000 | -1.9728340000 |
| C | -4.3675420000 | -3.5445510000 | -0.8101540000 |
| H | -3.1058530000 | -4.2296520000 | 0.8077560000 |
| H | -3.2867080000 | -5.3716920000 | -0.5171390000 |
| H | -5.2699290000 | -4.0636420000 | -0.4746920000 |
| C | -3.4290510000 | -1.1356970000 | -0.9833550000 |
| H | -3.7206720000 | -0.1012330000 | -0.7905690000 |
| C | -4.4740000000 | -2.0806460000 | -0.3741840000 |
| H | -3.4203750000 | -1.2606560000 | -2.0734850000 |
| H | -5.4608310000 | -1.7085950000 | -0.6629770000 |
| H | -4.3752540000 | -3.5949050000 | -1.9065250000 |
| H | -4.4202940000 | -2.0188000000 | 0.7177020000 |
| H | -1.3982230000 | 0.6986380000 | -2.8151290000 |
| H | 0.1271180000 | 0.7795270000 | -1.9284720000 |
| H | -0.4215560000 | 2.1752040000 | -2.8755920000 |
| H | -1.8125010000 | 0.2691110000 | 2.7559540000 |
| H | -3.3057300000 | -0.2955280000 | 1.9713560000 |
| H | -3.3766710000 | 1.0874940000 | 3.0752820000 |
| H | -4.2253480000 | 5.1575230000 | -0.0763930000 |
| H | -2.6497030000 | 5.7342570000 | -0.6246620000 |
| H | -2.9886000000 | 5.5794590000 | 1.1063100000 |
| H | 0.7369920000 | 1.3261660000 | 0.8913640000 |

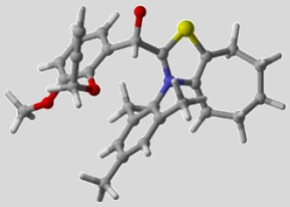
Thermochemie

| | |
|---|---|
| Zero-point correction= | 0.531841 (Hartree/Particle) |
| Thermal correction to Energy= | 0.564107 |
| Thermal correction to Enthalpy= | 0.565051 |
| Thermal correction to Gibbs Free Energy= | 0.467456 |
| Sum of electronic and zero-point Energies= | -1763.382938 |
| Sum of electronic and thermal Energies= | -1763.350672 |
| Sum of electronic and thermal Enthalpies= | -1763.349728 |
| Sum of electronic and thermal Free Energies= | -1763.447322 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 353.982 | 123.293 | 205.406 |

**22a (anti)**



64

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 3.2341640000 | -1.3751700000 | -2.1935250000 |
| C | 2.2564030000 | -2.3721540000 | -2.2662220000 |
| C | 1.3165130000 | -2.5138820000 | -1.2611240000 |
| C | 1.3223480000 | -1.6520460000 | -0.1601660000 |
| C | 2.3102260000 | -0.6817820000 | -0.0680930000 |
| C | 3.2713310000 | -0.5361660000 | -1.0858670000 |
| H | 3.9620200000 | -1.2792660000 | -2.9880220000 |
| H | 2.2491020000 | -3.0405400000 | -3.1194470000 |
| H | 0.5764460000 | -3.3067430000 | -1.2736290000 |
| C | 0.2343360000 | -1.8481690000 | 0.9225600000 |
| O | 2.3634950000 | 0.1822440000 | 1.0025870000 |
| O | 4.1910470000 | 0.4504080000 | -0.8896100000 |
| C | 5.1551980000 | 0.6448290000 | -1.9013010000 |
| H | 5.7763110000 | -0.2466210000 | -2.0357700000 |
| H | 5.7781260000 | 1.4739750000 | -1.5717850000 |
| H | 4.6812490000 | 0.9022860000 | -2.8544580000 |
| O | -0.0537590000 | -3.1092690000 | 1.2070400000 |
| C | 3.3361880000 | -0.1820170000 | 1.9847860000 |
| H | 4.3305290000 | -0.2143320000 | 1.5288600000 |
| C | 3.0094190000 | -1.4713000000 | 2.6012930000 |
| H | 3.3179510000 | 0.6207870000 | 2.7234280000 |
| C | 2.6262730000 | -2.5441790000 | 2.9778280000 |
| H | 2.2487120000 | -3.4933180000 | 3.2784660000 |
| N | -1.3832040000 | 0.0272010000 | -0.0151570000 |
| C | -1.0512750000 | -1.2066390000 | 0.3550310000 |
| S | -2.3453480000 | -2.2884660000 | 0.1925290000 |
| C | -3.3646640000 | -1.0154700000 | -0.4225380000 |
| C | -2.7041840000 | 0.1669850000 | -0.4659600000 |
| C | -0.4559850000 | 1.1295690000 | 0.1132260000 |
| C | -0.3296680000 | 1.7400250000 | 1.3586960000 |
| C | 0.5859890000 | 2.7844280000 | 1.4703620000 |
| C | 1.3597060000 | 3.1935180000 | 0.3885900000 |
| C | 1.1784810000 | 2.5675900000 | -0.8442910000 |
| C | 0.2676060000 | 1.5308950000 | -1.0108050000 |
| C | -1.1272720000 | 1.2651980000 | 2.5433940000 |
| H | 0.7096270000 | 3.2725600000 | 2.4322780000 |
| C | 2.4116410000 | 4.2580690000 | 0.5483580000 |
| H | 1.7740840000 | 2.8827710000 | -1.6957860000 |

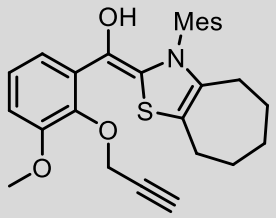
| | | | |
|---|---|---|---|
| C | 0.0847030000 | 0.8484860000 | -2.3388310000 |
| C | -4.7987890000 | -1.2468630000 | -0.8001210000 |
| C | -5.7827200000 | -0.3446520000 | -0.0426660000 |
| H | -5.0477770000 | -2.2937650000 | -0.6107850000 |
| H | -4.9193960000 | -1.0906800000 | -1.8791170000 |
| C | -5.7694990000 | 1.1253350000 | -0.4734750000 |
| H | -5.5797820000 | -0.4186980000 | 1.0311400000 |
| H | -6.7908220000 | -0.7376530000 | -0.2018740000 |
| H | -6.6216490000 | 1.6246320000 | -0.0033780000 |
| C | -3.2481390000 | 1.4946540000 | -0.9018710000 |
| H | -2.4704990000 | 2.2517060000 | -0.7815100000 |
| C | -4.5059230000 | 1.9199460000 | -0.1312790000 |
| H | -3.4811930000 | 1.4497430000 | -1.9730490000 |
| H | -4.6939450000 | 2.9738260000 | -0.3544020000 |
| H | -5.9415490000 | 1.1808030000 | -1.5559450000 |
| H | -4.3075430000 | 1.8562450000 | 0.9440210000 |
| H | -0.9681490000 | 0.8300290000 | -2.6358500000 |
| H | 0.4347470000 | -0.1872110000 | -2.2956310000 |
| H | 0.6488980000 | 1.3677100000 | -3.1134680000 |
| H | -0.7256400000 | 0.3209730000 | 2.9233660000 |
| H | -2.1744520000 | 1.0909050000 | 2.2824480000 |
| H | -1.0887580000 | 1.9985100000 | 3.3487400000 |
| H | 2.2174220000 | 4.8822420000 | 1.4215160000 |
| H | 2.4620330000 | 4.9002930000 | -0.3327630000 |
| H | 3.3921870000 | 3.7902330000 | 0.6762620000 |
| H | 0.5189950000 | -1.1976530000 | 1.7757150000 |

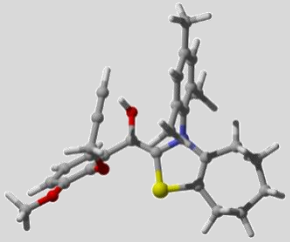
Thermochemie

Zero-point correction= 0.531542 (Hartree/Particle)
Thermal correction to Energy= 0.563795
Thermal correction to Enthalpy= 0.564740
Thermal correction to Gibbs Free Energy= 0.467907
Sum of electronic and zero-point Energies= -1763.381757
Sum of electronic and thermal Energies= -1763.349504
Sum of electronic and thermal Enthalpies= -1763.348560
Sum of electronic and thermal Free Energies= -1763.445392

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 353.787 | 123.292 | 203.801 |

**23a**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 5.0498460000 | -0.6005970000 | 1.3121680000 |
| C | 4.2865570000 | -0.4544860000 | 2.4735440000 |
| C | 2.9296160000 | -0.2095930000 | 2.4026350000 |
| C | 2.2876310000 | -0.1108840000 | 1.1572760000 |
| C | 3.0528210000 | -0.2319260000 | -0.0004670000 |
| C | 4.4355390000 | -0.4827820000 | 0.0720080000 |
| H | 6.1100800000 | -0.7989290000 | 1.3888760000 |
| H | 4.7719940000 | -0.5432520000 | 3.4381390000 |
| H | 2.3357840000 | -0.0937480000 | 3.3008370000 |
| C | 0.8442200000 | 0.1828550000 | 1.1083360000 |

| | | | |
|---|---|---|---|
| O | 2.4718840000 | -0.0979540000 | -1.2377880000 |
| O | 5.0775790000 | -0.5654040000 | -1.1232780000 |
| C | 6.4612680000 | -0.8491850000 | -1.1006890000 |
| H | 7.0185250000 | -0.0626350000 | -0.5820880000 |
| H | 6.7765940000 | -0.8924020000 | -2.1408670000 |
| H | 6.6565670000 | -1.8129150000 | -0.6205860000 |
| O | 0.4210760000 | 1.2611500000 | 1.8692660000 |
| C | 2.7021180000 | 1.1673130000 | -1.8423560000 |
| H | 3.7724880000 | 1.3918320000 | -1.8559170000 |
| C | 1.9627230000 | 2.2599210000 | -1.1893180000 |
| H | 2.3551640000 | 1.0706010000 | -2.8725850000 |
| C | 1.3439420000 | 3.1719200000 | -0.7111090000 |
| H | 0.7715020000 | 3.9746850000 | -0.3073290000 |
| H | 0.7722060000 | 2.0641970000 | 1.4635010000 |
| N | -1.4425290000 | -0.2987310000 | 0.3817570000 |
| C | -0.0728250000 | -0.5880470000 | 0.4925360000 |
| S | 0.2711390000 | -2.1717960000 | -0.2239190000 |
| C | -1.4512460000 | -2.4175570000 | -0.5521770000 |
| C | -2.1815110000 | -1.3561930000 | -0.1960720000 |
| C | -1.8582970000 | 1.0610020000 | 0.1542310000 |
| C | -2.5090080000 | 1.7543560000 | 1.1793390000 |
| C | -2.9121330000 | 3.0639650000 | 0.9368580000 |
| C | -2.6818980000 | 3.6858810000 | -0.2917000000 |
| C | -2.0339940000 | 2.9647870000 | -1.2907500000 |
| C | -1.6176790000 | 1.6474680000 | -1.0906830000 |
| C | -2.7390230000 | 1.0942840000 | 2.5098320000 |
| H | -3.4161770000 | 3.6143130000 | 1.7262420000 |
| C | -3.1595420000 | 5.0942520000 | -0.5390420000 |
| H | -1.8447560000 | 3.4341430000 | -2.2521770000 |
| C | -0.9371400000 | 0.8721450000 | -2.1872860000 |
| C | -1.9495930000 | -3.7124580000 | -1.1239750000 |
| C | -2.9819250000 | -4.4135130000 | -0.2311300000 |
| H | -1.1006690000 | -4.3808990000 | -1.2854210000 |
| H | -2.3920360000 | -3.5330870000 | -2.1126100000 |
| C | -4.3571680000 | -3.7399080000 | -0.2012740000 |
| H | -2.5808210000 | -4.4863070000 | 0.7851630000 |
| H | -3.1140740000 | -5.4365460000 | -0.5970200000 |
| H | -5.0489480000 | -4.3983880000 | 0.3330330000 |
| C | -3.6751950000 | -1.2493920000 | -0.3163820000 |
| H | -3.9919170000 | -0.2708500000 | 0.0499950000 |
| C | -4.4231120000 | -2.3528660000 | 0.4460830000 |
| H | -3.9594620000 | -1.2879940000 | -1.3757510000 |
| H | -5.4760450000 | -2.0627860000 | 0.5168820000 |
| H | -4.7371180000 | -3.6665810000 | -1.2285750000 |
| H | -4.0371070000 | -2.4026860000 | 1.4700670000 |
| H | -1.5802000000 | 0.0613980000 | -2.5441200000 |
| H | -0.0107340000 | 0.4126620000 | -1.8328730000 |
| H | -0.7046470000 | 1.5259080000 | -3.0290020000 |
| H | -1.7781670000 | 0.8790000000 | 2.9825950000 |
| H | -3.2637180000 | 0.1426120000 | 2.3916430000 |
| H | -3.3264410000 | 1.7381930000 | 3.1654580000 |
| H | -4.2079600000 | 5.0953770000 | -0.8508150000 |
| H | -2.5798620000 | 5.5768160000 | -1.3276520000 |
| H | -3.0848580000 | 5.7012110000 | 0.3651380000 |

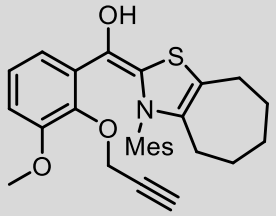
Thermochemie

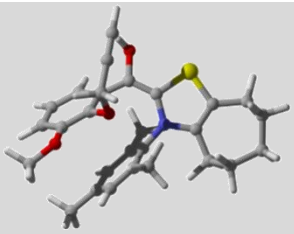
Zero-point correction= 0.531645 (Hartree/Particle)
Thermal correction to Energy= 0.564314
Thermal correction to Enthalpy= 0.565259
Thermal correction to Gibbs Free Energy= 0.467910
Sum of electronic and zero-point Energies= -1763.412946
Sum of electronic and thermal Energies= -1763.380277

Sum of electronic and thermal Enthalpies= -1763.379332
Sum of electronic and thermal Free Energies= -1763.476681

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 354.113 | 125.107 | 204.887 |

**23a (anti)**



64
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.0912450000 | 0.4569180000 | 0.4917660000 |
| C | 3.6788590000 | 1.0570840000 | 1.6850560000 |
| C | 2.3927910000 | 1.5424370000 | 1.8313950000 |
| C | 1.4702550000 | 1.4292540000 | 0.7777280000 |
| C | 1.9079750000 | 0.9024650000 | -0.4332910000 |
| C | 3.2058140000 | 0.3912760000 | -0.5784550000 |
| H | 5.0951220000 | 0.0629650000 | 0.4064320000 |
| H | 4.3793070000 | 1.1253920000 | 2.5089860000 |
| H | 2.0684910000 | 1.9921450000 | 2.7623700000 |
| C | 0.0781080000 | 1.8657010000 | 0.9428830000 |
| O | 1.0506890000 | 0.8401540000 | -1.5053120000 |
| O | 3.4951060000 | -0.1279560000 | -1.8013400000 |
| C | 4.7021330000 | -0.8508220000 | -1.9221570000 |
| H | 5.5730280000 | -0.2015800000 | -1.7884990000 |
| H | 4.7106750000 | -1.2606340000 | -2.9300000000 |
| H | 4.7381130000 | -1.6669370000 | -1.1929850000 |
| O | -0.1086910000 | 3.1323160000 | 1.4857030000 |
| C | 1.2139660000 | 1.9033020000 | -2.4302020000 |
| H | 2.2660200000 | 1.9931120000 | -2.7189950000 |
| C | 0.7223170000 | 3.1967130000 | -1.9294740000 |
| H | 0.6367830000 | 1.6222020000 | -3.3126620000 |
| C | 0.3179960000 | 4.2760700000 | -1.5916690000 |
| H | -0.0539660000 | 5.2326440000 | -1.3082590000 |
| H | 0.2818410000 | 3.7658380000 | 0.8705110000 |
| N | -1.2150550000 | -0.1956790000 | 0.3811100000 |
| C | -1.0473120000 | 1.1516270000 | 0.7140410000 |
| S | -2.6288750000 | 1.9191560000 | 0.8957430000 |
| C | -3.4415850000 | 0.4041950000 | 0.4934070000 |
| C | -2.5672400000 | -0.5856910000 | 0.2729610000 |
| C | -0.1323220000 | -1.1269290000 | 0.4707990000 |
| C | 0.3450500000 | -1.7637410000 | -0.6792740000 |
| C | 1.4879580000 | -2.5580170000 | -0.5681780000 |
| C | 2.1508970000 | -2.7240140000 | 0.6420120000 |
| C | 1.6117810000 | -2.1263140000 | 1.7815830000 |
| C | 0.4648810000 | -1.3436860000 | 1.7242890000 |
| C | -0.3245350000 | -1.6087030000 | -2.0190480000 |
| H | 1.8814740000 | -3.0305960000 | -1.4639210000 |
| C | 3.4244040000 | -3.5236780000 | 0.7393990000 |
| H | 2.0990470000 | -2.2728820000 | 2.7415710000 |
| C | -0.1070200000 | -0.7363480000 | 2.9768210000 |
| C | -4.9398030000 | 0.3203830000 | 0.4600210000 |
| C | -5.5002870000 | -0.2191970000 | -0.8625950000 |
| H | -5.3514580000 | 1.3162450000 | 0.6412520000 |
| H | -5.2939810000 | -0.3109590000 | 1.2856900000 |

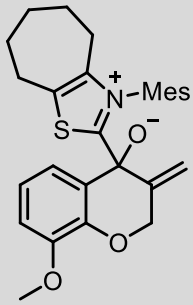
| | | | |
|---|---|---|---|
| C | -5.2802590000 | -1.7185700000 | -1.0836640000 |
| H | -5.0608910000 | 0.3463350000 | -1.6909610000 |
| H | -6.5777570000 | -0.0282890000 | -0.8810120000 |
| H | -5.8486590000 | -2.0221790000 | -1.9680010000 |
| C | -2.9440150000 | -2.0099120000 | -0.0243050000 |
| H | -2.0411310000 | -2.6109810000 | -0.1316890000 |
| C | -3.8276850000 | -2.1666520000 | -1.2704490000 |
| H | -3.4792810000 | -2.4171320000 | 0.8427590000 |
| H | -3.8323070000 | -3.2243840000 | -1.5515890000 |
| H | -5.7130610000 | -2.2680420000 | -0.2378500000 |
| H | -3.3751970000 | -1.6179590000 | -2.1027930000 |
| H | -1.1973580000 | -0.6881450000 | 2.9315020000 |
| H | 0.2532700000 | 0.2863730000 | 3.1170740000 |
| H | 0.1839240000 | -1.3259180000 | 3.8470340000 |
| H | -0.9725740000 | -0.7331860000 | -2.0367700000 |
| H | -0.9255840000 | -2.4934770000 | -2.2545120000 |
| H | 0.4306660000 | -1.4920760000 | -2.7977550000 |
| H | 3.6822640000 | -3.9780660000 | -0.2186840000 |
| H | 3.3334470000 | -4.3217450000 | 1.4801540000 |
| H | 4.2540990000 | -2.8818520000 | 1.0511450000 |

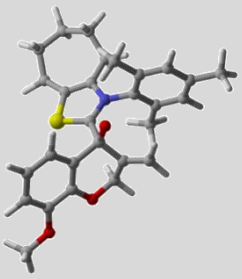
Thermochemie

| | |
|---|---|
| Zero-point correction= | 0.532826 (Hartree/Particle) |
| Thermal correction to Energy= | 0.564955 |
| Thermal correction to Enthalpy= | 0.565899 |
| Thermal correction to Gibbs Free Energy= | 0.470855 |
| Sum of electronic and zero-point Energies= | -1763.415429 |
| Sum of electronic and thermal Energies= | -1763.383300 |
| Sum of electronic and thermal Enthalpies= | -1763.382356 |
| Sum of electronic and thermal Free Energies= | -1763.477400 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 354.515 | 124.672 | 200.038 |

**[24a + A]**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0119530000 | 0.5444300000 | 1.1747160000 |
| C | -4.0587110000 | 0.7209580000 | 2.1843390000 |
| C | -2.7722290000 | 0.2510670000 | 2.0121870000 |
| C | -2.4018400000 | -0.3839660000 | 0.8228510000 |
| C | -3.3503380000 | -0.5825000000 | -0.1749950000 |
| C | -4.6703970000 | -0.1126300000 | 0.0023650000 |
| H | -6.0191900000 | 0.9105940000 | 1.3216440000 |
| H | -4.3456850000 | 1.2152800000 | 3.1045580000 |
| H | -2.0165680000 | 0.3273240000 | 2.7854500000 |
| C | -0.9400730000 | -0.8994570000 | 0.6976180000 |
| O | -5.5222220000 | -0.3590080000 | -1.0272940000 |
| C | -6.8611510000 | 0.0495320000 | -0.8687670000 |
| H | -7.3255230000 | -0.4376390000 | -0.0048580000 |
| H | -7.3784660000 | -0.2536600000 | -1.7767020000 |

| | | | |
|---|---|---|---|
| H | -6.9360580000 | 1.1363950000 | -0.7540590000 |
| O | -0.3595760000 | -1.1891470000 | 1.8372630000 |
| N | 1.2012650000 | 0.3241380000 | -0.1235020000 |
| C | -0.1165790000 | 0.3082200000 | 0.0855470000 |
| S | -0.7587770000 | 1.8727900000 | -0.1222510000 |
| C | 0.7974260000 | 2.5427370000 | -0.4970850000 |
| C | 1.7455850000 | 1.5782870000 | -0.4486100000 |
| C | 2.0417000000 | -0.8554540000 | -0.0229260000 |
| C | 2.6571600000 | -1.1196510000 | 1.2040820000 |
| C | 3.4879640000 | -2.2325000000 | 1.2705740000 |
| C | 3.7179440000 | -3.0492940000 | 0.1625280000 |
| C | 3.1165110000 | -2.7181950000 | -1.0466190000 |
| C | 2.2706790000 | -1.6150650000 | -1.1656680000 |
| C | 2.4225470000 | -0.2373060000 | 2.3952150000 |
| H | 3.9691500000 | -2.4674300000 | 2.2147260000 |
| C | 4.5883580000 | -4.2727910000 | 0.2810120000 |
| H | 3.3042250000 | -3.3298960000 | -1.9241660000 |
| C | 1.6249960000 | -1.3083740000 | -2.4904880000 |
| C | 0.9719420000 | 3.9962200000 | -0.8312420000 |
| C | 2.0388720000 | 4.7056040000 | 0.0107050000 |
| H | 0.0123450000 | 4.5022840000 | -0.7015440000 |
| H | 1.2275610000 | 4.0891490000 | -1.8939580000 |
| C | 3.4776340000 | 4.2971910000 | -0.3127500000 |
| H | 1.8331900000 | 4.5310620000 | 1.0719850000 |
| H | 1.9376690000 | 5.7809300000 | -0.1603260000 |
| H | 4.1519370000 | 4.9929700000 | 0.1944970000 |
| C | 3.2119200000 | 1.7521830000 | -0.7218470000 |
| H | 3.7230350000 | 0.8104710000 | -0.5171710000 |
| C | 3.8715230000 | 2.8747070000 | 0.0915760000 |
| H | 3.3469610000 | 1.9544970000 | -1.7919240000 |
| H | 4.9532490000 | 2.7710450000 | -0.0297060000 |
| H | 3.6548520000 | 4.4275380000 | -1.3878990000 |
| H | 3.6596200000 | 2.7221050000 | 1.1548440000 |
| H | 1.2573990000 | -0.2825540000 | -2.5515510000 |
| H | 0.7760760000 | -1.9791460000 | -2.6507450000 |
| H | 2.3352990000 | -1.4672620000 | -3.3036950000 |
| H | 1.3689780000 | -0.3265750000 | 2.6801170000 |
| H | 2.6324610000 | 0.8109740000 | 2.1586780000 |
| H | 3.0635000000 | -0.5349420000 | 3.2249770000 |
| H | 5.3716570000 | -4.1291030000 | 1.0268590000 |
| H | 5.0588080000 | -4.5177670000 | -0.6723610000 |
| H | 3.9905730000 | -5.1348410000 | 0.5896900000 |
| C | -1.0058880000 | -1.9974640000 | -0.3710990000 |
| C | -1.7688420000 | -1.6253800000 | -1.6062740000 |
| H | -1.2834370000 | -0.7804800000 | -2.1167370000 |
| O | -3.1169450000 | -1.2415620000 | -1.3393920000 |
| H | -1.8304060000 | -2.4603890000 | -2.3055570000 |
| C | -0.4663420000 | -3.1866710000 | -0.1458960000 |
| H | 0.0700130000 | -3.3439890000 | 0.7851630000 |
| H | -0.5522200000 | -3.9994340000 | -0.8606220000 |

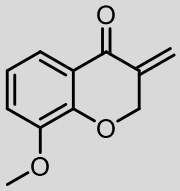
Thermochemie

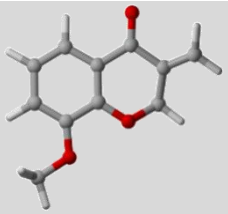
Zero-point correction= 0.534073 (Hartree/Particle)
Thermal correction to Energy= 0.564925
Thermal correction to Enthalpy= 0.565869
Thermal correction to Gibbs Free Energy= 0.472662
Sum of electronic and zero-point Energies= -1763.436249
Sum of electronic and thermal Energies= -1763.405397
Sum of electronic and thermal Enthalpies= -1763.404452
Sum of electronic and thermal Free Energies= -1763.497660

| | E (Thermal) | CV | S |
|---|---|---|---|

| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 354.496 | 120.744 | 196.171 |

**24a**





24

XYZ-Matrix in Ångström

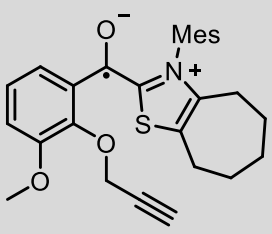
| | | | |
|---|---|---|---|
| C | 2.2559120000 | 1.1675390000 | 0.0072500000 |
| C | 1.4166390000 | 2.2889800000 | 0.0867370000 |
| C | 0.0502150000 | 2.1320320000 | 0.1154350000 |
| C | -0.5045490000 | 0.8435710000 | 0.0796210000 |
| C | 0.3247120000 | -0.2767320000 | 0.0199070000 |
| C | 1.7266160000 | -0.1123690000 | -0.0314020000 |
| H | 3.3277510000 | 1.3117990000 | -0.0189540000 |
| H | 1.8571310000 | 3.2774550000 | 0.1183220000 |
| H | -0.6256220000 | 2.9772060000 | 0.1514330000 |
| C | -1.9774370000 | 0.6716640000 | -0.0045360000 |
| O | -0.1394770000 | -1.5457800000 | -0.0226110000 |
| O | 2.4463430000 | -1.2546110000 | -0.1100140000 |
| C | 3.8512470000 | -1.1327770000 | -0.1829160000 |
| H | 4.1524020000 | -0.5637110000 | -1.0681470000 |
| H | 4.2365300000 | -2.1470340000 | -0.2551710000 |
| H | 4.2537060000 | -0.6527450000 | 0.7149310000 |
| O | -2.7392450000 | 1.6046630000 | -0.1203880000 |
| C | -2.4387190000 | -0.7535830000 | 0.0144570000 |
| C | -1.4328470000 | -1.7322340000 | 0.5463030000 |
| H | -1.3401740000 | -1.6079560000 | 1.6336340000 |
| H | -1.7149590000 | -2.7612180000 | 0.3296180000 |
| C | -3.6616450000 | -1.0742380000 | -0.3935160000 |
| H | -4.0043480000 | -2.1030630000 | -0.4097850000 |
| H | -4.3442590000 | -0.2960320000 | -0.7158200000 |

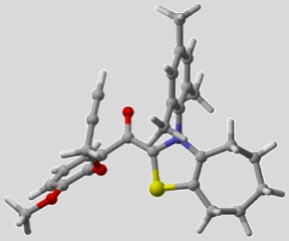
Thermochemie

Zero-point correction= 0.189864 (Hartree/Particle)
Thermal correction to Energy= 0.201512
Thermal correction to Enthalpy= 0.202456
Thermal correction to Gibbs Free Energy= 0.152012
Sum of electronic and zero-point Energies= -650.545582
Sum of electronic and thermal Energies= -650.533934
Sum of electronic and thermal Enthalpies= -650.532990
Sum of electronic and thermal Free Energies= -650.583435

| | E (Thermal) | CV | S |
|---|---|---|---|
| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 126.451 | 45.182 | 106.170 |

**21a**



63

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0639590000 | 0.4118280000 | 1.2633190000 |
| C | -4.3386920000 | 0.2011200000 | 2.4376600000 |
| C | -2.9804000000 | -0.0468910000 | 2.3910470000 |
| C | -2.3072740000 | -0.0697110000 | 1.1639320000 |
| C | -3.0262110000 | 0.1295210000 | -0.0109830000 |
| C | -4.4131630000 | 0.3664690000 | 0.0365970000 |
| H | -6.1272460000 | 0.6015350000 | 1.3177910000 |
| H | -4.8548240000 | 0.2291740000 | 3.3897100000 |
| H | -2.4128130000 | -0.2380200000 | 3.2932980000 |
| C | -0.8358220000 | -0.3775010000 | 1.1822920000 |
| O | -2.4093830000 | 0.1011740000 | -1.2390640000 |
| O | -5.0212230000 | 0.5227040000 | -1.1688910000 |
| C | -6.4113630000 | 0.7724920000 | -1.1698740000 |
| H | -6.9625170000 | -0.0555120000 | -0.7128140000 |
| H | -6.6992400000 | 0.8683240000 | -2.2144500000 |
| H | -6.6448840000 | 1.7019280000 | -0.6413230000 |
| O | -0.4217210000 | -1.3651020000 | 1.8111190000 |
| C | -2.5963050000 | -1.1216950000 | -1.9545990000 |
| H | -3.6632920000 | -1.3428690000 | -2.0456570000 |
| C | -1.8840660000 | -2.2274900000 | -1.3086470000 |
| H | -2.1932390000 | -0.9392690000 | -2.9519740000 |
| C | -1.2621110000 | -3.0541320000 | -0.7012360000 |
| H | -0.6961850000 | -3.7577070000 | -0.1370000000 |
| N | 1.3893200000 | 0.3007320000 | 0.3271640000 |
| C | 0.0409300000 | 0.5317810000 | 0.5285530000 |
| S | -0.3763290000 | 2.1487040000 | 0.0366990000 |
| C | 1.2897530000 | 2.4810750000 | -0.3939040000 |
| C | 2.0748060000 | 1.4035430000 | -0.1897730000 |
| C | 1.8885730000 | -1.0404190000 | 0.1394690000 |
| C | 2.5410770000 | -1.6863540000 | 1.1910940000 |
| C | 3.0283210000 | -2.9680240000 | 0.9623200000 |
| C | 2.8695700000 | -3.6041280000 | -0.2707260000 |
| C | 2.2194690000 | -2.9224830000 | -1.2947020000 |
| C | 1.7216170000 | -1.6313660000 | -1.1122070000 |
| C | 2.6769270000 | -1.0129750000 | 2.5264670000 |
| H | 3.5361890000 | -3.4889310000 | 1.7688090000 |
| C | 3.3710290000 | -5.0110660000 | -0.4730280000 |
| H | 2.0889590000 | -3.4027380000 | -2.2600830000 |
| C | 1.0477580000 | -0.8910960000 | -2.2380450000 |
| C | 1.6998710000 | 3.8260190000 | -0.9191090000 |
| C | 2.8264010000 | 4.4853150000 | -0.1136400000 |
| H | 0.8272450000 | 4.4834030000 | -0.9225500000 |
| H | 2.0139170000 | 3.7279810000 | -1.9661710000 |
| C | 4.2000770000 | 3.8327420000 | -0.2904660000 |
| H | 2.5515400000 | 4.4903860000 | 0.9465270000 |
| H | 2.9015380000 | 5.5304150000 | -0.4286760000 |
| H | 4.9474470000 | 4.4754300000 | 0.1842090000 |
| C | 3.5524150000 | 1.3323880000 | -0.4479580000 |
| H | 3.9142770000 | 0.3487160000 | -0.1430520000 |
| C | 4.3523430000 | 2.4207740000 | 0.2817310000 |
| H | 3.7366280000 | 1.4095840000 | -1.5268970000 |
| H | 5.4100120000 | 2.1457800000 | 0.2332600000 |
| H | 4.4491240000 | 3.8114040000 | -1.3592240000 |
| H | 4.0729900000 | 2.4187980000 | 1.3410900000 |
| H | 1.7328240000 | -0.1623120000 | -2.6843760000 |
| H | 0.1670640000 | -0.3464140000 | -1.8887560000 |
| H | 0.7357600000 | -1.5893300000 | -3.0157140000 |
| H | 1.6831550000 | -0.8889730000 | 2.9641760000 |
| H | 3.1256760000 | -0.0205220000 | 2.4273410000 |
| H | 3.2941050000 | -1.6083840000 | 3.1998360000 |
| H | 4.3416860000 | -5.1556530000 | 0.0052390000 |

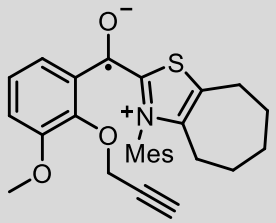
| | | | |
|---|---|---|---|
| H | 3.4724010000 | -5.2452980000 | -1.5335510000 |
| H | 2.6769280000 | -5.7339390000 | -0.0351630000 |

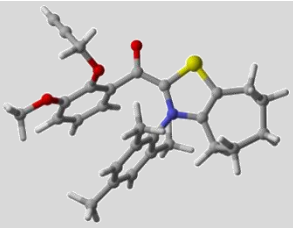
Thermochemie

Zero-point correction= 0.520940 (Hartree/Particle)
Thermal correction to Energy= 0.552837
Thermal correction to Enthalpy= 0.553781
Thermal correction to Gibbs Free Energy= 0.457720
Sum of electronic and zero-point Energies= -1762.818373
Sum of electronic and thermal Energies= -1762.786476
Sum of electronic and thermal Enthalpies= -1762.785531
Sum of electronic and thermal Free Energies= -1762.881592

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 346.910 | 122.573 | 202.177 |

**21a (anti)**



63

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 3.7120820000 | 1.0425660000 | -0.7166060000 |
| C | 2.7669640000 | 1.1897680000 | -1.7321740000 |
| C | 1.6535480000 | 0.3691200000 | -1.7822150000 |
| C | 1.4643940000 | -0.6200610000 | -0.8145430000 |
| C | 2.4120920000 | -0.7806330000 | 0.1889460000 |
| C | 3.5331710000 | 0.0599860000 | 0.2508090000 |
| H | 4.5781930000 | 1.6905970000 | -0.6917290000 |
| H | 2.9110690000 | 1.9550180000 | -2.4860250000 |
| H | 0.9249750000 | 0.4799120000 | -2.5770430000 |
| C | 0.3146310000 | -1.5886930000 | -0.8798240000 |
| O | 2.1976880000 | -1.7284920000 | 1.1491760000 |
| O | 4.3766760000 | -0.1673920000 | 1.2935280000 |
| C | 5.6197300000 | 0.5021710000 | 1.2788440000 |
| H | 6.1688810000 | 0.2828220000 | 0.3578180000 |
| H | 6.1771310000 | 0.1264940000 | 2.1344020000 |
| H | 5.4890290000 | 1.5843380000 | 1.3808010000 |
| O | 0.5425210000 | -2.7869740000 | -1.1134800000 |
| C | 3.1850030000 | -2.7491410000 | 1.3313860000 |
| H | 3.8467710000 | -2.4630030000 | 2.1518540000 |
| C | 3.9874720000 | -3.0301820000 | 0.1411510000 |
| H | 2.6238960000 | -3.6424490000 | 1.6094980000 |
| C | 4.6608030000 | -3.2579740000 | -0.8244560000 |
| H | 5.2348790000 | -3.4707660000 | -1.6942060000 |
| N | -1.6130800000 | 0.0303770000 | -0.3255740000 |
| C | -1.0394510000 | -1.1778500000 | -0.6842670000 |
| S | -2.2696490000 | -2.4032510000 | -0.8420200000 |
| C | -3.5182470000 | -1.2416730000 | -0.4486400000 |
| C | -3.0033610000 | -0.0202340000 | -0.1999240000 |
| C | -0.8493370000 | 1.2266110000 | -0.1244220000 |
| C | -0.1207200000 | 1.3674230000 | 1.0588200000 |
| C | 0.6888950000 | 2.4917430000 | 1.1884950000 |
| C | 0.7555290000 | 3.4654700000 | 0.1925600000 |
| C | -0.0350830000 | 3.3167610000 | -0.9445350000 |
| C | -0.8400540000 | 2.1954440000 | -1.1276960000 |
| C | -0.2077710000 | 0.3268840000 | 2.1412000000 |

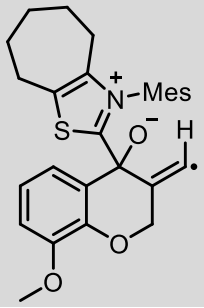
| | | | |
|---|---|---|---|
| H | 1.2866420000 | 2.6062330000 | 2.0879350000 |
| C | 1.7062000000 | 4.6250630000 | 0.3258020000 |
| H | 0.0022570000 | 4.0724510000 | -1.7235800000 |
| C | -1.6494560000 | 2.0068210000 | -2.3830330000 |
| C | -4.9608420000 | -1.6407910000 | -0.3471990000 |
| C | -5.5556670000 | -1.4226990000 | 1.0517330000 |
| H | -5.0559460000 | -2.6941660000 | -0.6209120000 |
| H | -5.5496880000 | -1.0778390000 | -1.0824810000 |
| C | -5.8066280000 | 0.0447760000 | 1.4117030000 |
| H | -4.8922380000 | -1.8796810000 | 1.7936780000 |
| H | -6.5101970000 | -1.9545180000 | 1.1060240000 |
| H | -6.3567410000 | 0.0765300000 | 2.3568130000 |
| C | -3.7955890000 | 1.1752930000 | 0.2445330000 |
| H | -3.1233810000 | 2.0261250000 | 0.3706180000 |
| C | -4.5662510000 | 0.9324740000 | 1.5511990000 |
| H | -4.5070670000 | 1.4464770000 | -0.5453760000 |
| H | -4.8870280000 | 1.9040270000 | 1.9382210000 |
| H | -6.4708640000 | 0.4851170000 | 0.6568120000 |
| H | -3.8839300000 | 0.5056890000 | 2.2940300000 |
| H | -2.7130600000 | 2.1889850000 | -2.1994940000 |
| H | -1.5590040000 | 0.9845150000 | -2.7594350000 |
| H | -1.3206250000 | 2.6977310000 | -3.1597460000 |
| H | 0.2594640000 | -0.6119190000 | 1.8331240000 |
| H | -1.2518670000 | 0.1076370000 | 2.3816430000 |
| H | 0.2944950000 | 0.6728350000 | 3.0447140000 |
| H | 1.7743570000 | 4.9661440000 | 1.3602890000 |
| H | 1.3995690000 | 5.4669230000 | -0.2965130000 |
| H | 2.7085480000 | 4.3193270000 | 0.0099160000 |

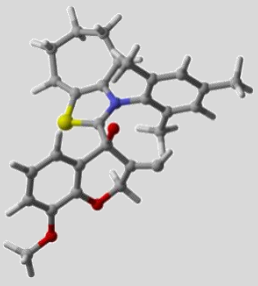
Thermochemie

Zero-point correction= 0.520136 (Hartree/Particle)
Thermal correction to Energy= 0.552342
Thermal correction to Enthalpy= 0.553286
Thermal correction to Gibbs Free Energy= 0.455724
Sum of electronic and zero-point Energies= -1762.814651
Sum of electronic and thermal Energies= -1762.782446
Sum of electronic and thermal Enthalpies= -1762.781502
Sum of electronic and thermal Free Energies= -1762.879064

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 346.600 | 122.926 | 205.337 |

**26a**



63

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0202650000 | 0.4922450000 | 1.1873600000 |
| C | -4.0681180000 | 0.6561950000 | 2.2001520000 |
| C | -2.7794640000 | 0.1958890000 | 2.0208290000 |
| C | -2.4042870000 | -0.4166960000 | 0.8205540000 |
| C | -3.3517960000 | -0.6023900000 | -0.1806750000 |
| C | -4.6746690000 | -0.1427130000 | 0.0044140000 |

| | | | |
|---|---|---|---|
| H | -6.0293830000 | 0.8507680000 | 1.3398950000 |
| H | -4.3576240000 | 1.1335140000 | 3.1285100000 |
| H | -2.0250410000 | 0.2636490000 | 2.7958910000 |
| C | -0.9393270000 | -0.9168070000 | 0.6953590000 |
| O | -5.5239100000 | -0.3759080000 | -1.0298270000 |
| C | -6.8650190000 | 0.0240740000 | -0.8665400000 |
| H | -7.3285090000 | -0.4796570000 | -0.0117690000 |
| H | -7.3794890000 | -0.2661660000 | -1.7802490000 |
| H | -6.9445930000 | 1.1085170000 | -0.7337300000 |
| O | -0.3609330000 | -1.2212930000 | 1.8261090000 |
| N | 1.1975520000 | 0.3117860000 | -0.1210920000 |
| C | -0.1199940000 | 0.2931710000 | 0.0880110000 |
| S | -0.7666100000 | 1.8559110000 | -0.1170840000 |
| C | 0.7878310000 | 2.5300040000 | -0.4914830000 |
| C | 1.7383950000 | 1.5675970000 | -0.4446250000 |
| C | 2.0406780000 | -0.8667620000 | -0.0252790000 |
| C | 2.6563190000 | -1.1346180000 | 1.2021690000 |
| C | 3.4901800000 | -2.2440530000 | 1.2641050000 |
| C | 3.7233270000 | -3.0562640000 | 0.1517880000 |
| C | 3.1199360000 | -2.7238360000 | -1.0548150000 |
| C | 2.2711520000 | -1.6209990000 | -1.1702510000 |
| C | 2.4175010000 | -0.2578260000 | 2.3966060000 |
| H | 3.9722710000 | -2.4819140000 | 2.2072510000 |
| C | 4.6077690000 | -4.2696280000 | 0.2710620000 |
| H | 3.3058860000 | -3.3331400000 | -1.9341160000 |
| C | 1.6243610000 | -1.3145490000 | -2.4944660000 |
| C | 0.9598470000 | 3.9846430000 | -0.8218560000 |
| C | 2.0225360000 | 4.6940150000 | 0.0256050000 |
| H | -0.0012740000 | 4.4882890000 | -0.6941150000 |
| H | 1.2188130000 | 4.0805090000 | -1.8834670000 |
| C | 3.4634020000 | 4.2903070000 | -0.2947040000 |
| H | 1.8139780000 | 4.5157270000 | 1.0857140000 |
| H | 1.9191740000 | 5.7695980000 | -0.1423920000 |
| H | 4.1341690000 | 4.9854020000 | 0.2181130000 |
| C | 3.2044760000 | 1.7465030000 | -0.7154490000 |
| H | 3.7177260000 | 0.8051530000 | -0.5145410000 |
| C | 3.8595620000 | 2.8670190000 | 0.1044530000 |
| H | 3.3403100000 | 1.9541440000 | -1.7843540000 |
| H | 4.9417940000 | 2.7664080000 | -0.0147330000 |
| H | 3.6440340000 | 4.4259730000 | -1.3685900000 |
| H | 3.6456340000 | 2.7092860000 | 1.1665810000 |
| H | 1.2339090000 | -0.2967150000 | -2.5465340000 |
| H | 0.7927560000 | -2.0047450000 | -2.6635280000 |
| H | 2.3418040000 | -1.4484870000 | -3.3059820000 |
| H | 1.3645660000 | -0.3520620000 | 2.6815670000 |
| H | 2.6232450000 | 0.7922070000 | 2.1643110000 |
| H | 3.0593750000 | -0.5560260000 | 3.2254240000 |
| H | 5.5051970000 | -4.0444710000 | 0.8506330000 |
| H | 4.9133900000 | -4.6355930000 | -0.7096700000 |
| H | 4.0788550000 | -5.0780960000 | 0.7827340000 |
| C | -0.9981110000 | -2.0079830000 | -0.4140860000 |
| C | -1.7728530000 | -1.6099880000 | -1.6392880000 |
| H | -1.2881190000 | -0.7506040000 | -2.1252050000 |
| O | -3.1180220000 | -1.2413530000 | -1.3556250000 |
| H | -1.8301630000 | -2.4283370000 | -2.3562890000 |
| C | -0.4326550000 | -3.1695470000 | -0.2285890000 |
| H | 0.1588610000 | -3.5838040000 | 0.5761980000 |

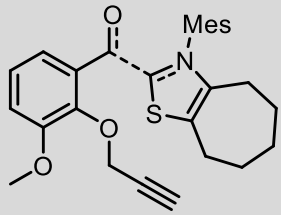
Thermochemie

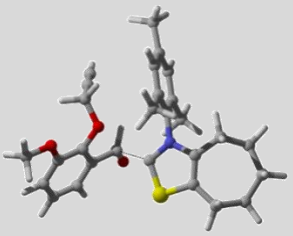
Zero-point correction= 0.520926 (Hartree/Particle)
Thermal correction to Energy= 0.551694
Thermal correction to Enthalpy= 0.552639

Thermal correction to Gibbs Free Energy= 0.459308
Sum of electronic and zero-point Energies= -1762.765791
Sum of electronic and thermal Energies= -1762.735022
Sum of electronic and thermal Enthalpies= -1762.734078
Sum of electronic and thermal Free Energies= -1762.827409

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 346.193 | 120.549 | 196.431 |

**TS-1a**



64
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.4749580000 | -2.3221150000 | 0.1081850000 |
| C | 3.9510790000 | -2.7756670000 | 1.3190580000 |
| C | 2.8197920000 | -2.1902720000 | 1.8641370000 |
| C | 2.1954720000 | -1.1331180000 | 1.2037120000 |
| C | 2.7136260000 | -0.6761690000 | -0.0007680000 |
| C | 3.8517470000 | -1.2734730000 | -0.5626880000 |
| H | 5.3562310000 | -2.7947640000 | -0.3039890000 |
| H | 4.4439250000 | -3.5932380000 | 1.8321350000 |
| H | 2.3952070000 | -2.5153890000 | 2.8065060000 |
| C | 0.9781530000 | -0.4812500000 | 1.8326150000 |
| O | 2.0374880000 | 0.2966740000 | -0.7033250000 |
| O | 4.2599360000 | -0.7696980000 | -1.7627300000 |
| C | 5.3649300000 | -1.3901520000 | -2.3856480000 |
| H | 6.2682690000 | -1.3005710000 | -1.7740570000 |
| H | 5.5128820000 | -0.8684540000 | -3.3288090000 |
| H | 5.1625050000 | -2.4475350000 | -2.5824910000 |
| O | 0.5492480000 | -0.9018660000 | 2.9214330000 |
| C | 2.6959590000 | 1.5516720000 | -0.8292760000 |
| H | 3.7540290000 | 1.4085060000 | -1.0588150000 |
| C | 2.5394110000 | 2.3790300000 | 0.3723500000 |
| H | 2.2231800000 | 2.0514560000 | -1.6775640000 |
| C | 2.3997400000 | 3.0468240000 | 1.3592560000 |
| H | 2.2714660000 | 3.6228460000 | 2.2445010000 |
| N | -1.3226740000 | -0.1500080000 | -0.0494910000 |
| C | -0.3911480000 | -0.9633270000 | 0.4519240000 |
| S | -0.9640730000 | -2.5636420000 | 0.3229280000 |
| C | -2.4657260000 | -2.0865600000 | -0.4186210000 |
| C | -2.5013840000 | -0.7416180000 | -0.5436820000 |
| C | -1.1097150000 | 1.2806210000 | -0.0535720000 |
| C | -1.3708740000 | 1.9929910000 | 1.1161600000 |
| C | -1.1288960000 | 3.3662620000 | 1.0958670000 |
| C | -0.6465140000 | 4.0092060000 | -0.0411160000 |
| C | -0.4356020000 | 3.2595970000 | -1.1973450000 |
| C | -0.6607720000 | 1.8859320000 | -1.2273330000 |
| C | -1.8833810000 | 1.2961210000 | 2.3477110000 |
| H | -1.3146540000 | 3.9421050000 | 1.9974570000 |
| C | -0.3098580000 | 5.4761550000 | -0.0135970000 |
| H | -0.0758700000 | 3.7536530000 | -2.0956170000 |
| C | -0.4329370000 | 1.0714600000 | -2.4720140000 |
| C | -3.5414930000 | -3.0565440000 | -0.8101630000 |
| C | -4.8909700000 | -2.7650660000 | -0.1402050000 |

| | | | |
|---|---|---|---|
| H | -3.2187380000 | -4.0673050000 | -0.5511500000 |
| H | -3.6656170000 | -3.0398690000 | -1.8999590000 |
| C | -5.6190480000 | -1.5287360000 | -0.6775750000 |
| H | -4.7381400000 | -2.6664170000 | 0.9397110000 |
| H | -5.5385490000 | -3.6335610000 | -0.2917140000 |
| H | -6.6289090000 | -1.5191810000 | -0.2573740000 |
| C | -3.6330670000 | 0.0725070000 | -1.0980290000 |
| H | -3.3734870000 | 1.1313540000 | -1.0339210000 |
| C | -4.9678970000 | -0.1740700000 | -0.3805080000 |
| H | -3.7518990000 | -0.1593340000 | -2.1639920000 |
| H | -5.6628210000 | 0.6124170000 | -0.6882100000 |
| H | -5.7408950000 | -1.6326140000 | -1.7635720000 |
| H | -4.8213030000 | -0.0612920000 | 0.6989110000 |
| H | -1.3689180000 | 0.6330270000 | -2.8319030000 |
| H | 0.2648800000 | 0.2557860000 | -2.2687550000 |
| H | -0.0267460000 | 1.6951910000 | -3.2692900000 |
| H | -1.1289760000 | 0.6253470000 | 2.7753020000 |
| H | -2.7579350000 | 0.6830280000 | 2.1098210000 |
| H | -2.1725650000 | 2.0263580000 | 3.1037470000 |
| H | -0.5250870000 | 5.9520140000 | -0.9719550000 |
| H | 0.7574360000 | 5.6067790000 | 0.1900120000 |
| H | -0.8673030000 | 5.9982800000 | 0.7653200000 |
| H | 0.9053920000 | 0.5873870000 | 1.5732600000 |

Thermochemie

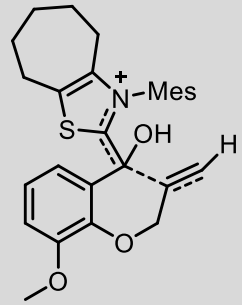
Zero-point correction= 0.530668 (Hartree/Particle)
Thermal correction to Energy= 0.562627
Thermal correction to Enthalpy= 0.563571
Thermal correction to Gibbs Free Energy= 0.467096
Sum of electronic and zero-point Energies= -1763.374920
Sum of electronic and thermal Energies= -1763.342961
Sum of electronic and thermal Enthalpies= -1763.342017
Sum of electronic and thermal Free Energies= -1763.438491

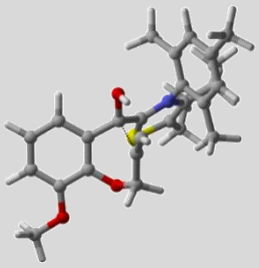
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 353.054 | 122.402 | 203.048 |

Imaginäre Frequenz

-158.3316

**TS-3a**



64

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0736770000 | -0.3315270000 | 1.3552910000 |
| C | -4.2228610000 | -0.8086340000 | 2.3560350000 |
| C | -2.8726550000 | -0.9915140000 | 2.1161110000 |
| C | -2.3483410000 | -0.6815090000 | 0.8578810000 |
| C | -3.1990970000 | -0.2476130000 | -0.1539390000 |
| C | -4.5688800000 | -0.0578140000 | 0.0874850000 |
| H | -6.1246390000 | -0.1941960000 | 1.5702270000 |
| H | -4.6353130000 | -1.0334690000 | 3.3324840000 |

| | | | |
|---|---|---|---|
| H | -2.2046950000 | -1.3728720000 | 2.8777310000 |
| C | -0.9066590000 | -0.8763060000 | 0.5417600000 |
| O | -5.3065180000 | 0.3713240000 | -0.9672600000 |
| C | -6.6902580000 | 0.5489310000 | -0.7598770000 |
| H | -7.1724290000 | -0.3905220000 | -0.4701710000 |
| H | -7.0959530000 | 0.8868220000 | -1.7111170000 |
| H | -6.8821580000 | 1.3066670000 | 0.0068890000 |
| O | -0.2408320000 | -1.8045100000 | 1.2783440000 |
| H | -0.1745270000 | -2.6066030000 | 0.6302980000 |
| N | 1.2100400000 | 0.3363980000 | 0.0669430000 |
| C | -0.1406960000 | 0.2804900000 | 0.2162830000 |
| S | -0.8133550000 | 1.8596390000 | -0.0112300000 |
| C | 0.7639410000 | 2.5578150000 | -0.2811770000 |
| C | 1.7237640000 | 1.6167420000 | -0.2041460000 |
| C | 2.0622460000 | -0.8294540000 | 0.0261330000 |
| C | 2.6775580000 | -1.2496870000 | 1.2099950000 |
| C | 3.5264770000 | -2.3450660000 | 1.1445710000 |
| C | 3.7689730000 | -3.0129200000 | -0.0597520000 |
| C | 3.1577140000 | -2.5449860000 | -1.2149870000 |
| C | 2.2980440000 | -1.4430420000 | -1.1987070000 |
| C | 2.3929160000 | -0.5406700000 | 2.5032750000 |
| H | 4.0064320000 | -2.6941270000 | 2.0538700000 |
| C | 4.6559490000 | -4.2303560000 | -0.0890310000 |
| H | 3.3433930000 | -3.0464440000 | -2.1604680000 |
| C | 1.6870530000 | -0.9512240000 | -2.4843410000 |
| C | 0.9164910000 | 4.0176690000 | -0.5965340000 |
| C | 1.9152380000 | 4.7467290000 | 0.3097460000 |
| H | -0.0611920000 | 4.4984900000 | -0.5125170000 |
| H | 1.2255940000 | 4.1320580000 | -1.6430480000 |
| C | 3.3805350000 | 4.3752980000 | 0.0708690000 |
| H | 1.6517520000 | 4.5584220000 | 1.3559820000 |
| H | 1.8003680000 | 5.8212660000 | 0.1403790000 |
| H | 4.0060460000 | 5.0762900000 | 0.6311580000 |
| C | 3.1968190000 | 1.8355390000 | -0.4005680000 |
| H | 3.7239880000 | 0.9036830000 | -0.1920650000 |
| C | 3.7826710000 | 2.9539400000 | 0.4715090000 |
| H | 3.3826390000 | 2.0659440000 | -1.4573930000 |
| H | 4.8722740000 | 2.8786950000 | 0.4131980000 |
| H | 3.6208790000 | 4.5289280000 | -0.9888960000 |
| H | 3.5108830000 | 2.7744090000 | 1.5173990000 |
| H | 1.1925840000 | -1.7768080000 | -2.9999160000 |
| H | 2.4624990000 | -0.5490740000 | -3.1429200000 |
| H | 0.9432710000 | -0.1721190000 | -2.3146660000 |
| H | 1.3476160000 | -0.7015670000 | 2.7787650000 |
| H | 2.5532890000 | 0.5375440000 | 2.4091920000 |
| H | 3.0340070000 | -0.9171370000 | 3.3003810000 |
| H | 4.0869270000 | -5.1215140000 | 0.1898910000 |
| H | 5.4827250000 | -4.1318210000 | 0.6165540000 |
| H | 5.0693710000 | -4.3954260000 | -1.0848970000 |
| C | -1.1798240000 | -1.9199480000 | -1.1528290000 |
| C | -2.0178750000 | -1.0628940000 | -2.0371150000 |
| H | -1.3995920000 | -0.5887810000 | -2.8034910000 |
| O | -2.6970390000 | 0.0229750000 | -1.3955000000 |
| H | -2.7617670000 | -1.6952960000 | -2.5322840000 |
| C | -0.6461670000 | -3.0392310000 | -0.9720450000 |
| H | -0.5421720000 | -4.0213100000 | -1.3955160000 |

Thermochemie

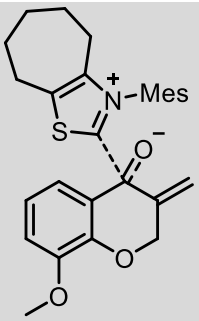
Zero-point correction= 0.530492 (Hartree/Particle)
Thermal correction to Energy= 0.561398
Thermal correction to Enthalpy= 0.562342
Thermal correction to Gibbs Free Energy= 0.469225

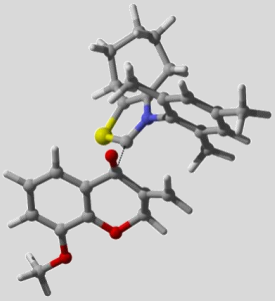
Sum of electronic and zero-point Energies= -1763.379222
Sum of electronic and thermal Energies= -1763.348316
Sum of electronic and thermal Enthalpies= -1763.347371
Sum of electronic and thermal Free Energies= -1763.440489

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 352.283 | 121.031 | 195.983 |

Imaginäre Frequenz
-475.8346

**TS-4a**



64
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -4.9191600000 | 0.8375850000 | 1.1565080000 |
| C | -3.9031890000 | 1.0681090000 | 2.0919720000 |
| C | -2.6700760000 | 0.4689160000 | 1.9380780000 |
| C | -2.4145890000 | -0.3556480000 | 0.8378000000 |
| C | -3.4224920000 | -0.5960010000 | -0.0905160000 |
| C | -4.6910050000 | 0.0038880000 | 0.0725660000 |
| H | -5.8848760000 | 1.3061060000 | 1.2918690000 |
| H | -4.1021270000 | 1.7081220000 | 2.9430330000 |
| H | -1.8764440000 | 0.5932110000 | 2.6656630000 |
| C | -1.0500120000 | -1.0496960000 | 0.7382980000 |
| O | -5.6095290000 | -0.3024350000 | -0.8792790000 |
| C | -6.9014050000 | 0.2395610000 | -0.7281060000 |
| H | -7.3613250000 | -0.0877000000 | 0.2102660000 |
| H | -7.4848820000 | -0.1338560000 | -1.5670900000 |
| H | -6.8804800000 | 1.3342170000 | -0.7591100000 |
| O | -0.4328700000 | -1.2839780000 | 1.8076220000 |
| N | 1.2660680000 | 0.3434620000 | -0.1923940000 |
| C | -0.0657530000 | 0.3216760000 | -0.1259750000 |
| S | -0.6481060000 | 1.9005090000 | -0.3929170000 |
| C | 0.9449780000 | 2.5637750000 | -0.6138850000 |
| C | 1.8691780000 | 1.5873990000 | -0.4610220000 |
| C | 2.0482480000 | -0.8694300000 | -0.0512770000 |
| C | 2.5850350000 | -1.1826730000 | 1.1977490000 |
| C | 3.3217730000 | -2.3594470000 | 1.2960500000 |
| C | 3.5317210000 | -3.1915380000 | 0.1966230000 |
| C | 3.0081370000 | -2.8154260000 | -1.0374560000 |
| C | 2.2591440000 | -1.6492750000 | -1.1849140000 |
| C | 2.3685980000 | -0.2841430000 | 2.3814880000 |
| H | 3.7398910000 | -2.6343130000 | 2.2594560000 |
| C | 4.2947590000 | -4.4812000000 | 0.3513940000 |
| H | 3.1792820000 | -3.4436170000 | -1.9062320000 |
| C | 1.6681030000 | -1.2687060000 | -2.5145830000 |
| C | 1.1746970000 | 4.0121380000 | -0.9361260000 |
| C | 2.1636880000 | 4.7117670000 | 0.0031820000 |
| H | 0.2155590000 | 4.5342530000 | -0.9046680000 |
| H | 1.5366140000 | 4.0945310000 | -1.9683930000 |
| C | 3.6211540000 | 4.2780530000 | -0.1687360000 |

| | | | |
|---|---|---|---|
| H | 1.8489770000 | 4.5507840000 | 1.0396460000 |
| H | 2.0990290000 | 5.7871720000 | -0.1850320000 |
| H | 4.2516220000 | 4.9698710000 | 0.3971140000 |
| C | 3.3596820000 | 1.7316620000 | -0.5730150000 |
| H | 3.8259930000 | 0.7837460000 | -0.2982640000 |
| C | 3.9495430000 | 2.8553870000 | 0.2904520000 |
| H | 3.6184840000 | 1.9131840000 | -1.6239120000 |
| H | 5.0363450000 | 2.7349980000 | 0.2848520000 |
| H | 3.9087780000 | 4.3926130000 | -1.2216550000 |
| H | 3.6247750000 | 2.7224690000 | 1.3277480000 |
| H | 1.7769380000 | -0.2005340000 | -2.7187830000 |
| H | 0.5995600000 | -1.5003730000 | -2.5266230000 |
| H | 2.1464990000 | -1.8255860000 | -3.3204600000 |
| H | 1.3091250000 | -0.3070030000 | 2.6510150000 |
| H | 2.6473980000 | 0.7483130000 | 2.1495680000 |
| H | 2.9665350000 | -0.6172390000 | 3.2298460000 |
| H | 5.1082460000 | -4.3733490000 | 1.0707150000 |
| H | 4.7150850000 | -4.8101680000 | -0.5999480000 |
| H | 3.6331500000 | -5.2716880000 | 0.7162790000 |
| C | -1.0922450000 | -2.0910550000 | -0.3664010000 |
| C | -1.9516830000 | -1.7277240000 | -1.5402070000 |
| H | -1.5470970000 | -0.8438350000 | -2.0527770000 |
| O | -3.2917170000 | -1.4234450000 | -1.1596550000 |
| H | -2.0224320000 | -2.5484750000 | -2.2539900000 |
| C | -0.4405720000 | -3.2393340000 | -0.2409610000 |
| H | 0.1640980000 | -3.4116910000 | 0.6443830000 |
| H | -0.4897090000 | -4.0094070000 | -1.0044880000 |

Thermochemie

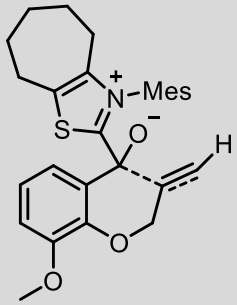
Zero-point correction= 0.532562 (Hartree/Particle)
Thermal correction to Energy= 0.563389
Thermal correction to Enthalpy= 0.564333
Thermal correction to Gibbs Free Energy= 0.470083
Sum of electronic and zero-point Energies= -1763.434226
Sum of electronic and thermal Energies= -1763.403400
Sum of electronic and thermal Enthalpies= -1763.402455
Sum of electronic and thermal Free Energies= -1763.496705

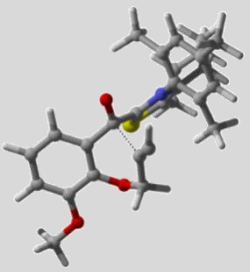
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 353.532 | 119.821 | 198.365 |

Imaginäre Frequenz

-191.4191

**TS-7a**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.1126030000 | -0.3463330000 | 1.2690220000 |
| C | -4.2995610000 | -0.7809590000 | 2.3188400000 |
| C | -2.9453650000 | -0.9902750000 | 2.1280930000 |
| C | -2.3785320000 | -0.7485620000 | 0.8750020000 |

| | | | |
|---|---|---|---|
| C | -3.1884760000 | -0.3433220000 | -0.1813760000 |
| C | -4.5645280000 | -0.1353720000 | 0.0071090000 |
| H | -6.1690740000 | -0.1919900000 | 1.4422710000 |
| H | -4.7453060000 | -0.9552030000 | 3.2911640000 |
| H | -2.2937140000 | -1.3438450000 | 2.9170000000 |
| C | -0.8908550000 | -0.9892450000 | 0.6904870000 |
| O | -5.2642470000 | 0.2549990000 | -1.0887120000 |
| C | -6.6544850000 | 0.4368390000 | -0.9368320000 |
| H | -7.1442910000 | -0.4910440000 | -0.6235880000 |
| H | -7.0280170000 | 0.7319120000 | -1.9150540000 |
| H | -6.8750160000 | 1.2261160000 | -0.2104970000 |
| O | -0.2713000000 | -1.6616180000 | 1.5664800000 |
| N | 1.1730530000 | 0.3275560000 | 0.0490860000 |
| C | -0.1539130000 | 0.2497240000 | 0.2329570000 |
| S | -0.8590460000 | 1.7984110000 | 0.0673550000 |
| C | 0.6734470000 | 2.5362040000 | -0.2689500000 |
| C | 1.6596060000 | 1.6105940000 | -0.2368930000 |
| C | 2.0557290000 | -0.8229020000 | 0.0145280000 |
| C | 2.6773510000 | -1.2284200000 | 1.2000930000 |
| C | 3.5613810000 | -2.2955470000 | 1.1229460000 |
| C | 3.8338390000 | -2.9414250000 | -0.0866750000 |
| C | 3.2211480000 | -2.4767400000 | -1.2427390000 |
| C | 2.3277530000 | -1.4024660000 | -1.2192260000 |
| C | 2.3914760000 | -0.5312950000 | 2.4982550000 |
| H | 4.0496930000 | -2.6370460000 | 2.0305870000 |
| C | 4.7721130000 | -4.1195120000 | -0.1201750000 |
| H | 3.4325570000 | -2.9562500000 | -2.1938690000 |
| C | 1.7231750000 | -0.9100100000 | -2.5081440000 |
| C | 0.7957500000 | 4.0028530000 | -0.5655340000 |
| C | 1.8018350000 | 4.7325950000 | 0.3330310000 |
| H | -0.1878080000 | 4.4663930000 | -0.4585280000 |
| H | 1.0846650000 | 4.1323100000 | -1.6157410000 |
| C | 3.2684560000 | 4.3942330000 | 0.0538590000 |
| H | 1.5650510000 | 4.5206120000 | 1.3810870000 |
| H | 1.6622700000 | 5.8073630000 | 0.1866940000 |
| H | 3.8920530000 | 5.0933300000 | 0.6183110000 |
| C | 3.1198540000 | 1.8639290000 | -0.4754370000 |
| H | 3.6707650000 | 0.9376580000 | -0.3082690000 |
| C | 3.7061380000 | 2.9719130000 | 0.4104190000 |
| H | 3.2656140000 | 2.1266350000 | -1.5307750000 |
| H | 4.7948540000 | 2.9180110000 | 0.3240820000 |
| H | 3.4829570000 | 4.5789970000 | -1.0063520000 |
| H | 3.4638030000 | 2.7611600000 | 1.4576460000 |
| H | 0.9561430000 | -0.1520760000 | -2.3460420000 |
| H | 1.2570940000 | -1.7428660000 | -3.0385810000 |
| H | 2.4989580000 | -0.4833660000 | -3.1508050000 |
| H | 1.3604250000 | -0.7486890000 | 2.7883290000 |
| H | 2.4982070000 | 0.5535510000 | 2.3971850000 |
| H | 3.0742040000 | -0.8727380000 | 3.2763350000 |
| H | 5.6902790000 | -3.9037700000 | 0.4301910000 |
| H | 5.0385440000 | -4.3848510000 | -1.1438280000 |
| H | 4.3063880000 | -4.9921750000 | 0.3449450000 |
| C | -1.0213440000 | -1.9004690000 | -0.9834840000 |
| C | -1.9411880000 | -1.2395510000 | -1.9618930000 |
| H | -1.3799560000 | -0.8296960000 | -2.8046510000 |
| O | -2.6545270000 | -0.1219020000 | -1.4192330000 |
| H | -2.6644730000 | -1.9662790000 | -2.3430650000 |
| C | -0.3996080000 | -3.0070290000 | -0.9879530000 |
| H | 0.2655460000 | -3.5781510000 | -0.3617120000 |

Thermochemie

Zero-point correction= 0.518972 (Hartree/Particle)

Thermal correction to Energy= 0.549753
Thermal correction to Enthalpy= 0.550697
Thermal correction to Gibbs Free Energy= 0.457490
Sum of electronic and zero-point Energies= -1762.759504
Sum of electronic and thermal Energies= -1762.728723
Sum of electronic and thermal Enthalpies= -1762.727779
Sum of electronic and thermal Free Energies= -1762.820986

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 344.975 | 120.462 | 196.171 |

Imaginäre Frequenz
-661.4438

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(u)M06-2X/6-311+G** SCRF=(PCM,Solvent=Tetrahydrofuran)

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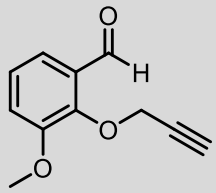
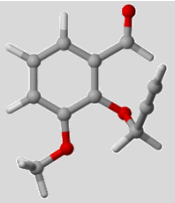
**19a**



24
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.7485080000 | -1.4569120000 | 0.5012870000 |
| C | 0.7644790000 | -2.4307060000 | 0.7007430000 |
| C | -0.5420630000 | -2.1993040000 | 0.3187530000 |
| C | -0.8853380000 | -0.9762950000 | -0.2703860000 |
| C | 0.0895810000 | -0.0042050000 | -0.4779370000 |
| C | 1.4213380000 | -0.2410110000 | -0.0885630000 |
| H | 2.7669060000 | -1.6614950000 | 0.8035710000 |
| H | 1.0416950000 | -3.3719890000 | 1.1589080000 |
| H | -1.3164630000 | -2.9419150000 | 0.4658420000 |
| C | -2.2897830000 | -0.7147900000 | -0.6733810000 |
| O | -0.2316380000 | 1.1744310000 | -1.0976100000 |
| O | 2.2937450000 | 0.7628060000 | -0.3364890000 |
| C | 3.6518960000 | 0.5595860000 | 0.0286490000 |
| H | 3.7467380000 | 0.4047360000 | 1.1065260000 |
| H | 4.1770340000 | 1.4667700000 | -0.2582600000 |
| H | 4.0740720000 | -0.2943340000 | -0.5072650000 |
| O | -3.1884830000 | -1.4995610000 | -0.4735940000 |
| H | -2.4785510000 | 0.2461780000 | -1.1737910000 |
| C | -0.2763710000 | 2.3121040000 | -0.2279200000 |
| H | 0.6713270000 | 2.4128050000 | 0.3059010000 |
| C | -1.3927790000 | 2.2168940000 | 0.7188980000 |
| H | -0.4053100000 | 3.1751810000 | -0.8801780000 |
| C | -2.3125830000 | 2.1089260000 | 1.4827130000 |
| H | -3.1277580000 | 2.0169410000 | 2.1631520000 |

Thermochemie
Zero-point correction= 0.186050 (Hartree/Particle)
Thermal correction to Energy= 0.199256
Thermal correction to Enthalpy= 0.200200
Thermal correction to Gibbs Free Energy= 0.145550
Sum of electronic and zero-point Energies= -650.492740
Sum of electronic and thermal Energies= -650.479534
Sum of electronic and thermal Enthalpies= -650.478590
Sum of electronic and thermal Free Energies= -650.533241

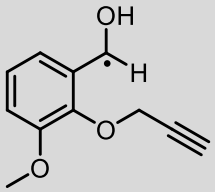
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 125.035 | 48.668 | 115.021 |

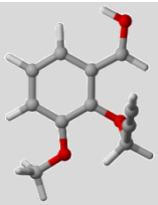
Volumen

Molar volume = 1705.805 bohr**3/mol (152.224 cm**3/mol)

Recommended a0 for SCRF calculation = 4.82 angstrom ( 9.10 bohr)

**25a**



25

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.6020710000 | -1.6027720000 | 0.5398490000 |
| C | 0.5193580000 | -2.4580940000 | 0.7660050000 |
| C | -0.7598260000 | -2.1204800000 | 0.3776110000 |
| C | -1.0144770000 | -0.8749420000 | -0.2569010000 |
| C | 0.0882460000 | -0.0125040000 | -0.4760730000 |
| C | 1.3807040000 | -0.3771400000 | -0.0942360000 |
| H | 2.5951370000 | -1.8992920000 | 0.8455820000 |
| H | 0.6956400000 | -3.4108240000 | 1.2510480000 |
| H | -1.5608760000 | -2.8274450000 | 0.5615370000 |
| C | -2.2949330000 | -0.4655030000 | -0.6770750000 |
| O | -0.1298280000 | 1.1736560000 | -1.1349890000 |
| O | 2.3571250000 | 0.5211760000 | -0.3849150000 |
| C | 3.6910580000 | 0.1801880000 | -0.0397710000 |
| H | 3.7932330000 | 0.0382620000 | 1.0392900000 |
| H | 4.3051000000 | 1.0197640000 | -0.3560920000 |
| H | 4.0098080000 | -0.7249110000 | -0.5632750000 |
| O | -3.4208070000 | -1.1854390000 | -0.4941940000 |
| H | -2.4645030000 | 0.4710160000 | -1.1835460000 |
| C | 0.0245520000 | 2.3494530000 | -0.3376400000 |
| H | 1.0342790000 | 2.3935470000 | 0.0755510000 |
| C | -0.9653680000 | 2.4227860000 | 0.7437860000 |
| H | -0.1098040000 | 3.1865790000 | -1.0226870000 |
| C | -1.7737410000 | 2.4818650000 | 1.6294650000 |
| H | -2.4921170000 | 2.5335190000 | 2.4147040000 |
| H | -3.2436770000 | -1.9925030000 | 0.0005560000 |

Thermochemie

Zero-point correction= 0.196090 (Hartree/Particle)

Thermal correction to Energy= 0.209911

Thermal correction to Enthalpy= 0.210855

Thermal correction to Gibbs Free Energy= 0.154426

Sum of electronic and zero-point Energies= -651.045251

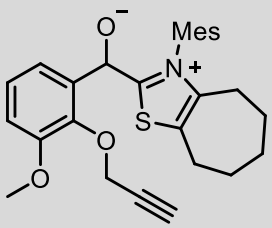
Sum of electronic and thermal Energies= -651.031430

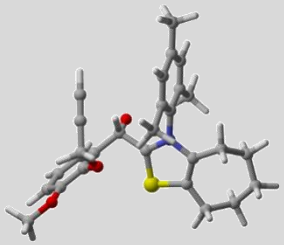
Sum of electronic and thermal Enthalpies= -651.030486

Sum of electronic and thermal Free Energies= -651.086914

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 131.721 | 51.612 | 118.764 |

**22a**



64

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.9575520000 | -0.7901780000 | 1.0829830000 |
| C | 4.2929190000 | -0.7335880000 | 2.3072950000 |
| C | 2.9630150000 | -0.3447070000 | 2.3757040000 |
| C | 2.2736630000 | 0.0101860000 | 1.2171680000 |
| C | 2.9384460000 | -0.0313850000 | -0.0032190000 |
| C | 4.2775920000 | -0.4488550000 | -0.0838880000 |
| H | 5.9909590000 | -1.1076270000 | 1.0457670000 |
| H | 4.8300050000 | -1.0014960000 | 3.2098100000 |
| H | 2.4213390000 | -0.2911690000 | 3.3116820000 |
| C | 0.8004630000 | 0.4485670000 | 1.3274450000 |
| O | 2.2473700000 | 0.2581010000 | -1.1640980000 |
| O | 4.8144250000 | -0.4982130000 | -1.3325230000 |
| C | 6.1687150000 | -0.9051170000 | -1.4482680000 |
| H | 6.8298860000 | -0.2234750000 | -0.9063120000 |
| H | 6.4020810000 | -0.8735470000 | -2.5096970000 |
| H | 6.3041500000 | -1.9232240000 | -1.0735910000 |
| O | 0.3115530000 | 0.4950950000 | 2.5748960000 |
| C | 2.6636880000 | 1.4456640000 | -1.8407070000 |
| H | 3.7510730000 | 1.4706770000 | -1.9302490000 |
| C | 2.1761760000 | 2.6602770000 | -1.1757110000 |
| H | 2.2392100000 | 1.3809430000 | -2.8437650000 |
| C | 1.7598320000 | 3.6475490000 | -0.6339780000 |
| H | 1.3874380000 | 4.5176640000 | -0.1443520000 |
| N | -1.2744190000 | -0.2837460000 | 0.0699780000 |
| C | -0.0627920000 | -0.5550130000 | 0.5448280000 |
| S | 0.2750280000 | -2.2125690000 | 0.4016060000 |
| C | -1.2755410000 | -2.5339650000 | -0.3151320000 |
| C | -1.9879230000 | -1.3878010000 | -0.4248030000 |
| C | -1.8066790000 | 1.0643050000 | 0.0627940000 |
| C | -2.5771520000 | 1.4770170000 | 1.1516010000 |
| C | -3.0728540000 | 2.7773300000 | 1.1204670000 |
| C | -2.8183430000 | 3.6358950000 | 0.0486880000 |
| C | -2.0612670000 | 3.1677090000 | -1.0230410000 |
| C | -1.5499760000 | 1.8702500000 | -1.0436470000 |
| C | -2.8517780000 | 0.5400980000 | 2.2936240000 |
| H | -3.6685190000 | 3.1302980000 | 1.9567690000 |
| C | -3.3804680000 | 5.0337020000 | 0.0469470000 |
| H | -1.8601420000 | 3.8229030000 | -1.8649310000 |
| C | -0.7874060000 | 1.3421160000 | -2.2274450000 |
| C | -1.6667970000 | -3.9133260000 | -0.7602130000 |
| C | -3.0251440000 | -4.3772440000 | -0.2213770000 |
| H | -0.8927150000 | -4.6165670000 | -0.4460170000 |
| H | -1.6829040000 | -3.9372850000 | -1.8561250000 |
| C | -4.2312420000 | -3.6602940000 | -0.8319100000 |
| H | -3.0385500000 | -4.2653460000 | 0.8678380000 |
| H | -3.1147730000 | -5.4459330000 | -0.4329100000 |
| H | -5.1342860000 | -4.1992240000 | -0.5324560000 |
| C | -3.3581170000 | -1.2297590000 | -1.0148760000 |
| H | -3.6896330000 | -0.2011840000 | -0.8607380000 |
| C | -4.4022270000 | -2.1927120000 | -0.4331080000 |
| H | -3.2917970000 | -1.3795580000 | -2.0993970000 |
| H | -5.3822860000 | -1.8535650000 | -0.7781620000 |

| | | | |
|---|---|---|---|
| H | -4.1769490000 | -3.7325350000 | -1.9253410000 |
| H | -4.4046730000 | -2.1071840000 | 0.6586350000 |
| H | -1.4266490000 | 0.6856500000 | -2.8274550000 |
| H | 0.0807000000 | 0.7605270000 | -1.9130880000 |
| H | -0.4524600000 | 2.1624270000 | -2.8626790000 |
| H | -1.8985970000 | 0.2410000000 | 2.7410260000 |
| H | -3.3690130000 | -0.3585980000 | 1.9427490000 |
| H | -3.4775240000 | 1.0231520000 | 3.0437910000 |
| H | -4.4525430000 | 5.0148090000 | -0.1666650000 |
| H | -2.8973870000 | 5.6523270000 | -0.7098380000 |
| H | -3.2478040000 | 5.5084650000 | 1.0208130000 |
| H | 0.7179120000 | 1.3938250000 | 0.7538050000 |

Thermochemie

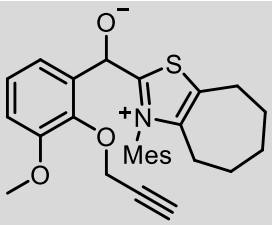
Zero-point correction= 0.531918 (Hartree/Particle)
Thermal correction to Energy= 0.564111
Thermal correction to Enthalpy= 0.565055
Thermal correction to Gibbs Free Energy= 0.467937
Sum of electronic and zero-point Energies= -1763.406671
Sum of electronic and thermal Energies= -1763.374479
Sum of electronic and thermal Enthalpies= -1763.373535
Sum of electronic and thermal Free Energies= -1763.470652

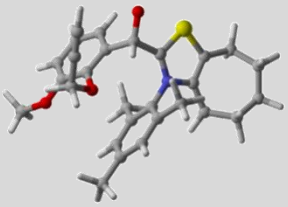
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 353.985 | 123.164 | 204.402 |

Volumen

Molar volume = 4101.568 bohr**3/mol (366.020 cm**3/mol)
Recommended a0 for SCRF calculation = 6.28 angstrom ( 11.87 bohr)

**22a (anti)**



64

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 3.0651010000 | -1.5646520000 | -2.2471610000 |
| C | 2.0780650000 | -2.5533040000 | -2.1986760000 |
| C | 1.1990080000 | -2.6191520000 | -1.1326350000 |
| C | 1.2871410000 | -1.7010680000 | -0.0802520000 |
| C | 2.2849630000 | -0.7356490000 | -0.1091740000 |
| C | 3.1705190000 | -0.6517030000 | -1.2040030000 |
| H | 3.7363350000 | -1.5167000000 | -3.0938620000 |
| H | 2.0063170000 | -3.2669790000 | -3.0110630000 |
| H | 0.4352110000 | -3.3868370000 | -1.0807060000 |
| C | 0.2592920000 | -1.7967350000 | 1.0693300000 |
| O | 2.3749050000 | 0.2054180000 | 0.8886950000 |
| O | 4.0773430000 | 0.3591210000 | -1.1517820000 |
| C | 4.9653190000 | 0.4986040000 | -2.2483720000 |
| H | 5.5910780000 | -0.3905000000 | -2.3631970000 |
| H | 5.5916560000 | 1.3576980000 | -2.0207510000 |
| H | 4.4148840000 | 0.6818580000 | -3.1754390000 |
| O | 0.0126850000 | -3.0408770000 | 1.4986090000 |
| C | 3.5071180000 | 0.0796230000 | 1.7435250000 |
| H | 4.4281900000 | 0.0490310000 | 1.1569420000 |
| C | 3.4189030000 | -1.1053000000 | 2.6054770000 |
| H | 3.5154160000 | 0.9843080000 | 2.3528300000 |

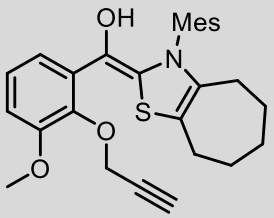
| | | | |
|---|---|---|---|
| C | 3.3302830000 | -2.0815670000 | 3.2986790000 |
| H | 3.2442640000 | -2.9523230000 | 3.9066900000 |
| N | -1.3779970000 | -0.0058250000 | 0.0627300000 |
| C | -1.0520150000 | -1.2193520000 | 0.4966380000 |
| S | -2.3523840000 | -2.2966810000 | 0.3572510000 |
| C | -3.3583170000 | -1.0611060000 | -0.3345510000 |
| C | -2.6914250000 | 0.1153870000 | -0.4176610000 |
| C | -0.4579380000 | 1.1090530000 | 0.1413600000 |
| C | -0.3370830000 | 1.7731270000 | 1.3601930000 |
| C | 0.5487140000 | 2.8476620000 | 1.4175430000 |
| C | 1.2880740000 | 3.2435130000 | 0.3053530000 |
| C | 1.1105510000 | 2.5621860000 | -0.8993850000 |
| C | 0.2352970000 | 1.4868870000 | -1.0094670000 |
| C | -1.1312670000 | 1.3433310000 | 2.5649000000 |
| H | 0.6633700000 | 3.3828150000 | 2.3550840000 |
| C | 2.2900580000 | 4.3629530000 | 0.4051940000 |
| H | 1.6737390000 | 2.8709340000 | -1.7747610000 |
| C | 0.0382050000 | 0.7602730000 | -2.3121100000 |
| C | -4.7810500000 | -1.3206190000 | -0.7363730000 |
| C | -5.7887360000 | -0.3889890000 | -0.0490830000 |
| H | -5.0294600000 | -2.3586750000 | -0.5063520000 |
| H | -4.8678540000 | -1.2128110000 | -1.8238480000 |
| C | -5.7638980000 | 1.0593060000 | -0.5456110000 |
| H | -5.6211580000 | -0.4149710000 | 1.0327670000 |
| H | -6.7884420000 | -0.7943440000 | -0.2254960000 |
| H | -6.6289950000 | 1.5776730000 | -0.1231650000 |
| C | -3.2324660000 | 1.4195220000 | -0.9222990000 |
| H | -2.4639640000 | 2.1875530000 | -0.8186440000 |
| C | -4.5111320000 | 1.8691380000 | -0.2000390000 |
| H | -3.4403940000 | 1.3220870000 | -1.9944500000 |
| H | -4.6919370000 | 2.9121690000 | -0.4718460000 |
| H | -5.9019050000 | 1.0655740000 | -1.6338700000 |
| H | -4.3416870000 | 1.8488510000 | 0.8817640000 |
| H | -0.9900220000 | 0.8667360000 | -2.6713040000 |
| H | 0.2420490000 | -0.3082440000 | -2.2012000000 |
| H | 0.7067490000 | 1.1607450000 | -3.0740210000 |
| H | -0.7541300000 | 0.3983780000 | 2.9663230000 |
| H | -2.1852080000 | 1.1935420000 | 2.3161960000 |
| H | -1.0658040000 | 2.0941410000 | 3.3515550000 |
| H | 2.0459040000 | 5.0424250000 | 1.2225640000 |
| H | 2.3379570000 | 4.9346440000 | -0.5228230000 |
| H | 3.2875220000 | 3.9556360000 | 0.5945400000 |
| H | 0.5872470000 | -1.0742370000 | 1.8422020000 |

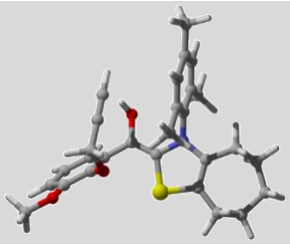
Thermochemie

Zero-point correction= 0.532110 (Hartree/Particle)
Thermal correction to Energy= 0.564218
Thermal correction to Enthalpy= 0.565163
Thermal correction to Gibbs Free Energy= 0.468799
Sum of electronic and zero-point Energies= -1763.408439
Sum of electronic and thermal Energies= -1763.376331
Sum of electronic and thermal Enthalpies= -1763.375387
Sum of electronic and thermal Free Energies= -1763.471750

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 354.052 | 123.203 | 202.814 |

**23a**



64

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 5.0419500000 | -0.6133430000 | 1.3219130000 |
| C | 4.2773440000 | -0.4489450000 | 2.4799980000 |
| C | 2.9209440000 | -0.1949690000 | 2.4041570000 |
| C | 2.2820430000 | -0.1000070000 | 1.1563740000 |
| C | 3.0499020000 | -0.2388530000 | 0.0015570000 |
| C | 4.4306600000 | -0.5046710000 | 0.0782230000 |
| H | 6.1002590000 | -0.8200990000 | 1.4026160000 |
| H | 4.7604110000 | -0.5321480000 | 3.4463460000 |
| H | 2.3294060000 | -0.0700560000 | 3.3029910000 |
| C | 0.8391840000 | 0.2022370000 | 1.1006080000 |
| O | 2.4727640000 | -0.1097770000 | -1.2394240000 |
| O | 5.0710240000 | -0.6164750000 | -1.1123650000 |
| C | 6.4675930000 | -0.8666970000 | -1.0846460000 |
| H | 6.9999950000 | -0.0583610000 | -0.5761460000 |
| H | 6.7838000000 | -0.9152740000 | -2.1236900000 |
| H | 6.6836610000 | -1.8181510000 | -0.5915190000 |
| O | 0.4215350000 | 1.2994360000 | 1.8397120000 |
| C | 2.7160810000 | 1.1512840000 | -1.8567740000 |
| H | 3.7900540000 | 1.3537180000 | -1.8908010000 |
| C | 2.0151320000 | 2.2606050000 | -1.1902010000 |
| H | 2.3477370000 | 1.0582310000 | -2.8793980000 |
| C | 1.4414600000 | 3.1955190000 | -0.6986710000 |
| H | 0.9262170000 | 4.0286220000 | -0.2767600000 |
| H | 0.7252850000 | 2.0964350000 | 1.3848440000 |
| N | -1.4468380000 | -0.2944800000 | 0.3683680000 |
| C | -0.0792570000 | -0.5771530000 | 0.4955230000 |
| S | 0.2697380000 | -2.1751100000 | -0.1898130000 |
| C | -1.4513100000 | -2.4291640000 | -0.5334780000 |
| C | -2.1820600000 | -1.3599830000 | -0.2017750000 |
| C | -1.8689380000 | 1.0647120000 | 0.1465870000 |
| C | -2.5449870000 | 1.7430860000 | 1.1650240000 |
| C | -2.9443230000 | 3.0559390000 | 0.9307970000 |
| C | -2.6832350000 | 3.6953410000 | -0.2833960000 |
| C | -2.0126210000 | 2.9868590000 | -1.2775880000 |
| C | -1.6021820000 | 1.6662010000 | -1.0857810000 |
| C | -2.8076490000 | 1.0640290000 | 2.4802840000 |
| H | -3.4660600000 | 3.5963130000 | 1.7155540000 |
| C | -3.1479260000 | 5.1095870000 | -0.5207690000 |
| H | -1.8009660000 | 3.4698180000 | -2.2273710000 |
| C | -0.9055640000 | 0.9002190000 | -2.1788310000 |
| C | -1.9401000000 | -3.7314580000 | -1.0980990000 |
| C | -2.9950450000 | -4.4172310000 | -0.2197280000 |
| H | -1.0900830000 | -4.4046430000 | -1.2304820000 |
| H | -2.3600160000 | -3.5639490000 | -2.0982230000 |
| C | -4.3672120000 | -3.7375770000 | -0.2283320000 |
| H | -2.6177900000 | -4.4815670000 | 0.8064510000 |
| H | -3.1220620000 | -5.4429660000 | -0.5786840000 |
| H | -5.0738810000 | -4.3876540000 | 0.2962200000 |
| C | -3.6731010000 | -1.2507070000 | -0.3508290000 |
| H | -3.9949960000 | -0.2686640000 | 0.0006110000 |
| C | -4.4406750000 | -2.3449860000 | 0.4056850000 |
| H | -3.9342530000 | -1.2988790000 | -1.4153570000 |

| | | | |
|---|---|---|---|
| H | -5.4928420000 | -2.0482220000 | 0.4496510000 |
| H | -4.7220130000 | -3.6710150000 | -1.2647400000 |
| H | -4.0787170000 | -2.3871860000 | 1.4388970000 |
| H | -1.5400120000 | 0.0852480000 | -2.5418010000 |
| H | 0.0214590000 | 0.4499100000 | -1.8151340000 |
| H | -0.6711230000 | 1.5561360000 | -3.0179960000 |
| H | -1.8604230000 | 0.8086050000 | 2.9605780000 |
| H | -3.3608430000 | 0.1316390000 | 2.3385820000 |
| H | -3.3819740000 | 1.7117280000 | 3.1433380000 |
| H | -4.1891750000 | 5.1205870000 | -0.8553040000 |
| H | -2.5476620000 | 5.5985290000 | -1.2894050000 |
| H | -3.0905660000 | 5.7017130000 | 0.3941660000 |

Thermochemie

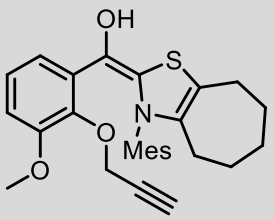
Zero-point correction= 0.531209 (Hartree/Particle)
Thermal correction to Energy= 0.563795
Thermal correction to Enthalpy= 0.564739
Thermal correction to Gibbs Free Energy= 0.467767
Sum of electronic and zero-point Energies= -1763.424977
Sum of electronic and thermal Energies= -1763.392390
Sum of electronic and thermal Enthalpies= -1763.391446
Sum of electronic and thermal Free Energies= -1763.488419

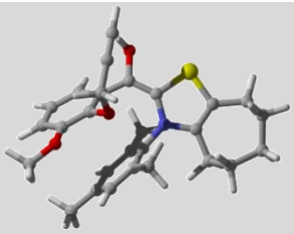
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 353.787 | 125.107 | 204.096 |

Volumen

Molar volume = 3901.102 bohr**3/mol (348.130 cm**3/mol)
Recommended a0 for SCRF calculation = 6.19 angstrom ( 11.69 bohr)

**23a (anti)**



64

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.0958650000 | 0.4571410000 | 0.5060530000 |
| C | 3.6787950000 | 1.0495420000 | 1.7014570000 |
| C | 2.3894840000 | 1.5293220000 | 1.8467300000 |
| C | 1.4730550000 | 1.4239320000 | 0.7871290000 |
| C | 1.9144640000 | 0.9044950000 | -0.4262570000 |
| C | 3.2132500000 | 0.3903650000 | -0.5673750000 |
| H | 5.0998600000 | 0.0630950000 | 0.4226270000 |
| H | 4.3762070000 | 1.1134190000 | 2.5284730000 |
| H | 2.0618580000 | 1.9640020000 | 2.7839680000 |
| C | 0.0790690000 | 1.8598980000 | 0.9509380000 |
| O | 1.0555690000 | 0.8415050000 | -1.4964990000 |
| O | 3.5079640000 | -0.1314940000 | -1.7851970000 |
| C | 4.7274880000 | -0.8444530000 | -1.9044670000 |
| H | 5.5884180000 | -0.1836390000 | -1.7705380000 |
| H | 4.7403490000 | -1.2551590000 | -2.9113560000 |
| H | 4.7694050000 | -1.6579520000 | -1.1737530000 |
| O | -0.1088640000 | 3.1300170000 | 1.4935920000 |
| C | 1.2384590000 | 1.8840640000 | -2.4453180000 |
| H | 2.2878030000 | 1.9384800000 | -2.7508320000 |
| C | 0.7963650000 | 3.1987370000 | -1.9524430000 |

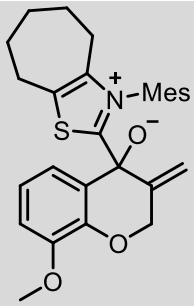
| | | | |
|---|---|---|---|
| H | 0.6408520000 | 1.6059430000 | -3.3145710000 |
| C | 0.4388140000 | 4.2908290000 | -1.6004270000 |
| H | 0.1171530000 | 5.2626550000 | -1.3023700000 |
| H | 0.2966300000 | 3.7664590000 | 0.8900550000 |
| N | -1.2229610000 | -0.1955620000 | 0.3812370000 |
| C | -1.0475000000 | 1.1472340000 | 0.7254800000 |
| S | -2.6291500000 | 1.9180690000 | 0.9210120000 |
| C | -3.4512560000 | 0.4090640000 | 0.5030340000 |
| C | -2.5780310000 | -0.5786880000 | 0.2681100000 |
| C | -0.1443210000 | -1.1342040000 | 0.4671320000 |
| C | 0.3330370000 | -1.7657030000 | -0.6861470000 |
| C | 1.4707060000 | -2.5679370000 | -0.5762650000 |
| C | 2.1275160000 | -2.7500750000 | 0.6358790000 |
| C | 1.5861660000 | -2.1588510000 | 1.7783900000 |
| C | 0.4463440000 | -1.3647190000 | 1.7210660000 |
| C | -0.3327490000 | -1.6012090000 | -2.0267970000 |
| H | 1.8658820000 | -3.0358160000 | -1.4737360000 |
| C | 3.3924240000 | -3.5636810000 | 0.7306800000 |
| H | 2.0645120000 | -2.3213300000 | 2.7405880000 |
| C | -0.1224570000 | -0.7598880000 | 2.9765980000 |
| C | -4.9502520000 | 0.3357250000 | 0.4659870000 |
| C | -5.5104170000 | -0.1739800000 | -0.8684520000 |
| H | -5.3571410000 | 1.3297670000 | 0.6668310000 |
| H | -5.3085340000 | -0.3120490000 | 1.2765150000 |
| C | -5.2988860000 | -1.6697530000 | -1.1140870000 |
| H | -5.0644710000 | 0.4027220000 | -1.6859620000 |
| H | -6.5859660000 | 0.0259540000 | -0.8848630000 |
| H | -5.8661370000 | -1.9549920000 | -2.0051550000 |
| C | -2.9623470000 | -1.9947310000 | -0.0579560000 |
| H | -2.0625400000 | -2.5969490000 | -0.1819580000 |
| C | -3.8481250000 | -2.1208510000 | -1.3066960000 |
| H | -3.4969550000 | -2.4175120000 | 0.8017640000 |
| H | -3.8563620000 | -3.1732100000 | -1.6065600000 |
| H | -5.7360070000 | -2.2305570000 | -0.2780910000 |
| H | -3.3917340000 | -1.5600450000 | -2.1292490000 |
| H | -1.2116340000 | -0.6907900000 | 2.9255960000 |
| H | 0.2602320000 | 0.2533080000 | 3.1286790000 |
| H | 0.1525880000 | -1.3626670000 | 3.8429740000 |
| H | -0.9741140000 | -0.7208440000 | -2.0445420000 |
| H | -0.9405700000 | -2.4803520000 | -2.2654260000 |
| H | 0.4230670000 | -1.4909690000 | -2.8058720000 |
| H | 3.6421860000 | -4.0212550000 | -0.2277040000 |
| H | 3.2938850000 | -4.3577100000 | 1.4747750000 |
| H | 4.2312840000 | -2.9321210000 | 1.0378250000 |

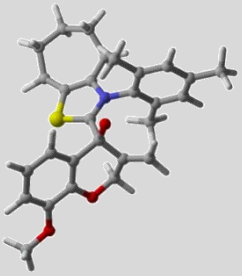
Thermochemie

Zero-point correction= 0.532671 (Hartree/Particle)
Thermal correction to Energy= 0.564525
Thermal correction to Enthalpy= 0.565469
Thermal correction to Gibbs Free Energy= 0.471574
Sum of electronic and zero-point Energies= -1763.427339
Sum of electronic and thermal Energies= -1763.395485
Sum of electronic and thermal Enthalpies= -1763.394540
Sum of electronic and thermal Free Energies= -1763.488435

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 354.245 | 124.407 | 197.618 |

**[24a + A]**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0346550000 | 0.4910720000 | 1.1790910000 |
| C | -4.0851080000 | 0.6616600000 | 2.1931480000 |
| C | -2.7938670000 | 0.2034440000 | 2.0184450000 |
| C | -2.4098060000 | -0.4185950000 | 0.8252560000 |
| C | -3.3543150000 | -0.6003970000 | -0.1806540000 |
| C | -4.6800720000 | -0.1443010000 | -0.0016490000 |
| H | -6.0449270000 | 0.8483090000 | 1.3262530000 |
| H | -4.3766230000 | 1.1475020000 | 3.1165450000 |
| H | -2.0455890000 | 0.2941970000 | 2.7967820000 |
| C | -0.9416150000 | -0.9284870000 | 0.7019770000 |
| O | -5.5253520000 | -0.3783980000 | -1.0395180000 |
| C | -6.8701790000 | 0.0394920000 | -0.8881460000 |
| H | -7.3436790000 | -0.4595270000 | -0.0377660000 |
| H | -7.3789580000 | -0.2453660000 | -1.8060430000 |
| H | -6.9337230000 | 1.1237080000 | -0.7570890000 |
| O | -0.4007680000 | -1.2933970000 | 1.8502950000 |
| N | 1.1964050000 | 0.3209240000 | -0.0824660000 |
| C | -0.1167400000 | 0.2966690000 | 0.1421910000 |
| S | -0.7725140000 | 1.8521410000 | -0.0681170000 |
| C | 0.7677370000 | 2.5336320000 | -0.4686930000 |
| C | 1.7261410000 | 1.5773590000 | -0.4245700000 |
| C | 2.0522010000 | -0.8492940000 | 0.0007360000 |
| C | 2.6787260000 | -1.1134670000 | 1.2213220000 |
| C | 3.5323520000 | -2.2100720000 | 1.2754170000 |
| C | 3.7765680000 | -3.0078640000 | 0.1549580000 |
| C | 3.1675510000 | -2.6714110000 | -1.0502320000 |
| C | 2.2991880000 | -1.5835270000 | -1.1554640000 |
| C | 2.4392270000 | -0.2341970000 | 2.4146380000 |
| H | 4.0266680000 | -2.4425170000 | 2.2134520000 |
| C | 4.6777600000 | -4.2107700000 | 0.2533610000 |
| H | 3.3741030000 | -3.2618240000 | -1.9379890000 |
| C | 1.6648890000 | -1.2545180000 | -2.4805270000 |
| C | 0.9198830000 | 3.9851510000 | -0.8205600000 |
| C | 1.9917490000 | 4.7129070000 | -0.0005940000 |
| H | -0.0430430000 | 4.4816160000 | -0.6831560000 |
| H | 1.1606960000 | 4.0641490000 | -1.8872990000 |
| C | 3.4299120000 | 4.3154980000 | -0.3393920000 |
| H | 1.8021200000 | 4.5498360000 | 1.0654720000 |
| H | 1.8753060000 | 5.7839780000 | -0.1848310000 |
| H | 4.1034320000 | 5.0230240000 | 0.1518790000 |
| C | 3.1862370000 | 1.7647960000 | -0.7186930000 |
| H | 3.7125590000 | 0.8321200000 | -0.5129160000 |
| C | 3.8425960000 | 2.9023280000 | 0.0768260000 |
| H | 3.3021940000 | 1.9588250000 | -1.7920210000 |
| H | 4.9230320000 | 2.8060700000 | -0.0574120000 |
| H | 3.5911300000 | 4.4337380000 | -1.4180470000 |
| H | 3.6442730000 | 2.7598130000 | 1.1443200000 |
| H | 1.3122860000 | -0.2229380000 | -2.5328150000 |
| H | 0.8108620000 | -1.9137050000 | -2.6603370000 |
| H | 2.3805270000 | -1.4118050000 | -3.2887680000 |

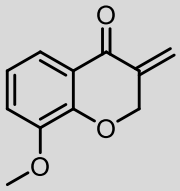
| | | | |
|---|---|---|---|
| H | 1.3809250000 | -0.2968970000 | 2.6827900000 |
| H | 2.6788260000 | 0.8096730000 | 2.1879680000 |
| H | 3.0557390000 | -0.5512200000 | 3.2555030000 |
| H | 5.4564630000 | -4.0595240000 | 1.0023250000 |
| H | 5.1518620000 | -4.4275720000 | -0.7048070000 |
| H | 4.1018940000 | -5.0925520000 | 0.5476610000 |
| C | -0.9924120000 | -1.9820800000 | -0.4144750000 |
| C | -1.7443260000 | -1.5609910000 | -1.6404220000 |
| H | -1.2785020000 | -0.6767370000 | -2.0960550000 |
| O | -3.1092980000 | -1.2311640000 | -1.3601930000 |
| H | -1.7781640000 | -2.3571100000 | -2.3842060000 |
| C | -0.4497500000 | -3.1816670000 | -0.2586380000 |
| H | 0.0949380000 | -3.4044410000 | 0.6526940000 |
| H | -0.5271250000 | -3.9441010000 | -1.0275700000 |

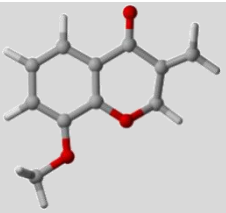
Thermochemie

Zero-point correction= 0.534610 (Hartree/Particle)
Thermal correction to Energy= 0.565185
Thermal correction to Enthalpy= 0.566129
Thermal correction to Gibbs Free Energy= 0.474098
Sum of electronic and zero-point Energies= -1763.458534
Sum of electronic and thermal Energies= -1763.427959
Sum of electronic and thermal Enthalpies= -1763.427015
Sum of electronic and thermal Free Energies= -1763.519046

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 354.659 | 120.477 | 193.696 |

**24a**



24

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 2.2570000000 | 1.1655470000 | 0.0045420000 |
| C | 1.4186880000 | 2.2879610000 | 0.0854720000 |
| C | 0.0515480000 | 2.1327700000 | 0.1167740000 |
| C | -0.5067200000 | 0.8446370000 | 0.0823530000 |
| C | 0.3230450000 | -0.2768940000 | 0.0240190000 |
| C | 1.7253130000 | -0.1137720000 | -0.0315290000 |
| H | 3.3288460000 | 1.3087680000 | -0.0237670000 |
| H | 1.8608840000 | 3.2756590000 | 0.1166550000 |
| H | -0.6174810000 | 2.9830930000 | 0.1562730000 |
| C | -1.9772210000 | 0.6707390000 | -0.0019740000 |
| O | -0.1427940000 | -1.5456470000 | -0.0137540000 |
| O | 2.4442680000 | -1.2561820000 | -0.1110890000 |
| C | 3.8558920000 | -1.1338070000 | -0.1895660000 |
| H | 4.1495950000 | -0.5652520000 | -1.0761060000 |
| H | 4.2400880000 | -2.1479140000 | -0.2625320000 |
| H | 4.2573290000 | -0.6534360000 | 0.7069260000 |
| O | -2.7397080000 | 1.6088610000 | -0.1189390000 |
| C | -2.4390630000 | -0.7508030000 | 0.0151640000 |
| C | -1.4399660000 | -1.7285010000 | 0.5604710000 |
| H | -1.3444810000 | -1.5950930000 | 1.6452160000 |
| H | -1.7250020000 | -2.7573410000 | 0.3509620000 |
| C | -3.6543790000 | -1.0786690000 | -0.4126020000 |
| H | -3.9894610000 | -2.1097560000 | -0.4294440000 |

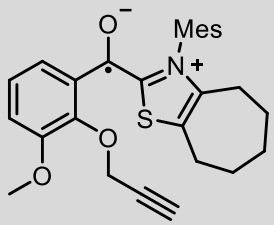
| | | | |
|---|---|---|---|
| H | -4.3392630000 | -0.3102370000 | -0.7526710000 |

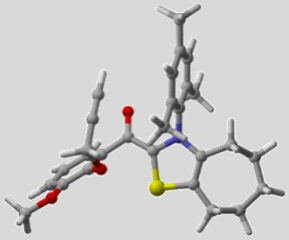
Thermochemie

Zero-point correction= 0.189750 (Hartree/Particle)
Thermal correction to Energy= 0.201394
Thermal correction to Enthalpy= 0.202338
Thermal correction to Gibbs Free Energy= 0.151933
Sum of electronic and zero-point Energies= -650.555239
Sum of electronic and thermal Energies= -650.543595
Sum of electronic and thermal Enthalpies= -650.542651
Sum of electronic and thermal Free Energies= -650.593055

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 126.376 | 45.225 | 106.086 |

**21a**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 5.0582480000 | -0.4298890000 | 1.2704140000 |
| C | 4.3310690000 | -0.2315560000 | 2.4456000000 |
| C | 2.9730790000 | 0.0260960000 | 2.3998970000 |
| C | 2.3030510000 | 0.0778260000 | 1.1709310000 |
| C | 3.0249760000 | -0.1123870000 | -0.0045510000 |
| C | 4.4100770000 | -0.3655690000 | 0.0418670000 |
| H | 6.1195890000 | -0.6300600000 | 1.3244430000 |
| H | 4.8437290000 | -0.2813910000 | 3.3987110000 |
| H | 2.4075960000 | 0.1936450000 | 3.3084630000 |
| C | 0.8340870000 | 0.3985540000 | 1.1833460000 |
| O | 2.4078290000 | -0.0707980000 | -1.2331030000 |
| O | 5.0158490000 | -0.5241030000 | -1.1609390000 |
| C | 6.4164320000 | -0.7539110000 | -1.1654760000 |
| H | 6.9506050000 | 0.0798400000 | -0.7018590000 |
| H | 6.7029540000 | -0.8355340000 | -2.2109720000 |
| H | 6.6613160000 | -1.6836620000 | -0.6451700000 |
| O | 0.4308680000 | 1.4054540000 | 1.7999520000 |
| C | 2.6216270000 | 1.1445230000 | -1.9565750000 |
| H | 3.6918120000 | 1.3526430000 | -2.0336900000 |
| C | 1.9142640000 | 2.2683460000 | -1.3345370000 |
| H | 2.2299360000 | 0.9631970000 | -2.9583470000 |
| C | 1.2962730000 | 3.1380560000 | -0.7843160000 |
| H | 0.7375640000 | 3.8944680000 | -0.2832860000 |
| N | -1.3881120000 | -0.3025420000 | 0.3269250000 |
| C | -0.0435870000 | -0.5187130000 | 0.5470160000 |
| S | 0.3876790000 | -2.1398820000 | 0.0817320000 |
| C | -1.2675170000 | -2.4890210000 | -0.3752810000 |
| C | -2.0625140000 | -1.4141130000 | -0.1895830000 |
| C | -1.9035050000 | 1.0334420000 | 0.1482800000 |
| C | -2.5867280000 | 1.6528040000 | 1.1958100000 |
| C | -3.0821120000 | 2.9346120000 | 0.9797330000 |
| C | -2.9031500000 | 3.5936020000 | -0.2393820000 |
| C | -2.2280340000 | 2.9334750000 | -1.2628530000 |
| C | -1.7212390000 | 1.6437180000 | -1.0922040000 |
| C | -2.7525270000 | 0.9487710000 | 2.5125880000 |

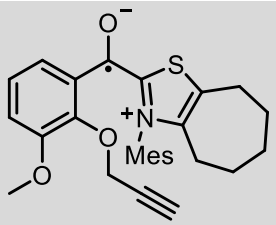
| | | | |
|---|---|---|---|
| H | -3.6142360000 | 3.4360520000 | 1.7828870000 |
| C | -3.4106630000 | 4.9999900000 | -0.4291560000 |
| H | -2.0888300000 | 3.4291490000 | -2.2192100000 |
| C | -1.0318060000 | 0.9213780000 | -2.2201800000 |
| C | -1.6511090000 | -3.8369010000 | -0.9136390000 |
| C | -2.8013570000 | -4.5047740000 | -0.1502050000 |
| H | -0.7751680000 | -4.4888750000 | -0.8879080000 |
| H | -1.9290430000 | -3.7358270000 | -1.9701450000 |
| C | -4.1704440000 | -3.8556110000 | -0.3674100000 |
| H | -2.5625560000 | -4.5192690000 | 0.9185890000 |
| H | -2.8596290000 | -5.5464870000 | -0.4781750000 |
| H | -4.9302770000 | -4.5060430000 | 0.0752460000 |
| C | -3.5347220000 | -1.3499040000 | -0.4782910000 |
| H | -3.9112350000 | -0.3738270000 | -0.1673110000 |
| C | -4.3453790000 | -2.4522760000 | 0.2179500000 |
| H | -3.6922200000 | -1.4133980000 | -1.5620280000 |
| H | -5.4017800000 | -2.1800330000 | 0.1434160000 |
| H | -4.3825750000 | -3.8213290000 | -1.4433860000 |
| H | -4.0948000000 | -2.4620620000 | 1.2844470000 |
| H | -1.7026020000 | 0.1793520000 | -2.6661100000 |
| H | -0.1398490000 | 0.3948750000 | -1.8719350000 |
| H | -0.7356310000 | 1.6257740000 | -2.9981180000 |
| H | -1.7702190000 | 0.7849520000 | 2.9629180000 |
| H | -3.2249710000 | -0.0290490000 | 2.3824160000 |
| H | -3.3629370000 | 1.5408370000 | 3.1946160000 |
| H | -4.3731840000 | 5.1414590000 | 0.0655190000 |
| H | -3.5265360000 | 5.2375880000 | -1.4873490000 |
| H | -2.7100220000 | 5.7211030000 | 0.0011000000 |

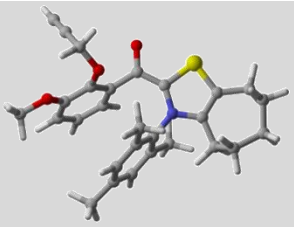
Thermochemie

Zero-point correction= 0.520073 (Hartree/Particle)
Thermal correction to Energy= 0.552096
Thermal correction to Enthalpy= 0.553040
Thermal correction to Gibbs Free Energy= 0.456531
Sum of electronic and zero-point Energies= -1762.833913
Sum of electronic and thermal Energies= -1762.801890
Sum of electronic and thermal Enthalpies= -1762.800946
Sum of electronic and thermal Free Energies= -1762.897455

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 346.445 | 122.844 | 203.120 |

**21a (anti)**



63

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 3.7207530000 | 1.0196420000 | -0.6554200000 |
| C | 2.8206850000 | 1.1736560000 | -1.7094320000 |
| C | 1.7100510000 | 0.3539260000 | -1.8110840000 |
| C | 1.4858500000 | -0.6453480000 | -0.8610070000 |
| C | 2.3937560000 | -0.8216900000 | 0.1771460000 |
| C | 3.5042430000 | 0.0301230000 | 0.2988490000 |
| H | 4.5766230000 | 1.6768260000 | -0.5809210000 |
| H | 2.9919940000 | 1.9500750000 | -2.4457790000 |
| H | 1.0046620000 | 0.4821000000 | -2.6239380000 |

| | | | |
|---|---|---|---|
| C | 0.3182490000 | -1.5846530000 | -0.9851840000 |
| O | 2.1305670000 | -1.7867040000 | 1.1149030000 |
| O | 4.2965980000 | -0.1841050000 | 1.3819790000 |
| C | 5.4417760000 | 0.6391160000 | 1.5316890000 |
| H | 6.1197150000 | 0.5251250000 | 0.6814790000 |
| H | 5.9361730000 | 0.3027620000 | 2.4398740000 |
| H | 5.1566250000 | 1.6895820000 | 1.6378310000 |
| O | 0.5209560000 | -2.7669130000 | -1.3433620000 |
| C | 3.1390150000 | -2.7671200000 | 1.3815180000 |
| H | 3.8418170000 | -2.3845660000 | 2.1228360000 |
| C | 3.8779810000 | -3.1889960000 | 0.1890180000 |
| H | 2.6025760000 | -3.6181830000 | 1.8023630000 |
| C | 4.5024480000 | -3.5336300000 | -0.7764030000 |
| H | 5.0467750000 | -3.8404060000 | -1.6394260000 |
| N | -1.5570010000 | 0.0178660000 | -0.2722010000 |
| C | -1.0180940000 | -1.1730040000 | -0.7171260000 |
| S | -2.2769420000 | -2.3610810000 | -0.9144900000 |
| C | -3.4927300000 | -1.2117290000 | -0.4048070000 |
| C | -2.9437470000 | -0.0163050000 | -0.1003800000 |
| C | -0.7926090000 | 1.2286940000 | -0.1455930000 |
| C | -0.0429600000 | 1.4376950000 | 1.0127010000 |
| C | 0.7334930000 | 2.5914660000 | 1.0791340000 |
| C | 0.7493740000 | 3.5239000000 | 0.0412530000 |
| C | -0.0564190000 | 3.3013910000 | -1.0738820000 |
| C | -0.8330860000 | 2.1507580000 | -1.1911200000 |
| C | -0.0925100000 | 0.4473690000 | 2.1437140000 |
| H | 1.3420000000 | 2.7663200000 | 1.9617110000 |
| C | 1.6584310000 | 4.7221830000 | 0.1117460000 |
| H | -0.0607630000 | 4.0246720000 | -1.8836920000 |
| C | -1.6713880000 | 1.8887690000 | -2.4133760000 |
| C | -4.9419530000 | -1.5909100000 | -0.3172770000 |
| C | -5.5413380000 | -1.4117290000 | 1.0845020000 |
| H | -5.0542150000 | -2.6317630000 | -0.6286400000 |
| H | -5.5158570000 | -0.9906400000 | -1.0340840000 |
| C | -5.7536670000 | 0.0458570000 | 1.5013980000 |
| H | -4.9013500000 | -1.9183630000 | 1.8146620000 |
| H | -6.5104330000 | -1.9181780000 | 1.1036410000 |
| H | -6.3196150000 | 0.0547140000 | 2.4372760000 |
| C | -3.6952670000 | 1.1752140000 | 0.4185250000 |
| H | -2.9920550000 | 1.9892240000 | 0.6027100000 |
| C | -4.4864030000 | 0.8808730000 | 1.7024610000 |
| H | -4.3879800000 | 1.5257470000 | -0.3561200000 |
| H | -4.7771990000 | 1.8405320000 | 2.1385580000 |
| H | -6.3870020000 | 0.5399890000 | 0.7538390000 |
| H | -3.8275870000 | 0.3900320000 | 2.4268510000 |
| H | -2.7382120000 | 1.9690880000 | -2.1840100000 |
| H | -1.5016690000 | 0.8797390000 | -2.7997070000 |
| H | -1.4400200000 | 2.6073670000 | -3.1994150000 |
| H | 0.2080100000 | -0.5506060000 | 1.8174240000 |
| H | -1.1100770000 | 0.3705600000 | 2.5387760000 |
| H | 0.5701760000 | 0.7559280000 | 2.9523540000 |
| H | 1.7287530000 | 5.1067740000 | 1.1305620000 |
| H | 1.3118500000 | 5.5240130000 | -0.5412060000 |
| H | 2.6677790000 | 4.4424460000 | -0.2061060000 |

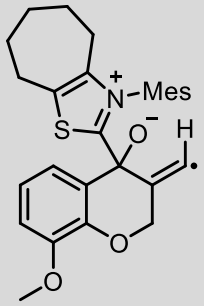
Thermochemie

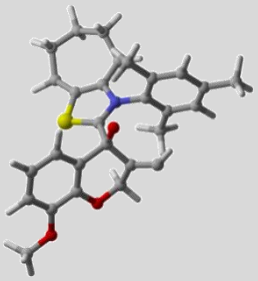
Zero-point correction= 0.519233 (Hartree/Particle)
Thermal correction to Energy= 0.551528
Thermal correction to Enthalpy= 0.552473
Thermal correction to Gibbs Free Energy= 0.454359
Sum of electronic and zero-point Energies= -1762.833891
Sum of electronic and thermal Energies= -1762.801595

Sum of electronic and thermal Enthalpies= -1762.800651
Sum of electronic and thermal Free Energies= -1762.898764

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 346.089 | 123.136 | 206.497 |

**26a**



63
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0484650000 | 0.4803730000 | 1.1674270000 |
| C | -4.0978930000 | 0.6635840000 | 2.1783040000 |
| C | -2.8050950000 | 0.2099890000 | 2.0057720000 |
| C | -2.4183500000 | -0.4186370000 | 0.8159790000 |
| C | -3.3639600000 | -0.6114790000 | -0.1866830000 |
| C | -4.6923070000 | -0.1621900000 | -0.0086260000 |
| H | -6.0602460000 | 0.8337110000 | 1.3134360000 |
| H | -4.3899290000 | 1.1554430000 | 3.0983030000 |
| H | -2.0577780000 | 0.3099080000 | 2.7838350000 |
| C | -0.9491580000 | -0.9217910000 | 0.7062590000 |
| O | -5.5371130000 | -0.4098060000 | -1.0429370000 |
| C | -6.8854390000 | -0.0023390000 | -0.8920220000 |
| H | -7.3522050000 | -0.4979220000 | -0.0359920000 |
| H | -7.3935300000 | -0.3001830000 | -1.8061340000 |
| H | -6.9581550000 | 1.0824180000 | -0.7708650000 |
| O | -0.4222690000 | -1.3004120000 | 1.8509820000 |
| N | 1.1989520000 | 0.3089020000 | -0.0739380000 |
| C | -0.1145360000 | 0.2956960000 | 0.1509660000 |
| S | -0.7587640000 | 1.8555680000 | -0.0590600000 |
| C | 0.7863690000 | 2.5246690000 | -0.4603330000 |
| C | 1.7377780000 | 1.5610840000 | -0.4161790000 |
| C | 2.0442030000 | -0.8701650000 | 0.0003800000 |
| C | 2.6593780000 | -1.1580490000 | 1.2225880000 |
| C | 3.4970320000 | -2.2660670000 | 1.2683290000 |
| C | 3.7387060000 | -3.0534720000 | 0.1387570000 |
| C | 3.1419590000 | -2.6949700000 | -1.0651110000 |
| C | 2.2884900000 | -1.5932150000 | -1.1624970000 |
| C | 2.4272560000 | -0.2867160000 | 2.4232560000 |
| H | 3.9823860000 | -2.5172460000 | 2.2063770000 |
| C | 4.6325390000 | -4.2620190000 | 0.2348380000 |
| H | 3.3436390000 | -3.2780970000 | -1.9585430000 |
| C | 1.6630340000 | -1.2455240000 | -2.4869050000 |
| C | 0.9492660000 | 3.9749200000 | -0.8124560000 |
| C | 2.0258490000 | 4.6947030000 | 0.0082700000 |
| H | -0.0100870000 | 4.4783830000 | -0.6758390000 |
| H | 1.1914170000 | 4.0516780000 | -1.8790380000 |
| C | 3.4610670000 | 4.2867080000 | -0.3297100000 |
| H | 1.8343240000 | 4.5331140000 | 1.0742130000 |
| H | 1.9173010000 | 5.7665530000 | -0.1761670000 |
| H | 4.1395240000 | 4.9891560000 | 0.1620190000 |
| C | 3.1993090000 | 1.7376470000 | -0.7095800000 |
| H | 3.7183680000 | 0.8009950000 | -0.5033340000 |

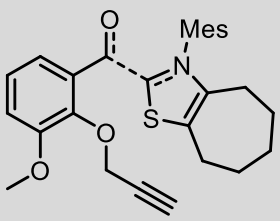
| | | | |
|---|---|---|---|
| C | 3.8631840000 | 2.8704060000 | 0.0866240000 |
| H | 3.3172820000 | 1.9305740000 | -1.7828790000 |
| H | 4.9429650000 | 2.7663170000 | -0.0468760000 |
| H | 3.6237940000 | 4.4039030000 | -1.4082390000 |
| H | 3.6628700000 | 2.7287880000 | 1.1538920000 |
| H | 1.3080260000 | -0.2142570000 | -2.5274070000 |
| H | 0.8124840000 | -1.9055160000 | -2.6810680000 |
| H | 2.3847530000 | -1.3895420000 | -3.2922590000 |
| H | 1.3679660000 | -0.3379300000 | 2.6896310000 |
| H | 2.6801850000 | 0.7559260000 | 2.2052550000 |
| H | 3.0384700000 | -0.6180770000 | 3.2624250000 |
| H | 5.5316880000 | -4.0374580000 | 0.8117840000 |
| H | 4.9318580000 | -4.6124530000 | -0.7532360000 |
| H | 4.1133700000 | -5.0801820000 | 0.7409910000 |
| C | -0.9833990000 | -1.9736280000 | -0.4429470000 |
| C | -1.7552140000 | -1.5442900000 | -1.6593960000 |
| H | -1.3040730000 | -0.6409870000 | -2.0915670000 |
| O | -3.1201790000 | -1.2523610000 | -1.3613870000 |
| H | -1.7734700000 | -2.3245860000 | -2.4187150000 |
| C | -0.3977480000 | -3.1333090000 | -0.3164660000 |
| H | 0.2177240000 | -3.5947420000 | 0.4422230000 |

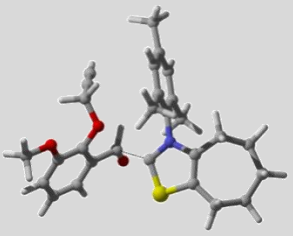
Thermochemie

Zero-point correction= 0.520830 (Hartree/Particle)
Thermal correction to Energy= 0.551565
Thermal correction to Enthalpy= 0.552509
Thermal correction to Gibbs Free Energy= 0.459217
Sum of electronic and zero-point Energies= -1762.788550
Sum of electronic and thermal Energies= -1762.757815
Sum of electronic and thermal Enthalpies= -1762.756871
Sum of electronic and thermal Free Energies= -1762.850163

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 346.112 | 120.566 | 196.349 |

**TS-1a**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.3973750000 | -2.4111020000 | 0.0088670000 |
| C | 3.9515630000 | -2.8181580000 | 1.2671140000 |
| C | 2.8884630000 | -2.1770340000 | 1.8824470000 |
| C | 2.2541800000 | -1.1068540000 | 1.2483780000 |
| C | 2.6969660000 | -0.6943550000 | -0.0028360000 |
| C | 3.7650840000 | -1.3518820000 | -0.6373160000 |
| H | 5.2239530000 | -2.9279810000 | -0.4600270000 |
| H | 4.4493780000 | -3.6448590000 | 1.7601110000 |
| H | 2.5344920000 | -2.4772360000 | 2.8608720000 |
| C | 1.1275640000 | -0.3873630000 | 1.9506970000 |
| O | 2.0138020000 | 0.2892300000 | -0.6745840000 |
| O | 4.0917600000 | -0.8947600000 | -1.8745250000 |
| C | 5.1601460000 | -1.5382880000 | -2.5508490000 |
| H | 6.0925630000 | -1.4469860000 | -1.9872700000 |
| H | 5.2604030000 | -1.0296450000 | -3.5065070000 |

| | | | |
|---|---|---|---|
| H | 4.9348420000 | -2.5944990000 | -2.7210310000 |
| O | 0.7801760000 | -0.7383000000 | 3.0855400000 |
| C | 2.7144060000 | 1.5153860000 | -0.8736800000 |
| H | 3.7528110000 | 1.3236560000 | -1.1515930000 |
| C | 2.6521780000 | 2.3762240000 | 0.3130410000 |
| H | 2.2195830000 | 2.0115660000 | -1.7101600000 |
| C | 2.5932180000 | 3.0802660000 | 1.2840910000 |
| H | 2.5349190000 | 3.7008030000 | 2.1483390000 |
| N | -1.3443690000 | -0.1480660000 | 0.0003860000 |
| C | -0.4452280000 | -0.9524960000 | 0.5730110000 |
| S | -1.0532110000 | -2.5436680000 | 0.4835720000 |
| C | -2.5191700000 | -2.0746780000 | -0.3335110000 |
| C | -2.5182860000 | -0.7349820000 | -0.5144230000 |
| C | -1.1044480000 | 1.2778980000 | -0.0412000000 |
| C | -1.3428700000 | 2.0224240000 | 1.1140210000 |
| C | -1.0714360000 | 3.3892310000 | 1.0677680000 |
| C | -0.5829990000 | 3.9995930000 | -0.0858030000 |
| C | -0.3932100000 | 3.2208860000 | -1.2268400000 |
| C | -0.6484040000 | 1.8510390000 | -1.2284360000 |
| C | -1.8656050000 | 1.3636880000 | 2.3627030000 |
| H | -1.2413410000 | 3.9872390000 | 1.9580320000 |
| C | -0.2248030000 | 5.4619500000 | -0.0888580000 |
| H | -0.0274220000 | 3.6876090000 | -2.1371940000 |
| C | -0.4484830000 | 1.0113850000 | -2.4608110000 |
| C | -3.5973440000 | -3.0420470000 | -0.7251220000 |
| C | -4.9655500000 | -2.6981160000 | -0.1209180000 |
| H | -3.3030920000 | -4.0462730000 | -0.4135710000 |
| H | -3.6786910000 | -3.0658920000 | -1.8184870000 |
| C | -5.6445910000 | -1.4697170000 | -0.7337970000 |
| H | -4.8548010000 | -2.5611280000 | 0.9601170000 |
| H | -5.6228620000 | -3.5597300000 | -0.2670860000 |
| H | -6.6693020000 | -1.4233890000 | -0.3543220000 |
| C | -3.6139700000 | 0.0762040000 | -1.1411100000 |
| H | -3.3386160000 | 1.1323740000 | -1.1114020000 |
| C | -4.9766770000 | -0.1185380000 | -0.4604530000 |
| H | -3.6994950000 | -0.1990510000 | -2.1994210000 |
| H | -5.6431000000 | 0.6699120000 | -0.8204470000 |
| H | -5.7240430000 | -1.6121970000 | -1.8188670000 |
| H | -4.8646610000 | 0.0295890000 | 0.6190570000 |
| H | 0.1791250000 | 0.1474790000 | -2.2329610000 |
| H | 0.0258820000 | 1.5948880000 | -3.2506170000 |
| H | -1.4049320000 | 0.6423690000 | -2.8434470000 |
| H | -1.1143330000 | 0.6997340000 | 2.8012220000 |
| H | -2.7469740000 | 0.7545280000 | 2.1426310000 |
| H | -2.1410840000 | 2.1155200000 | 3.1022840000 |
| H | -0.8158450000 | 6.0168440000 | 0.6410320000 |
| H | -0.3783010000 | 5.9064960000 | -1.0734650000 |
| H | 0.8308490000 | 5.5865730000 | 0.1711830000 |
| H | 0.9777320000 | 0.6440880000 | 1.6046380000 |

Thermochemie

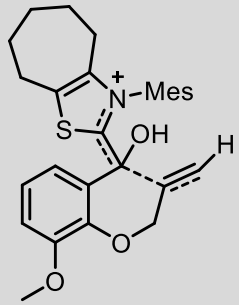
Zero-point correction= 0.530346 (Hartree/Particle)
Thermal correction to Energy= 0.562496
Thermal correction to Enthalpy= 0.563440
Thermal correction to Gibbs Free Energy= 0.465485
Sum of electronic and zero-point Energies= -1763.392814
Sum of electronic and thermal Energies= -1763.360664
Sum of electronic and thermal Enthalpies= -1763.359720
Sum of electronic and thermal Free Energies= -1763.457676

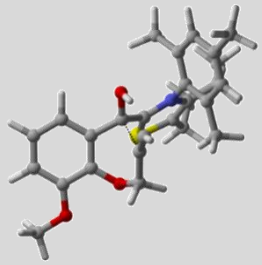
| | E (Thermal) | CV | S |
|---|---|---|---|
| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |

| | | | |
|---|---|---|---|
| Total | 352.972 | 122.604 | 206.165 |

Imaginäre Frequenz
-127.2541

**TS-3a**



64
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0042160000 | -0.4696410000 | 1.4583890000 |
| C | -4.0699900000 | -0.9399360000 | 2.3869530000 |
| C | -2.7481110000 | -1.1077040000 | 2.0237850000 |
| C | -2.3257760000 | -0.8042870000 | 0.7212600000 |
| C | -3.2590770000 | -0.3728980000 | -0.2179940000 |
| C | -4.6076920000 | -0.1882680000 | 0.1579750000 |
| H | -6.0349400000 | -0.3383250000 | 1.7579910000 |
| H | -4.3926450000 | -1.1675930000 | 3.3956600000 |
| H | -2.0145050000 | -1.4739640000 | 2.7311950000 |
| C | -0.8925280000 | -0.9810960000 | 0.3377600000 |
| O | -5.4342910000 | 0.2546860000 | -0.8222610000 |
| C | -6.8045370000 | 0.4111940000 | -0.4967490000 |
| H | -7.2434900000 | -0.5383890000 | -0.1775550000 |
| H | -7.2922370000 | 0.7494240000 | -1.4078620000 |
| H | -6.9393790000 | 1.1597210000 | 0.2891560000 |
| O | -0.2395740000 | -1.9894440000 | 1.0262400000 |
| H | -0.1490480000 | -2.7338840000 | 0.4033310000 |
| N | 1.2086250000 | 0.3187740000 | -0.0282430000 |
| C | -0.1344620000 | 0.2077080000 | 0.1525540000 |
| S | -0.8709230000 | 1.7721040000 | 0.0347690000 |
| C | 0.6684390000 | 2.5363120000 | -0.2853990000 |
| C | 1.6631390000 | 1.6289820000 | -0.2694920000 |
| C | 2.1199940000 | -0.7999670000 | 0.0196370000 |
| C | 2.6048620000 | -1.2100700000 | 1.2655150000 |
| C | 3.5016580000 | -2.2708160000 | 1.2921960000 |
| C | 3.9157660000 | -2.9100800000 | 0.1194320000 |
| C | 3.4302560000 | -2.4488690000 | -1.1004060000 |
| C | 2.5343160000 | -1.3790690000 | -1.1760070000 |
| C | 2.1479150000 | -0.5228960000 | 2.5215520000 |
| H | 3.8872670000 | -2.6114390000 | 2.2487000000 |
| C | 4.8727920000 | -4.0715970000 | 0.1886480000 |
| H | 3.7579270000 | -2.9223760000 | -2.0206820000 |
| C | 2.0878280000 | -0.8338010000 | -2.5050350000 |
| C | 0.7739410000 | 4.0154840000 | -0.5165980000 |
| C | 1.7305150000 | 4.7180100000 | 0.4560030000 |
| H | -0.2203200000 | 4.4590240000 | -0.4290290000 |
| H | 1.1035300000 | 4.1954610000 | -1.5469010000 |
| C | 3.2136550000 | 4.4190940000 | 0.2214130000 |
| H | 1.4548770000 | 4.4524310000 | 1.4822320000 |
| H | 1.5776540000 | 5.7959450000 | 0.3537920000 |
| H | 3.8005030000 | 5.0912710000 | 0.8538040000 |
| C | 3.1204400000 | 1.9300150000 | -0.4679120000 |
| H | 3.6946710000 | 1.0082370000 | -0.3644290000 |
| C | 3.6649660000 | 2.9847100000 | 0.5064020000 |

| | | | |
|---|---|---|---|
| H | 3.2700840000 | 2.2800140000 | -1.4963980000 |
| H | 4.7562240000 | 2.9526390000 | 0.4491440000 |
| H | 3.4683840000 | 4.6714830000 | -0.8156290000 |
| H | 3.3936610000 | 2.7059910000 | 1.5304200000 |
| H | 2.6546460000 | 0.0692670000 | -2.7552960000 |
| H | 1.0297320000 | -0.5740900000 | -2.4928160000 |
| H | 2.2524700000 | -1.5662330000 | -3.2952250000 |
| H | 1.0828130000 | -0.7092200000 | 2.6810220000 |
| H | 2.2878870000 | 0.5595420000 | 2.4518650000 |
| H | 2.7019600000 | -0.8882130000 | 3.3859130000 |
| H | 5.7573030000 | -3.8114150000 | 0.7741740000 |
| H | 5.1957670000 | -4.3775770000 | -0.8065720000 |
| H | 4.4006760000 | -4.9303440000 | 0.6723730000 |
| C | -1.1535130000 | -1.7640590000 | -1.4458600000 |
| C | -1.8551800000 | -0.6850130000 | -2.1831570000 |
| H | -1.1529030000 | 0.1220850000 | -2.4214260000 |
| O | -2.9608440000 | -0.0649510000 | -1.5060650000 |
| H | -2.2535150000 | -1.0850620000 | -3.1151900000 |
| C | -0.7220040000 | -2.9290960000 | -1.6708530000 |
| H | -0.1233670000 | -3.7059050000 | -1.2217550000 |

Thermochemie

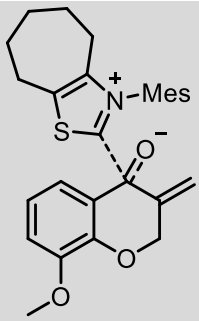
Zero-point correction= 0.530303 (Hartree/Particle)
Thermal correction to Energy= 0.561906
Thermal correction to Enthalpy= 0.562850
Thermal correction to Gibbs Free Energy= 0.467542
Sum of electronic and zero-point Energies= -1763.389079
Sum of electronic and thermal Energies= -1763.357476
Sum of electronic and thermal Enthalpies= -1763.356532
Sum of electronic and thermal Free Energies= -1763.451840

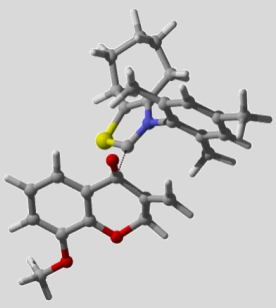
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 352.601 | 122.623 | 200.593 |

Imaginäre Frequenz

-619.0145

**TS-4a**



64

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -4.9345980000 | 0.7568920000 | 1.1547750000 |
| C | -3.9435900000 | 0.9189440000 | 2.1306110000 |
| C | -2.7198760000 | 0.2953240000 | 1.9889550000 |
| C | -2.4502630000 | -0.4908330000 | 0.8636700000 |
| C | -3.4310010000 | -0.6541020000 | -0.1103640000 |
| C | -4.6893290000 | -0.0299020000 | 0.0385680000 |
| H | -5.8913300000 | 1.2457090000 | 1.2803420000 |
| H | -4.1520620000 | 1.5320050000 | 2.9990800000 |
| H | -1.9446420000 | 0.3898440000 | 2.7404540000 |
| C | -1.1133530000 | -1.2190140000 | 0.7650480000 |
| O | -5.5818380000 | -0.2622240000 | -0.9570940000 |

| | | | |
|---|---|---|---|
| C | -6.8525970000 | 0.3548470000 | -0.8472870000 |
| H | -7.3784040000 | 0.0155040000 | 0.0496970000 |
| H | -7.4102480000 | 0.0545990000 | -1.7310870000 |
| H | -6.7588860000 | 1.4444230000 | -0.8263300000 |
| O | -0.5426220000 | -1.5579160000 | 1.8239420000 |
| N | 1.2621590000 | 0.3630990000 | -0.1701260000 |
| C | -0.0611850000 | 0.3177260000 | -0.0196160000 |
| S | -0.6730610000 | 1.8951260000 | -0.2280880000 |
| C | 0.8940510000 | 2.5862580000 | -0.5328590000 |
| C | 1.8362820000 | 1.6178790000 | -0.4577910000 |
| C | 2.0665610000 | -0.8349320000 | -0.0407740000 |
| C | 2.5574310000 | -1.1706050000 | 1.2195260000 |
| C | 3.3214020000 | -2.3313560000 | 1.3194590000 |
| C | 3.5988200000 | -3.1251340000 | 0.2058610000 |
| C | 3.1106520000 | -2.7299080000 | -1.0392610000 |
| C | 2.3377400000 | -1.5797380000 | -1.1861540000 |
| C | 2.2712910000 | -0.2994530000 | 2.4103980000 |
| H | 3.7113700000 | -2.6204920000 | 2.2905250000 |
| C | 4.3971120000 | -4.3944730000 | 0.3520570000 |
| H | 3.3334560000 | -3.3299120000 | -1.9162960000 |
| C | 1.7995460000 | -1.1554550000 | -2.5249180000 |
| C | 1.0918870000 | 4.0441480000 | -0.8306870000 |
| C | 2.1222990000 | 4.7249650000 | 0.0783040000 |
| H | 0.1314630000 | 4.5553370000 | -0.7368530000 |
| H | 1.4012590000 | 4.1541280000 | -1.8769690000 |
| C | 3.5736920000 | 4.3147060000 | -0.1811770000 |
| H | 1.8631640000 | 4.5296050000 | 1.1244070000 |
| H | 2.0365950000 | 5.8041460000 | -0.0747110000 |
| H | 4.2238410000 | 4.9945980000 | 0.3765600000 |
| C | 3.3138950000 | 1.7846950000 | -0.6606860000 |
| H | 3.8088750000 | 0.8330720000 | -0.4581650000 |
| C | 3.9430100000 | 2.8815000000 | 0.2100180000 |
| H | 3.4986350000 | 2.0156880000 | -1.7170620000 |
| H | 5.0283990000 | 2.7744330000 | 0.1347650000 |
| H | 3.8053380000 | 4.4671710000 | -1.2426520000 |
| H | 3.6812660000 | 2.7068710000 | 1.2590610000 |
| H | 2.0959670000 | -0.1310390000 | -2.7678530000 |
| H | 0.7065680000 | -1.1868540000 | -2.5246190000 |
| H | 2.1624550000 | -1.8152600000 | -3.3124420000 |
| H | 1.1943460000 | -0.2790470000 | 2.5936510000 |
| H | 2.6119090000 | 0.7258140000 | 2.2373520000 |
| H | 2.7754250000 | -0.6837200000 | 3.2968780000 |
| H | 5.1579160000 | -4.2927580000 | 1.1275570000 |
| H | 4.8880600000 | -4.6618630000 | -0.5844930000 |
| H | 3.7443180000 | -5.2244550000 | 0.6360880000 |
| C | -1.0671540000 | -2.1106920000 | -0.4573270000 |
| C | -1.9124040000 | -1.6534650000 | -1.6084110000 |
| H | -1.5285340000 | -0.7120970000 | -2.0204090000 |
| O | -3.2714760000 | -1.4286330000 | -1.2182150000 |
| H | -1.9466240000 | -2.4001030000 | -2.4007070000 |
| C | -0.3426560000 | -3.2228260000 | -0.4678170000 |
| H | 0.2653370000 | -3.4759310000 | 0.3947460000 |
| H | -0.3198630000 | -3.8789160000 | -1.3319970000 |

Thermochemie

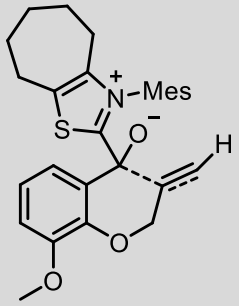
Zero-point correction= 0.532810 (Hartree/Particle)
Thermal correction to Energy= 0.563628
Thermal correction to Enthalpy= 0.564572
Thermal correction to Gibbs Free Energy= 0.470680
Sum of electronic and zero-point Energies= -1763.452412
Sum of electronic and thermal Energies= -1763.421594
Sum of electronic and thermal Enthalpies= -1763.420649

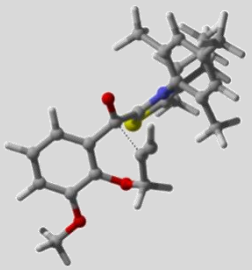
Sum of electronic and thermal Free Energies= -1763.514542

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 353.682 | 119.849 | 197.613 |

Imaginäre Frequenz
-173.7995

**TS-7a**



63
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.1126030000 | -0.3463330000 | 1.2690220000 |
| C | -4.2995610000 | -0.7809590000 | 2.3188400000 |
| C | -2.9453650000 | -0.9902750000 | 2.1280930000 |
| C | -2.3785320000 | -0.7485620000 | 0.8750020000 |
| C | -3.1884760000 | -0.3433220000 | -0.1813760000 |
| C | -4.5645280000 | -0.1353720000 | 0.0071090000 |
| H | -6.1690740000 | -0.1919900000 | 1.4422710000 |
| H | -4.7453060000 | -0.9552030000 | 3.2911640000 |
| H | -2.2937140000 | -1.3438450000 | 2.9170000000 |
| C | -0.8908550000 | -0.9892450000 | 0.6904870000 |
| O | -5.2642470000 | 0.2549990000 | -1.0887120000 |
| C | -6.6544850000 | 0.4368390000 | -0.9368320000 |
| H | -7.1442910000 | -0.4910440000 | -0.6235880000 |
| H | -7.0280170000 | 0.7319120000 | -1.9150540000 |
| H | -6.8750160000 | 1.2261160000 | -0.2104970000 |
| O | -0.2713000000 | -1.6616180000 | 1.5664800000 |
| N | 1.1730530000 | 0.3275560000 | 0.0490860000 |
| C | -0.1539130000 | 0.2497240000 | 0.2329570000 |
| S | -0.8590460000 | 1.7984110000 | 0.0673550000 |
| C | 0.6734470000 | 2.5362040000 | -0.2689500000 |
| C | 1.6596060000 | 1.6105940000 | -0.2368930000 |
| C | 2.0557290000 | -0.8229020000 | 0.0145280000 |
| C | 2.6773510000 | -1.2284200000 | 1.2000930000 |
| C | 3.5613810000 | -2.2955470000 | 1.1229460000 |
| C | 3.8338390000 | -2.9414250000 | -0.0866750000 |
| C | 3.2211480000 | -2.4767400000 | -1.2427390000 |
| C | 2.3277530000 | -1.4024660000 | -1.2192260000 |
| C | 2.3914760000 | -0.5312950000 | 2.4982550000 |
| H | 4.0496930000 | -2.6370460000 | 2.0305870000 |
| C | 4.7721130000 | -4.1195120000 | -0.1201750000 |
| H | 3.4325570000 | -2.9562500000 | -2.1938690000 |
| C | 1.7231750000 | -0.9100100000 | -2.5081440000 |
| C | 0.7957500000 | 4.0028530000 | -0.5655340000 |
| C | 1.8018350000 | 4.7325950000 | 0.3330310000 |
| H | -0.1878080000 | 4.4663930000 | -0.4585280000 |
| H | 1.0846650000 | 4.1323100000 | -1.6157410000 |
| C | 3.2684560000 | 4.3942330000 | 0.0538590000 |
| H | 1.5650510000 | 4.5206120000 | 1.3810870000 |
| H | 1.6622700000 | 5.8073630000 | 0.1866940000 |
| H | 3.8920530000 | 5.0933300000 | 0.6183110000 |

| | | | |
|---|---|---|---|
| C | 3.1198540000 | 1.8639290000 | -0.4754370000 |
| H | 3.6707650000 | 0.9376580000 | -0.3082690000 |
| C | 3.7061380000 | 2.9719130000 | 0.4104190000 |
| H | 3.2656140000 | 2.1266350000 | -1.5307750000 |
| H | 4.7948540000 | 2.9180110000 | 0.3240820000 |
| H | 3.4829570000 | 4.5789970000 | -1.0063520000 |
| H | 3.4638030000 | 2.7611600000 | 1.4576460000 |
| H | 0.9561430000 | -0.1520760000 | -2.3460420000 |
| H | 1.2570940000 | -1.7428660000 | -3.0385810000 |
| H | 2.4989580000 | -0.4833660000 | -3.1508050000 |
| H | 1.3604250000 | -0.7486890000 | 2.7883290000 |
| H | 2.4982070000 | 0.5535510000 | 2.3971850000 |
| H | 3.0742040000 | -0.8727380000 | 3.2763350000 |
| H | 5.6902790000 | -3.9037700000 | 0.4301910000 |
| H | 5.0385440000 | -4.3848510000 | -1.1438280000 |
| H | 4.3063880000 | -4.9921750000 | 0.3449450000 |
| C | -1.0213440000 | -1.9004690000 | -0.9834840000 |
| C | -1.9411880000 | -1.2395510000 | -1.9618930000 |
| H | -1.3799560000 | -0.8296960000 | -2.8046510000 |
| O | -2.6545270000 | -0.1219020000 | -1.4192330000 |
| H | -2.6644730000 | -1.9662790000 | -2.3430650000 |
| C | -0.3996080000 | -3.0070290000 | -0.9879530000 |
| H | 0.2655460000 | -3.5781510000 | -0.3617120000 |

Thermochemie

Zero-point correction= 0.518475 (Hartree/Particle)
Thermal correction to Energy= 0.549351
Thermal correction to Enthalpy= 0.550295
Thermal correction to Gibbs Free Energy= 0.456772
Sum of electronic and zero-point Energies= -1762.779426
Sum of electronic and thermal Energies= -1762.748550
Sum of electronic and thermal Enthalpies= -1762.747606
Sum of electronic and thermal Free Energies= -1762.841129

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 344.723 | 120.641 | 196.836 |

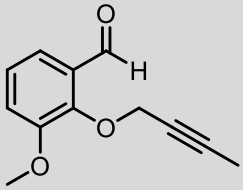
Imaginäre Frequenz

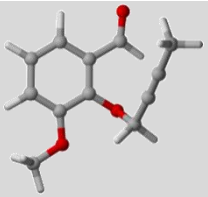
-615.9667

## *O*-propargylierte Aldehyde: Me-Substituent

(u)M06-2X/6-311+G** SCRF=(PCM,Solvent=Tetrahydrofuran)

**19b**



27

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -2.2254520000 | 1.1407460000 | 0.7168510000 |
| C | -1.3976910000 | 2.2602560000 | 0.8499950000 |
| C | -0.1390780000 | 2.2774690000 | 0.2816920000 |
| C | 0.3091620000 | 1.1648200000 | -0.4402730000 |
| C | -0.5122430000 | 0.0503760000 | -0.5865810000 |

| | | | |
|---|---|---|---|
| C | -1.7892690000 | 0.0287300000 | 0.0044620000 |
| H | -3.2072850000 | 1.1489650000 | 1.1708570000 |
| H | -1.7569070000 | 3.1167840000 | 1.4070690000 |
| H | 0.5160460000 | 3.1343390000 | 0.3782390000 |
| C | 1.6613820000 | 1.1695990000 | -1.0522680000 |
| O | -0.0946360000 | -1.0306470000 | -1.3139730000 |
| O | -2.5008600000 | -1.1070490000 | -0.1793670000 |
| C | -3.7955500000 | -1.1738200000 | 0.4010120000 |
| H | -3.7408360000 | -1.0774280000 | 1.4885750000 |
| H | -4.1887760000 | -2.1529470000 | 0.1401330000 |
| H | -4.4464880000 | -0.3966520000 | -0.0077650000 |
| O | 2.4813990000 | 2.0328490000 | -0.8336290000 |
| H | 1.8851200000 | 0.3370260000 | -1.7344400000 |
| C | 0.3840400000 | -2.1264770000 | -0.5148710000 |
| H | -0.3953160000 | -2.4343360000 | 0.1869690000 |
| C | 1.6149710000 | -1.7651860000 | 0.1933780000 |
| H | 0.5628910000 | -2.9387430000 | -1.2184190000 |
| C | 2.6136570000 | -1.3859730000 | 0.7472180000 |
| C | 3.8217620000 | -0.9041150000 | 1.4099390000 |
| H | 3.7095950000 | -0.9411880000 | 2.4943520000 |
| H | 4.0145140000 | 0.1311130000 | 1.1193340000 |
| H | 4.6860730000 | -1.5067030000 | 1.1275310000 |

Thermochemie

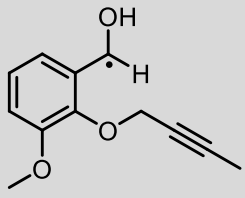
Zero-point correction= 0.214613 (Hartree/Particle)
Thermal correction to Energy= 0.229445
Thermal correction to Enthalpy= 0.230389
Thermal correction to Gibbs Free Energy= 0.172064
Sum of electronic and zero-point Energies= -689.777799
Sum of electronic and thermal Energies= -689.762967
Sum of electronic and thermal Enthalpies= -689.762023
Sum of electronic and thermal Free Energies= -689.820348

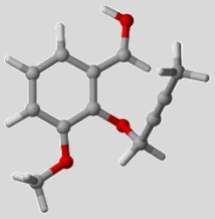
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 143.979 | 53.909 | 122.757 |

Volumen

Molar volume = 1662.171 bohr**3/mol (148.330 cm**3/mol)
Recommended a0 for SCRF calculation = 4.78 angstrom ( 9.03 bohr)

**25b**



28

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -2.2042760000 | 0.9551110000 | 0.9109310000 |
| C | -1.4321400000 | 2.0922870000 | 1.1668200000 |
| C | -0.2079350000 | 2.2830450000 | 0.5617430000 |
| C | 0.3089090000 | 1.3134510000 | -0.3394250000 |
| C | -0.4758720000 | 0.1591820000 | -0.5847810000 |
| C | -1.7221030000 | -0.0103560000 | 0.0227100000 |
| H | -3.1640720000 | 0.8375990000 | 1.3933850000 |
| H | -1.8095930000 | 2.8383960000 | 1.8560040000 |
| H | 0.3520890000 | 3.1811050000 | 0.7970180000 |
| C | 1.5492110000 | 1.4458910000 | -0.9940040000 |
| O | -0.0165800000 | -0.7673960000 | -1.4870060000 |

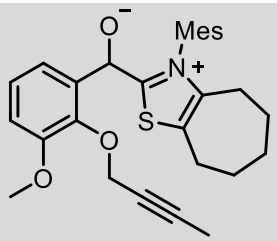
| | | | |
|---|---|---|---|
| O | -2.3959860000 | -1.1399190000 | -0.3166560000 |
| C | -3.6636000000 | -1.3556400000 | 0.2838110000 |
| H | -3.5751420000 | -1.4250940000 | 1.3713120000 |
| H | -4.0261300000 | -2.3005450000 | -0.1133260000 |
| H | -4.3619960000 | -0.5567190000 | 0.0212160000 |
| O | 2.3751700000 | 2.5035600000 | -0.8503880000 |
| H | 1.9354450000 | 0.6889590000 | -1.6575880000 |
| C | 0.3860230000 | -2.0195760000 | -0.9165800000 |
| H | -0.4566300000 | -2.4727150000 | -0.3902050000 |
| C | 1.5352310000 | -1.8739340000 | -0.0174150000 |
| H | 0.6455210000 | -2.6509050000 | -1.7665380000 |
| C | 2.4764800000 | -1.7290130000 | 0.7174930000 |
| C | 3.6195150000 | -1.5351640000 | 1.6057440000 |
| H | 1.9806140000 | 3.1815760000 | -0.2918290000 |
| H | 4.0741290000 | -0.5589670000 | 1.4263580000 |
| H | 4.3769850000 | -2.3012860000 | 1.4331310000 |
| H | 3.3112860000 | -1.5830530000 | 2.6511850000 |

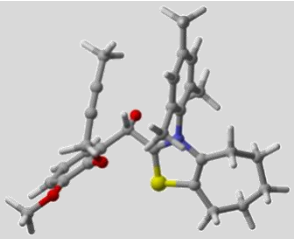
Thermochemie

Zero-point correction= 0.225153 (Hartree/Particle)
Thermal correction to Energy= 0.240580
Thermal correction to Enthalpy= 0.241524
Thermal correction to Gibbs Free Energy= 0.181203
Sum of electronic and zero-point Energies= -690.329197
Sum of electronic and thermal Energies= -690.313770
Sum of electronic and thermal Enthalpies= -690.312826
Sum of electronic and thermal Free Energies= -690.373147

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 150.966 | 56.674 | 126.957 |

**22b**



67

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.9138450000 | -1.1893790000 | 0.9780430000 |
| C | 4.2638710000 | -1.1834820000 | 2.2115940000 |
| C | 2.9513030000 | -0.7473620000 | 2.3193980000 |
| C | 2.2633680000 | -0.2975060000 | 1.1933210000 |
| C | 2.9114640000 | -0.2945950000 | -0.0369200000 |
| C | 4.2352400000 | -0.7513890000 | -0.1567470000 |
| H | 5.9342110000 | -1.5415140000 | 0.9091360000 |
| H | 4.7986420000 | -1.5262080000 | 3.0899460000 |
| H | 2.4210810000 | -0.7286650000 | 3.2631510000 |
| C | 0.8124040000 | 0.1962330000 | 1.3543050000 |
| O | 2.2271580000 | 0.0800140000 | -1.1747710000 |
| O | 4.7584720000 | -0.7371740000 | -1.4121760000 |
| C | 6.0962530000 | -1.1816910000 | -1.5692290000 |
| H | 6.7854390000 | -0.5628430000 | -0.9883150000 |
| H | 6.3225640000 | -1.0842730000 | -2.6282630000 |
| H | 6.1990270000 | -2.2277690000 | -1.2678870000 |
| O | 0.3520180000 | 0.2094970000 | 2.6154570000 |
| C | 2.6476920000 | 1.3206210000 | -1.7583510000 |
| H | 3.7375920000 | 1.3788290000 | -1.7644530000 |

| | | | |
|---|---|---|---|
| C | 2.0607030000 | 2.4692890000 | -1.0609880000 |
| H | 2.3022380000 | 1.2916130000 | -2.7930880000 |
| C | 1.5217280000 | 3.3588340000 | -0.4558530000 |
| C | 0.8448270000 | 4.3922470000 | 0.3220150000 |
| N | -1.3018750000 | -0.3930010000 | 0.0802840000 |
| C | -0.1090460000 | -0.7382910000 | 0.5560310000 |
| S | 0.1313530000 | -2.4121020000 | 0.4048150000 |
| C | -1.4366930000 | -2.6384190000 | -0.3101040000 |
| C | -2.0805700000 | -1.4523970000 | -0.4142340000 |
| C | -1.7406540000 | 0.9883880000 | 0.0396200000 |
| C | -2.4572760000 | 1.4936070000 | 1.1261200000 |
| C | -2.8606310000 | 2.8249640000 | 1.0549700000 |
| C | -2.5726130000 | 3.6220400000 | -0.0548200000 |
| C | -1.8873140000 | 3.0579530000 | -1.1285660000 |
| C | -1.4619600000 | 1.7303630000 | -1.1064930000 |
| C | -2.7818700000 | 0.6181640000 | 2.3036220000 |
| H | -3.4106730000 | 3.2507780000 | 1.8886260000 |
| C | -2.9686790000 | 5.0749320000 | -0.0709580000 |
| H | -1.6653830000 | 3.6632570000 | -2.0023880000 |
| C | -0.7667210000 | 1.1069960000 | -2.2851610000 |
| C | -1.9158030000 | -3.9894360000 | -0.7537880000 |
| C | -3.2863880000 | -4.3748870000 | -0.1837520000 |
| H | -1.1773380000 | -4.7389870000 | -0.4620410000 |
| H | -1.9601650000 | -4.0043500000 | -1.8491180000 |
| C | -4.4628410000 | -3.5893590000 | -0.7679870000 |
| H | -3.2680080000 | -4.2622400000 | 0.9052900000 |
| H | -3.4432550000 | -5.4364870000 | -0.3917780000 |
| H | -5.3886130000 | -4.0697750000 | -0.4395490000 |
| C | -3.4452100000 | -1.2192900000 | -0.9917230000 |
| H | -3.7128210000 | -0.1704450000 | -0.8502060000 |
| C | -4.5360480000 | -2.1102630000 | -0.3806540000 |
| H | -3.4027110000 | -1.3897670000 | -2.0743570000 |
| H | -5.5000720000 | -1.7162560000 | -0.7125230000 |
| H | -4.4426740000 | -3.6732480000 | -1.8617000000 |
| H | -4.5127840000 | -2.0137520000 | 0.7099450000 |
| H | -1.4525480000 | 0.4460580000 | -2.8259500000 |
| H | 0.0905860000 | 0.5101600000 | -1.9694490000 |
| H | -0.4236550000 | 1.8777200000 | -2.9757270000 |
| H | -1.8484770000 | 0.2490500000 | 2.7410890000 |
| H | -3.3832160000 | -0.2417490000 | 1.9910730000 |
| H | -3.3461640000 | 1.1756280000 | 3.0509640000 |
| H | -3.9647090000 | 5.2169510000 | 0.3521740000 |
| H | -2.9597670000 | 5.4765670000 | -1.0847960000 |
| H | -2.2701890000 | 5.6639230000 | 0.5311230000 |
| H | 0.7556340000 | 1.1652190000 | 0.8230600000 |
| H | 0.2796230000 | 5.0619410000 | -0.3293770000 |
| H | 1.5609360000 | 4.9823960000 | 0.8958860000 |
| H | 0.1416710000 | 3.9228580000 | 1.0161200000 |

Thermochemie

Zero-point correction= 0.561001 (Hartree/Particle)
Thermal correction to Energy= 0.594401
Thermal correction to Enthalpy= 0.595345
Thermal correction to Gibbs Free Energy= 0.496629
Sum of electronic and zero-point Energies= -1802.693485
Sum of electronic and thermal Energies= -1802.660085
Sum of electronic and thermal Enthalpies= -1802.659141
Sum of electronic and thermal Free Energies= -1802.757857

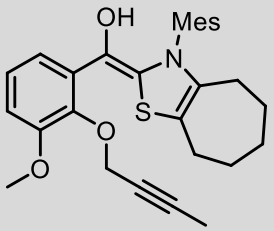
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 372.992 | 128.160 | 207.765 |

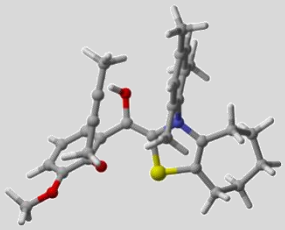
Thermochemie

| | |
|---|---|
| Zero-point correction= | 0.560055 (Hartree/Particle) |
| Thermal correction to Energy= | 0.593962 |
| Thermal correction to Enthalpy= | 0.594906 |
| Thermal correction to Gibbs Free Energy= | 0.494001 |
| Sum of electronic and zero-point Energies= | -1802.694175 |
| Sum of electronic and thermal Energies= | -1802.660269 |
| Sum of electronic and thermal Enthalpies= | -1802.659325 |
| Sum of electronic and thermal Free Energies= | -1802.760229 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 372.717 | 128.486 | 212.372 |

**23b**



67

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 5.0518470000 | -0.8408430000 | 1.2526500000 |
| C | 4.3004080000 | -0.7340570000 | 2.4259430000 |
| C | 2.9452700000 | -0.4665170000 | 2.3770650000 |
| C | 2.2961780000 | -0.2990090000 | 1.1422870000 |
| C | 3.0492620000 | -0.3832700000 | -0.0278900000 |
| C | 4.4290930000 | -0.6627140000 | 0.0225190000 |
| H | 6.1096100000 | -1.0579880000 | 1.3109130000 |
| H | 4.7919510000 | -0.8722290000 | 3.3816180000 |
| H | 2.3626970000 | -0.3879040000 | 3.2871160000 |
| C | 0.8564240000 | 0.0232450000 | 1.1178180000 |
| O | 2.4636960000 | -0.1887740000 | -1.2538080000 |
| O | 5.0579300000 | -0.7182690000 | -1.1779640000 |
| C | 6.4518810000 | -0.9832400000 | -1.1760210000 |
| H | 6.9976550000 | -0.2035280000 | -0.6377190000 |
| H | 6.7571830000 | -0.9887030000 | -2.2194650000 |
| H | 6.6631660000 | -1.9577890000 | -0.7278140000 |
| O | 0.4630900000 | 1.0992880000 | 1.8970680000 |
| C | 2.6922980000 | 1.1138800000 | -1.7986160000 |
| H | 3.7654830000 | 1.3224190000 | -1.8197940000 |
| C | 1.9768910000 | 2.1706800000 | -1.0693060000 |
| H | 2.3294340000 | 1.0668720000 | -2.8263930000 |
| C | 1.3745640000 | 3.0530810000 | -0.5131090000 |
| C | 0.6307840000 | 4.1071680000 | 0.1755550000 |
| H | 0.9293320000 | 1.8793710000 | 1.5710420000 |
| N | -1.4462740000 | -0.4132280000 | 0.3972020000 |
| C | -0.0769830000 | -0.7148470000 | 0.4906970000 |
| S | 0.2508290000 | -2.2934830000 | -0.2527640000 |
| C | -1.4822440000 | -2.5349630000 | -0.5439370000 |
| C | -2.1991640000 | -1.4704710000 | -0.1705510000 |
| C | -1.8625660000 | 0.9447080000 | 0.1478260000 |
| C | -2.5327760000 | 1.6458700000 | 1.1548110000 |
| C | -2.9813700000 | 2.9356150000 | 0.8762690000 |
| C | -2.7756850000 | 3.5295760000 | -0.3704500000 |
| C | -2.1001280000 | 2.8040600000 | -1.3489690000 |

| | | | |
|---|---|---|---|
| C | -1.6369170000 | 1.5087710000 | -1.1120190000 |
| C | -2.7572440000 | 1.0118620000 | 2.4995970000 |
| H | -3.5011750000 | 3.4910940000 | 1.6516940000 |
| C | -3.2814090000 | 4.9213490000 | -0.6508340000 |
| H | -1.9239740000 | 3.2549390000 | -2.3217580000 |
| C | -0.9256030000 | 0.7289260000 | -2.1851750000 |
| C | -1.9919840000 | -3.8218680000 | -1.1251600000 |
| C | -3.0254820000 | -4.5259430000 | -0.2360600000 |
| H | -1.1486810000 | -4.4945420000 | -1.2972160000 |
| H | -2.4381590000 | -3.6283700000 | -2.1091720000 |
| C | -4.3946600000 | -3.8416550000 | -0.1908480000 |
| H | -2.6208840000 | -4.6174370000 | 0.7775480000 |
| H | -3.1661040000 | -5.5419170000 | -0.6171240000 |
| H | -5.0888620000 | -4.5008880000 | 0.3390210000 |
| C | -3.6937220000 | -1.3550650000 | -0.2778260000 |
| H | -4.0041400000 | -0.3806750000 | 0.1037050000 |
| C | -4.4442060000 | -2.4633560000 | 0.4753200000 |
| H | -3.9836240000 | -1.3788460000 | -1.3359230000 |
| H | -5.4934790000 | -2.1640510000 | 0.5557320000 |
| H | -4.7781660000 | -3.7510990000 | -1.2151360000 |
| H | -4.0530480000 | -2.5294500000 | 1.4965840000 |
| H | -1.5084090000 | -0.1508870000 | -2.4765280000 |
| H | 0.0434970000 | 0.3712890000 | -1.8282330000 |
| H | -0.7677060000 | 1.3488840000 | -3.0684050000 |
| H | -1.7966550000 | 0.7862210000 | 2.9675150000 |
| H | -3.3002440000 | 0.0677260000 | 2.4030240000 |
| H | -3.3270530000 | 1.6757750000 | 3.1504860000 |
| H | -4.3270160000 | 4.8957520000 | -0.9708540000 |
| H | -2.7036650000 | 5.3979710000 | -1.4444500000 |
| H | -3.2262100000 | 5.5466840000 | 0.2421050000 |
| H | 1.2688020000 | 4.6354390000 | 0.8865710000 |
| H | -0.2250610000 | 3.6807910000 | 0.7070750000 |
| H | 0.2398830000 | 4.8296140000 | -0.5438390000 |

Thermochemie

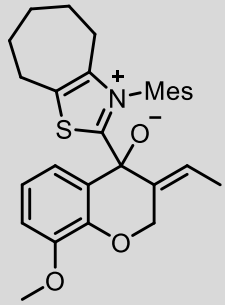
Zero-point correction= 0.560553 (Hartree/Particle)
Thermal correction to Energy= 0.594578
Thermal correction to Enthalpy= 0.595523
Thermal correction to Gibbs Free Energy= 0.495105
Sum of electronic and zero-point Energies= -1802.711128
Sum of electronic and thermal Energies= -1802.677102
Sum of electronic and thermal Enthalpies= -1802.676158
Sum of electronic and thermal Free Energies= -1802.776575

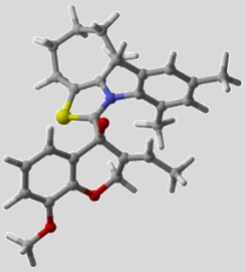
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 373.104 | 130.017 | 211.346 |

Volumen

Molar volume = 3874.580 bohr**3/mol (345.763 cm**3/mol)
Recommended a0 for SCRF calculation = 6.17 angstrom ( 11.67 bohr)

**[24b + A]**
**(E)**



67
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0283680000 | 0.7871380000 | 1.1786090000 |
| C | -4.0663870000 | 1.0313630000 | 2.1653260000 |
| C | -2.7790970000 | 0.5544700000 | 2.0125940000 |
| C | -2.4097630000 | -0.1604280000 | 0.8668500000 |
| C | -3.3659740000 | -0.4096100000 | -0.1133230000 |
| C | -4.6885290000 | 0.0630290000 | 0.0453460000 |
| H | -6.0357870000 | 1.1584660000 | 1.3097300000 |
| H | -4.3454490000 | 1.5877670000 | 3.0521700000 |
| H | -2.0248910000 | 0.6994260000 | 2.7771320000 |
| C | -0.9530700000 | -0.7036000000 | 0.7732760000 |
| O | -5.5463050000 | -0.2450740000 | -0.9629610000 |
| C | -6.8910580000 | 0.1769330000 | -0.8233830000 |
| H | -7.3488280000 | -0.2590370000 | 0.0692760000 |
| H | -7.4112260000 | -0.1782050000 | -1.7099140000 |
| H | -6.9594990000 | 1.2676080000 | -0.7730690000 |
| O | -0.4218970000 | -1.0154690000 | 1.9436840000 |
| N | 1.2157950000 | 0.4442010000 | -0.0739670000 |
| C | -0.0956300000 | 0.4730380000 | 0.1624460000 |
| S | -0.7028270000 | 2.0380700000 | -0.1116170000 |
| C | 0.8555980000 | 2.6508190000 | -0.5526040000 |
| C | 1.7828680000 | 1.6669330000 | -0.4748550000 |
| C | 2.0336410000 | -0.7473600000 | 0.0671150000 |
| C | 2.6597070000 | -0.9636930000 | 1.2980380000 |
| C | 3.4713620000 | -2.0859970000 | 1.4130380000 |
| C | 3.6771750000 | -2.9589340000 | 0.3410620000 |
| C | 3.0682490000 | -2.6739800000 | -0.8763390000 |
| C | 2.2378680000 | -1.5627890000 | -1.0411280000 |
| C | 2.4564530000 | -0.0119800000 | 2.4416240000 |
| H | 3.9621490000 | -2.2816350000 | 2.3614890000 |
| C | 4.5383930000 | -4.1827730000 | 0.5109940000 |
| H | 3.2404570000 | -3.3259310000 | -1.7279030000 |
| C | 1.5955000000 | -1.3042400000 | -2.3777750000 |
| C | 1.0518030000 | 4.0796670000 | -0.9686790000 |
| C | 2.1496570000 | 4.8071610000 | -0.1839050000 |
| H | 0.1056430000 | 4.6118750000 | -0.8511090000 |
| H | 1.2914820000 | 4.1041520000 | -2.0382870000 |
| C | 3.5717800000 | 4.3533260000 | -0.5168490000 |
| H | 1.9631930000 | 4.6909310000 | 0.8888620000 |
| H | 2.0640540000 | 5.8734270000 | -0.4086860000 |
| H | 4.2711090000 | 5.0581900000 | -0.0588890000 |
| C | 3.2452860000 | 1.7960130000 | -0.7890830000 |
| H | 3.7453600000 | 0.8570910000 | -0.5486980000 |
| C | 3.9455430000 | 2.9451830000 | -0.0485790000 |
| H | 3.3553450000 | 1.9414710000 | -1.8707050000 |
| H | 5.0208650000 | 2.8102090000 | -0.1904360000 |
| H | 3.7271090000 | 4.4249570000 | -1.6004710000 |
| H | 3.7559100000 | 2.8525120000 | 1.0259300000 |
| H | 1.1745830000 | -0.3007720000 | -2.4551650000 |
| H | 0.7881000000 | -2.0228510000 | -2.5486420000 |
| H | 2.3265760000 | -1.4314550000 | -3.1780790000 |

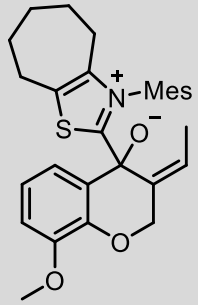
| | | | |
|---|---|---|---|
| H | 1.3976750000 | -0.0232260000 | 2.7146970000 |
| H | 2.7321730000 | 1.0087620000 | 2.1586690000 |
| H | 3.0640360000 | -0.3049910000 | 3.2976520000 |
| H | 5.4215900000 | -3.9593180000 | 1.1122320000 |
| H | 4.8640310000 | -4.5743030000 | -0.4532830000 |
| H | 3.9818180000 | -4.9715030000 | 1.0244130000 |
| C | -0.9994530000 | -1.8108450000 | -0.2958580000 |
| C | -1.7594860000 | -1.4282190000 | -1.5281490000 |
| H | -1.3156770000 | -0.5368890000 | -1.9925560000 |
| O | -3.1318080000 | -1.1248250000 | -1.2458620000 |
| H | -1.7876020000 | -2.2192620000 | -2.2747680000 |
| C | -0.4131190000 | -2.9808800000 | -0.0608360000 |
| C | -0.3394320000 | -4.1744290000 | -0.9619770000 |
| H | -0.6384580000 | -5.0775560000 | -0.4238090000 |
| H | 0.6969980000 | -4.3297090000 | -1.2836080000 |
| H | -0.9634500000 | -4.0875080000 | -1.8517210000 |
| H | 0.1062680000 | -3.0501810000 | 0.8943220000 |

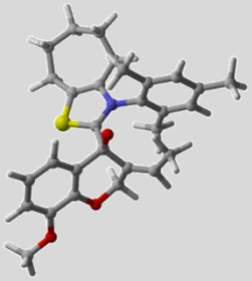
Thermochemie

Zero-point correction= 0.562697 (Hartree/Particle)
Thermal correction to Energy= 0.594947
Thermal correction to Enthalpy= 0.595892
Thermal correction to Gibbs Free Energy= 0.500133
Sum of electronic and zero-point Energies= -1802.738482
Sum of electronic and thermal Energies= -1802.706231
Sum of electronic and thermal Enthalpies= -1802.705287
Sum of electronic and thermal Free Energies= -1802.801046

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 373.335 | 125.990 | 201.541 |

**[24b + A]**
**(Z)**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0879060000 | 0.5671230000 | 1.1251080000 |
| C | -4.1456390000 | 0.7585190000 | 2.1421690000 |
| C | -2.8481480000 | 0.3129490000 | 1.9796790000 |
| C | -2.4479230000 | -0.3160860000 | 0.7951910000 |
| C | -3.3867100000 | -0.5200560000 | -0.2114760000 |
| C | -4.7184980000 | -0.0775570000 | -0.0458830000 |
| H | -6.1029000000 | 0.9148320000 | 1.2625280000 |
| H | -4.4476270000 | 1.2497480000 | 3.0594040000 |
| H | -2.1062460000 | 0.4158360000 | 2.7623710000 |
| C | -0.9678460000 | -0.8133750000 | 0.6972420000 |
| O | -5.5539620000 | -0.3334090000 | -1.0871820000 |
| C | -6.9041550000 | 0.0714410000 | -0.9504340000 |
| H | -7.3785130000 | -0.4223030000 | -0.0974130000 |
| H | -7.4031750000 | -0.2301470000 | -1.8684250000 |
| H | -6.9807390000 | 1.1564550000 | -0.8331590000 |
| O | -0.4467170000 | -1.1124540000 | 1.8758300000 |
| N | 1.1636490000 | 0.4444470000 | -0.0973660000 |

| | | | |
|---|---|---|---|
| C | -0.1482520000 | 0.4164370000 | 0.1340510000 |
| S | -0.8045340000 | 1.9765980000 | -0.0390340000 |
| C | 0.7346260000 | 2.6667880000 | -0.4312000000 |
| C | 1.6925350000 | 1.7098150000 | -0.4132050000 |
| C | 2.0301690000 | -0.7206340000 | -0.0463730000 |
| C | 2.6916350000 | -0.9886440000 | 1.1562910000 |
| C | 3.5969440000 | -2.0439950000 | 1.1659370000 |
| C | 3.8574940000 | -2.8002260000 | 0.0208600000 |
| C | 3.2046470000 | -2.4677090000 | -1.1618040000 |
| C | 2.2859500000 | -1.4175720000 | -1.2241160000 |
| C | 2.4430020000 | -0.1441010000 | 2.3727430000 |
| H | 4.1189920000 | -2.2770640000 | 2.0889020000 |
| C | 4.8111150000 | -3.9641510000 | 0.0792450000 |
| H | 3.4170120000 | -3.0284630000 | -2.0671330000 |
| C | 1.6227390000 | -1.0778190000 | -2.5325140000 |
| C | 0.8847290000 | 4.1252060000 | -0.7546910000 |
| C | 1.9594390000 | 4.8384090000 | 0.0741590000 |
| H | -0.0779090000 | 4.6181900000 | -0.6034820000 |
| H | 1.1207430000 | 4.2254890000 | -1.8207220000 |
| C | 3.3962930000 | 4.4487730000 | -0.2787540000 |
| H | 1.7748370000 | 4.6551040000 | 1.1378200000 |
| H | 1.8413240000 | 5.9127270000 | -0.0893110000 |
| H | 4.0716920000 | 5.1456430000 | 0.2250910000 |
| C | 3.1511470000 | 1.9061390000 | -0.7110170000 |
| H | 3.6813100000 | 0.9709660000 | -0.5285510000 |
| C | 3.8101260000 | 3.0271360000 | 0.1057460000 |
| H | 3.2614050000 | 2.1235470000 | -1.7805270000 |
| H | 4.8901380000 | 2.9337440000 | -0.0339150000 |
| H | 3.5532570000 | 4.5900190000 | -1.3552540000 |
| H | 3.6151860000 | 2.8626110000 | 1.1706580000 |
| H | 1.2527750000 | -0.0513590000 | -2.5602520000 |
| H | 0.7762470000 | -1.7470570000 | -2.7092830000 |
| H | 2.3273440000 | -1.2088240000 | -3.3548840000 |
| H | 1.3838400000 | -0.2169050000 | 2.6359650000 |
| H | 2.6774900000 | 0.9065180000 | 2.1726260000 |
| H | 3.0609830000 | -0.4785100000 | 3.2057500000 |
| H | 5.6845680000 | -3.7263650000 | 0.6891020000 |
| H | 5.1485580000 | -4.2509570000 | -0.9172000000 |
| H | 4.3204880000 | -4.8311510000 | 0.5310770000 |
| C | -0.9898090000 | -1.8805680000 | -0.4104510000 |
| C | -1.7399790000 | -1.4373140000 | -1.6348080000 |
| H | -1.3000760000 | -0.5214980000 | -2.0530840000 |
| O | -3.1222290000 | -1.1633760000 | -1.3782030000 |
| H | -1.7318050000 | -2.2067970000 | -2.4067060000 |
| C | -0.4617350000 | -3.1048910000 | -0.3583970000 |
| C | 0.3687520000 | -3.7257600000 | 0.7233370000 |
| H | 1.3132530000 | -4.0795260000 | 0.2980240000 |
| H | -0.1452750000 | -4.6026690000 | 1.1305900000 |
| H | 0.5640400000 | -3.0136920000 | 1.5200080000 |
| H | -0.6393820000 | -3.7405750000 | -1.2278960000 |

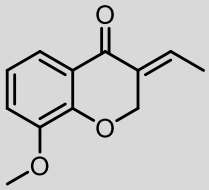
Thermochemie

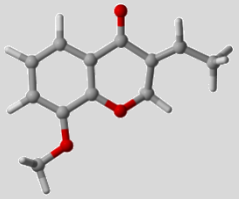
Zero-point correction= 0.562395 (Hartree/Particle)
Thermal correction to Energy= 0.594620
Thermal correction to Enthalpy= 0.595565
Thermal correction to Gibbs Free Energy= 0.499822
Sum of electronic and zero-point Energies= -1802.735651
Sum of electronic and thermal Energies= -1802.703426
Sum of electronic and thermal Enthalpies= -1802.702482
Sum of electronic and thermal Free Energies= -1802.798224

| | E (Thermal) | CV | S |
|---|---|---|---|

| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 373.130 | 126.043 | 201.506 |

**24b (E)**





27

XYZ-Matrix in Ångström

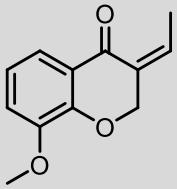
| | | | |
|---|---|---|---|
| C | 2.7952180000 | 0.8429980000 | -0.0437880000 |
| C | 2.1817450000 | 2.1026780000 | 0.0296540000 |
| C | 0.8101640000 | 2.2051750000 | 0.0886440000 |
| C | 0.0219590000 | 1.0432600000 | 0.0901020000 |
| C | 0.6273950000 | -0.2124620000 | 0.0404120000 |
| C | 2.0336680000 | -0.3154040000 | -0.0440710000 |
| H | 3.8742320000 | 0.7838220000 | -0.0947440000 |
| H | 2.8005580000 | 2.9912010000 | 0.0322990000 |
| H | 0.3114950000 | 3.1655320000 | 0.1233310000 |
| C | -1.4587850000 | 1.1432680000 | 0.0300180000 |
| O | -0.0722430000 | -1.3694340000 | 0.0385320000 |
| O | 2.5252670000 | -1.5736100000 | -0.1125290000 |
| C | 3.9336900000 | -1.7193000000 | -0.2040020000 |
| H | 4.3189540000 | -1.2365090000 | -1.1062790000 |
| H | 4.1206770000 | -2.7888570000 | -0.2543920000 |
| H | 4.4275780000 | -1.3016970000 | 0.6776180000 |
| O | -2.0229400000 | 2.2111390000 | -0.1176820000 |
| C | -2.1812640000 | -0.1585780000 | 0.1111680000 |
| C | -1.3603300000 | -1.2904350000 | 0.6583460000 |
| H | -1.2001120000 | -1.1469570000 | 1.7342580000 |
| H | -1.8227240000 | -2.2606630000 | 0.4996530000 |
| C | -3.4625630000 | -0.2199840000 | -0.2652220000 |
| C | -4.3601530000 | -1.4119540000 | -0.2684750000 |
| H | -3.9053880000 | 0.7160880000 | -0.5989310000 |
| H | -5.1693150000 | -1.2615120000 | 0.4525030000 |
| H | -3.8502970000 | -2.3409920000 | -0.0199410000 |
| H | -4.8307840000 | -1.5197800000 | -1.2486620000 |

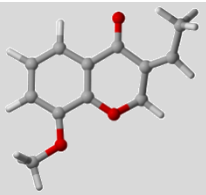
Thermochemie

Zero-point correction= 0.217943 (Hartree/Particle)
Thermal correction to Energy= 0.231239
Thermal correction to Enthalpy= 0.232184
Thermal correction to Gibbs Free Energy= 0.177922
Sum of electronic and zero-point Energies= -689.835730
Sum of electronic and thermal Energies= -689.822434
Sum of electronic and thermal Enthalpies= -689.821490
Sum of electronic and thermal Free Energies= -689.875751

| | E (Thermal) | CV | S |
|---|---|---|---|
| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 145.105 | 50.711 | 114.202 |

**24b (Z)**





27

XYZ-Matrix in Ångström

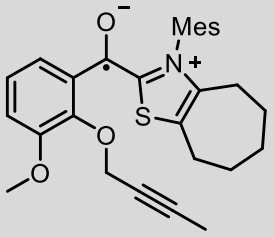
| | | | |
|---|---|---|---|
| C | -2.6272070000 | 1.1303490000 | 0.1330540000 |
| C | -1.8193170000 | 2.2713620000 | 0.0135460000 |
| C | -0.4574760000 | 2.1445880000 | -0.1406760000 |
| C | 0.1262920000 | 0.8686140000 | -0.1912940000 |
| C | -0.6757170000 | -0.2703480000 | -0.0980990000 |
| C | -2.0705630000 | -0.1378160000 | 0.0850190000 |
| H | -3.6950090000 | 1.2507280000 | 0.2583790000 |
| H | -2.2799380000 | 3.2504010000 | 0.0525940000 |
| H | 0.1904920000 | 3.0091990000 | -0.2100190000 |
| C | 1.6075470000 | 0.7310540000 | -0.2289170000 |
| O | -0.1861560000 | -1.5286160000 | -0.1552150000 |
| O | -2.7591460000 | -1.2975350000 | 0.1904530000 |
| C | -4.1644060000 | -1.2078710000 | 0.3638730000 |
| H | -4.4116420000 | -0.6741400000 | 1.2855680000 |
| H | -4.5235830000 | -2.2317640000 | 0.4279580000 |
| H | -4.6325820000 | -0.7078940000 | -0.4885190000 |
| O | 2.3418220000 | 1.7014030000 | -0.2180320000 |
| C | 2.0877390000 | -0.6762660000 | -0.2377650000 |
| C | 1.0855480000 | -1.6410720000 | -0.8046160000 |
| H | 0.9257010000 | -1.4440530000 | -1.8718610000 |
| H | 1.4032000000 | -2.6736620000 | -0.6747570000 |
| C | 3.2749790000 | -1.0745970000 | 0.2339850000 |
| C | 4.3647240000 | -0.2312060000 | 0.8124950000 |
| H | 3.4757800000 | -2.1443760000 | 0.1983430000 |
| H | 4.8447650000 | -0.7610470000 | 1.6370050000 |
| H | 4.0038500000 | 0.7372760000 | 1.1503190000 |
| H | 5.1339500000 | -0.0534280000 | 0.0537120000 |

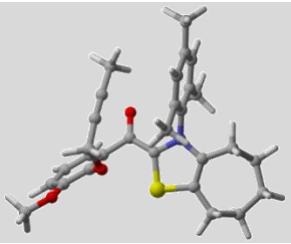
Thermochemie

| | |
|---|---|
| Zero-point correction= | 0.217893 (Hartree/Particle) |
| Thermal correction to Energy= | 0.231095 |
| Thermal correction to Enthalpy= | 0.232039 |
| Thermal correction to Gibbs Free Energy= | 0.178166 |
| Sum of electronic and zero-point Energies= | -689.834313 |
| Sum of electronic and thermal Energies= | -689.821111 |
| Sum of electronic and thermal Enthalpies= | -689.820166 |
| Sum of electronic and thermal Free Energies= | -689.874040 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 145.014 | 50.655 | 113.386 |

**21b**



66

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 5.0606830000 | -0.6141340000 | 1.2292430000 |
| C | 4.3448290000 | -0.4209480000 | 2.4122520000 |
| C | 2.9891210000 | -0.1500620000 | 2.3793830000 |
| C | 2.3101960000 | -0.0799050000 | 1.1560550000 |
| C | 3.0197760000 | -0.2662620000 | -0.0282390000 |
| C | 4.4034730000 | -0.5313420000 | 0.0065210000 |
| H | 6.1205740000 | -0.8244660000 | 1.2728250000 |

| | | | |
|---|---|---|---|
| H | 4.8641980000 | -0.4851810000 | 3.3608890000 |
| H | 2.4321760000 | 0.0133310000 | 3.2939830000 |
| C | 0.8444420000 | 0.2524060000 | 1.1854860000 |
| O | 2.3968740000 | -0.2067240000 | -1.2509430000 |
| O | 5.0001230000 | -0.6828780000 | -1.2019380000 |
| C | 6.3982030000 | -0.9245860000 | -1.2177450000 |
| H | 6.9427640000 | -0.1008210000 | -0.7482530000 |
| H | 6.6777930000 | -0.9969730000 | -2.2658480000 |
| H | 6.6386860000 | -1.8622010000 | -0.7094070000 |
| O | 0.4525200000 | 1.2505880000 | 1.8239200000 |
| C | 2.5925190000 | 1.0317930000 | -1.9503550000 |
| H | 3.6624630000 | 1.2359650000 | -2.0430970000 |
| C | 1.8965180000 | 2.1356850000 | -1.2859250000 |
| H | 2.1846100000 | 0.8645690000 | -2.9482520000 |
| C | 1.2813560000 | 2.9671100000 | -0.6705810000 |
| C | 0.5190350000 | 3.9308280000 | 0.1155310000 |
| N | -1.3916340000 | -0.4149910000 | 0.3381960000 |
| C | -0.0465940000 | -0.6466750000 | 0.5428880000 |
| S | 0.3648200000 | -2.2692650000 | 0.0649980000 |
| C | -1.3003880000 | -2.6033180000 | -0.3665450000 |
| C | -2.0828150000 | -1.5216020000 | -0.1694060000 |
| C | -1.8963000000 | 0.9233140000 | 0.1408770000 |
| C | -2.5658170000 | 1.5679320000 | 1.1821500000 |
| C | -3.0777150000 | 2.8387520000 | 0.9358530000 |
| C | -2.9325510000 | 3.4591390000 | -0.3074080000 |
| C | -2.2710590000 | 2.7742500000 | -1.3235460000 |
| C | -1.7424210000 | 1.4984170000 | -1.1213430000 |
| C | -2.7153060000 | 0.8959950000 | 2.5175340000 |
| H | -3.5987760000 | 3.3597850000 | 1.7338140000 |
| C | -3.4436660000 | 4.8592720000 | -0.5264860000 |
| H | -2.1545780000 | 3.2424760000 | -2.2968740000 |
| C | -1.0621240000 | 0.7470340000 | -2.2355050000 |
| C | -1.7030720000 | -3.9478300000 | -0.8995900000 |
| C | -2.8500930000 | -4.6045570000 | -0.1219350000 |
| H | -0.8329200000 | -4.6078090000 | -0.8836310000 |
| H | -1.9926540000 | -3.8451730000 | -1.9528160000 |
| C | -4.2155840000 | -3.9434190000 | -0.3238810000 |
| H | -2.5989430000 | -4.6199630000 | 0.9440400000 |
| H | -2.9214410000 | -5.6460610000 | -0.4479800000 |
| H | -4.9763560000 | -4.5869490000 | 0.1272030000 |
| C | -3.5579140000 | -1.4433140000 | -0.4404550000 |
| H | -3.9220280000 | -0.4645530000 | -0.1235020000 |
| C | -4.3712450000 | -2.5386700000 | 0.2636080000 |
| H | -3.7290250000 | -1.5031040000 | -1.5224410000 |
| H | -5.4258090000 | -2.2565260000 | 0.2003020000 |
| H | -4.4394030000 | -3.9069990000 | -1.3974300000 |
| H | -4.1094820000 | -2.5508690000 | 1.3273980000 |
| H | -1.7168960000 | -0.0405910000 | -2.6230600000 |
| H | -0.1416160000 | 0.2714690000 | -1.8884630000 |
| H | -0.8166760000 | 1.4215270000 | -3.0562140000 |
| H | -1.7272740000 | 0.7294020000 | 2.9533990000 |
| H | -3.2016020000 | -0.0785710000 | 2.4154370000 |
| H | -3.3082320000 | 1.5094800000 | 3.1961260000 |
| H | -4.3893320000 | 5.0212450000 | -0.0063580000 |
| H | -3.5907420000 | 5.0652240000 | -1.5874520000 |
| H | -2.7263880000 | 5.5896690000 | -0.1398040000 |
| H | 1.1814450000 | 4.5379810000 | 0.7352060000 |
| H | -0.1657570000 | 3.3787950000 | 0.7655190000 |
| H | -0.0635220000 | 4.5893690000 | -0.5315050000 |

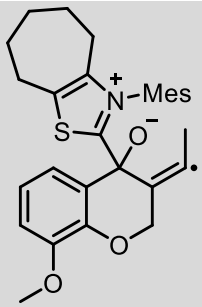
Thermochemie

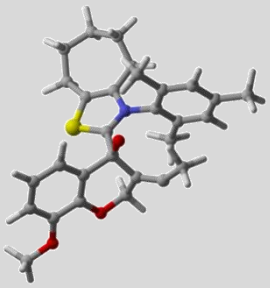
Zero-point correction= 0.548891 (Hartree/Particle)

Thermal correction to Energy= 0.582398
Thermal correction to Enthalpy= 0.583342
Thermal correction to Gibbs Free Energy= 0.484127
Sum of electronic and zero-point Energies= -1802.122454
Sum of electronic and thermal Energies= -1802.088948
Sum of electronic and thermal Enthalpies= -1802.088003
Sum of electronic and thermal Free Energies= -1802.187218

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 365.460 | 127.998 | 208.816 |

**26b**



66
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0858240000 | 0.5012380000 | 1.1583740000 |
| C | -4.1398910000 | 0.6722310000 | 2.1757370000 |
| C | -2.8402920000 | 0.2419250000 | 1.9938450000 |
| C | -2.4417420000 | -0.3518690000 | 0.7902470000 |
| C | -3.3831510000 | -0.5338990000 | -0.2189630000 |
| C | -4.7177510000 | -0.1066990000 | -0.0322830000 |
| H | -6.1028830000 | 0.8363190000 | 1.3107020000 |
| H | -4.4408320000 | 1.1357610000 | 3.1075930000 |
| H | -2.0952950000 | 0.3317930000 | 2.7752370000 |
| C | -0.9644660000 | -0.8327950000 | 0.6723790000 |
| O | -5.5571330000 | -0.3394220000 | -1.0751820000 |
| C | -6.9091250000 | 0.0529320000 | -0.9203220000 |
| H | -7.3761340000 | -0.4674900000 | -0.0792100000 |
| H | -7.4110570000 | -0.2257970000 | -1.8438790000 |
| H | -6.9914350000 | 1.1337060000 | -0.7720360000 |
| O | -0.4312410000 | -1.2012030000 | 1.8206960000 |
| N | 1.1630580000 | 0.4403420000 | -0.0863830000 |
| C | -0.1498470000 | 0.4036990000 | 0.1364860000 |
| S | -0.8173050000 | 1.9578550000 | -0.0442260000 |
| C | 0.7183120000 | 2.6579570000 | -0.4309240000 |
| C | 1.6835370000 | 1.7080830000 | -0.4034060000 |
| C | 2.0351460000 | -0.7207410000 | -0.0361740000 |
| C | 2.6811900000 | -1.0012880000 | 1.1716680000 |
| C | 3.5867800000 | -2.0565190000 | 1.1808370000 |
| C | 3.8634730000 | -2.7986540000 | 0.0299390000 |
| C | 3.2264290000 | -2.4523790000 | -1.1572630000 |
| C | 2.3053690000 | -1.4041750000 | -1.2187010000 |
| C | 2.4178580000 | -0.1697820000 | 2.3940550000 |
| H | 4.0975440000 | -2.2997020000 | 2.1074810000 |
| C | 4.8182030000 | -3.9617760000 | 0.0867850000 |
| H | 3.4497690000 | -3.0033100000 | -2.0659170000 |
| C | 1.6501170000 | -1.0561750000 | -2.5289190000 |
| C | 0.8610630000 | 4.1167980000 | -0.7554430000 |
| C | 1.9202910000 | 4.8384790000 | 0.0861030000 |
| H | -0.1069780000 | 4.6028540000 | -0.6168350000 |
| H | 1.1094320000 | 4.2169690000 | -1.8186420000 |
| C | 3.3645320000 | 4.4595880000 | -0.2485680000 |

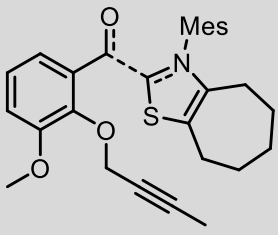
| | | | |
|---|---|---|---|
| H | 1.7237100000 | 4.6543810000 | 1.1474900000 |
| H | 1.7962180000 | 5.9117690000 | -0.0794820000 |
| H | 4.0279610000 | 5.1605950000 | 0.2652880000 |
| C | 3.1428900000 | 1.9164110000 | -0.6880110000 |
| H | 3.6785310000 | 0.9847910000 | -0.5033750000 |
| C | 3.7843170000 | 3.0403910000 | 0.1385960000 |
| H | 3.2612080000 | 2.1380360000 | -1.7557380000 |
| H | 4.8665240000 | 2.9553690000 | 0.0112070000 |
| H | 3.5344640000 | 4.6038580000 | -1.3226510000 |
| H | 3.5784160000 | 2.8721400000 | 1.2009120000 |
| H | 1.2871700000 | -0.0269970000 | -2.5556240000 |
| H | 0.7995640000 | -1.7201920000 | -2.7075070000 |
| H | 2.3565330000 | -1.1904100000 | -3.3491290000 |
| H | 1.3586870000 | -0.2553090000 | 2.6525400000 |
| H | 2.6430110000 | 0.8847340000 | 2.2041450000 |
| H | 3.0349160000 | -0.5051540000 | 3.2273330000 |
| H | 5.6873120000 | -3.7269360000 | 0.7039830000 |
| H | 5.1626390000 | -4.2411350000 | -0.9093490000 |
| H | 4.3260220000 | -4.8326540000 | 0.5293580000 |
| C | -0.9896810000 | -1.8774510000 | -0.4871360000 |
| C | -1.7545140000 | -1.4175780000 | -1.6967790000 |
| H | -1.3120920000 | -0.4988520000 | -2.1055270000 |
| O | -3.1276750000 | -1.1407200000 | -1.4074490000 |
| H | -1.7610970000 | -2.1789220000 | -2.4753340000 |
| C | -0.4311140000 | -3.0581510000 | -0.3983010000 |
| C | 0.3934530000 | -3.8331650000 | 0.5370310000 |
| H | 1.3142050000 | -4.1735620000 | 0.0558250000 |
| H | -0.1475010000 | -4.7117020000 | 0.8983070000 |
| H | 0.6419660000 | -3.1820830000 | 1.3852820000 |

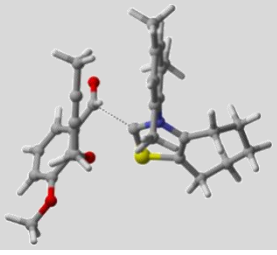
Thermochemie

Zero-point correction= 0.549193 (Hartree/Particle)
Thermal correction to Energy= 0.581491
Thermal correction to Enthalpy= 0.582436
Thermal correction to Gibbs Free Energy= 0.485685
Sum of electronic and zero-point Energies= -1802.076419
Sum of electronic and thermal Energies= -1802.044120
Sum of electronic and thermal Enthalpies= -1802.043176
Sum of electronic and thermal Free Energies= -1802.139927

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 364.891 | 125.821 | 203.629 |

**TS-1b**



67

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.7613720000 | -1.6580750000 | 0.8561560000 |
| C | 4.2830620000 | -1.4583890000 | 2.1522290000 |
| C | 3.1163090000 | -0.7452650000 | 2.3731640000 |
| C | 2.4011900000 | -0.2162150000 | 1.2968190000 |
| C | 2.8696970000 | -0.4173290000 | 0.0030580000 |
| C | 4.0527190000 | -1.1422500000 | -0.2253170000 |
| H | 5.6742000000 | -2.2173360000 | 0.7013320000 |

| | | | |
|---|---|---|---|
| H | 4.8399430000 | -1.8658690000 | 2.9877660000 |
| H | 2.7371800000 | -0.5716740000 | 3.3726960000 |
| C | 1.1591460000 | 0.6038030000 | 1.5640200000 |
| O | 2.1331480000 | 0.0046660000 | -1.0768450000 |
| O | 4.4104780000 | -1.2899140000 | -1.5275340000 |
| C | 5.6008400000 | -2.0113770000 | -1.8012810000 |
| H | 6.4676350000 | -1.5244980000 | -1.3461120000 |
| H | 5.7095540000 | -2.0123610000 | -2.8830330000 |
| H | 5.5257910000 | -3.0404870000 | -1.4398430000 |
| O | 0.8200220000 | 0.8565280000 | 2.7277320000 |
| C | 2.6737620000 | 1.1125260000 | -1.8074820000 |
| H | 3.7641040000 | 1.0557190000 | -1.8261900000 |
| C | 2.2156370000 | 2.3851760000 | -1.2422190000 |
| H | 2.3100530000 | 1.0031690000 | -2.8306410000 |
| C | 1.7750950000 | 3.3850160000 | -0.7382710000 |
| C | 1.2212780000 | 4.5683120000 | -0.0865840000 |
| N | -1.3548500000 | -0.3992250000 | 0.0962830000 |
| C | -0.2146810000 | -0.8001430000 | 0.6609950000 |
| S | -0.1783680000 | -2.5028160000 | 0.5856490000 |
| C | -1.7222730000 | -2.6275800000 | -0.2162030000 |
| C | -2.2249260000 | -1.3866560000 | -0.4062720000 |
| C | -1.6559190000 | 1.0145580000 | 0.0332520000 |
| C | -2.2026070000 | 1.6231650000 | 1.1654510000 |
| C | -2.4504150000 | 2.9915970000 | 1.1020850000 |
| C | -2.1646410000 | 3.7358000000 | -0.0450820000 |
| C | -1.6277730000 | 3.0829750000 | -1.1514940000 |
| C | -1.3627620000 | 1.7129600000 | -1.1350880000 |
| C | -2.4880140000 | 0.8178270000 | 2.4036880000 |
| H | -2.8711080000 | 3.4903950000 | 1.9701570000 |
| C | -2.4068860000 | 5.2229520000 | -0.0632490000 |
| H | -1.3918850000 | 3.6502020000 | -2.0471330000 |
| C | -0.7859570000 | 1.0087390000 | -2.3326230000 |
| C | -2.3505210000 | -3.9345190000 | -0.6032960000 |
| C | -3.7611560000 | -4.1262720000 | -0.0317220000 |
| H | -1.7070360000 | -4.7502780000 | -0.2674760000 |
| H | -2.3914270000 | -4.0003080000 | -1.6972580000 |
| C | -4.8360620000 | -3.2474380000 | -0.6772270000 |
| H | -3.7374540000 | -3.9513590000 | 1.0491710000 |
| H | -4.0411350000 | -5.1730600000 | -0.1787380000 |
| H | -5.8128040000 | -3.5935740000 | -0.3273810000 |
| C | -3.5374170000 | -1.0409550000 | -1.0454380000 |
| H | -3.6808430000 | 0.0403730000 | -0.9972570000 |
| C | -4.7376390000 | -1.7450980000 | -0.3965370000 |
| H | -3.4960950000 | -1.3066820000 | -2.1088480000 |
| H | -5.6451760000 | -1.2671980000 | -0.7751430000 |
| H | -4.8230590000 | -3.4084090000 | -1.7624710000 |
| H | -4.7158440000 | -1.5714390000 | 0.6846350000 |
| H | -1.5592450000 | 0.4341370000 | -2.8534750000 |
| H | 0.0006670000 | 0.3138880000 | -2.0308480000 |
| H | -0.3696810000 | 1.7325270000 | -3.0344090000 |
| H | -1.5459740000 | 0.4919400000 | 2.8537030000 |
| H | -3.0769040000 | -0.0730000000 | 2.1679340000 |
| H | -3.0374280000 | 1.4152300000 | 3.1310890000 |
| H | -1.7142100000 | 5.7321070000 | 0.6131610000 |
| H | -3.4199830000 | 5.4590480000 | 0.2690840000 |
| H | -2.2672380000 | 5.6345240000 | -1.0636220000 |
| H | 0.8922740000 | 1.2795120000 | 0.7419660000 |
| H | 0.5903220000 | 5.1325970000 | -0.7765170000 |
| H | 2.0152250000 | 5.2223510000 | 0.2773320000 |
| H | 0.6034750000 | 4.2621510000 | 0.7619850000 |

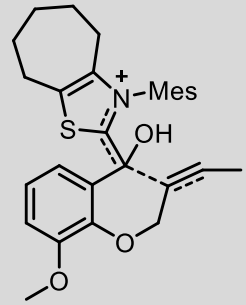
Thermochemie

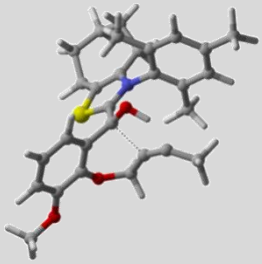
Zero-point correction= 0.559223 (Hartree/Particle)
Thermal correction to Energy= 0.592750
Thermal correction to Enthalpy= 0.593694
Thermal correction to Gibbs Free Energy= 0.493524
Sum of electronic and zero-point Energies= -1802.677090
Sum of electronic and thermal Energies= -1802.643563
Sum of electronic and thermal Enthalpies= -1802.642619
Sum of electronic and thermal Free Energies= -1802.742789

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 371.956 | 127.669 | 210.825 |

Imaginäre Frequenz
-127.0934

**TS-3b (E)**



67
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0521070000 | -0.2010820000 | 1.5009670000 |
| C | -4.1571100000 | -0.6565170000 | 2.4740310000 |
| C | -2.8195980000 | -0.8297240000 | 2.1712700000 |
| C | -2.3423620000 | -0.5401750000 | 0.8858200000 |
| C | -3.2386510000 | -0.1297200000 | -0.0992670000 |
| C | -4.6012820000 | 0.0569700000 | 0.2119790000 |
| H | -6.0943400000 | -0.0649720000 | 1.7551440000 |
| H | -4.5231400000 | -0.8678840000 | 3.4716150000 |
| H | -2.1162510000 | -1.1869920000 | 2.9130810000 |
| C | -0.9048160000 | -0.7425930000 | 0.5536360000 |
| O | -5.3890200000 | 0.4763920000 | -0.8110810000 |
| C | -6.7697360000 | 0.6462080000 | -0.5423420000 |
| H | -7.2276860000 | -0.2950550000 | -0.2249360000 |
| H | -7.2193580000 | 0.9727520000 | -1.4771370000 |
| H | -6.9303810000 | 1.4082250000 | 0.2255880000 |
| O | -0.2669990000 | -1.7387650000 | 1.2261660000 |
| N | 1.2218460000 | 0.4480650000 | 0.0373910000 |
| C | -0.1212910000 | 0.4018990000 | 0.2388960000 |
| S | -0.7969360000 | 1.9787450000 | 0.0039470000 |
| C | 0.7687140000 | 2.6622280000 | -0.3649660000 |
| C | 1.7273100000 | 1.7194630000 | -0.2962760000 |
| C | 2.0898500000 | -0.7025500000 | 0.1423250000 |
| C | 2.5972660000 | -1.0283480000 | 1.4038190000 |
| C | 3.4425630000 | -2.1259150000 | 1.5004020000 |
| C | 3.7854530000 | -2.8855190000 | 0.3769930000 |
| C | 3.2826860000 | -2.5062020000 | -0.8627030000 |
| C | 2.4335020000 | -1.4051450000 | -1.0080760000 |
| C | 2.2016230000 | -0.2223430000 | 2.6089410000 |
| H | 3.8397160000 | -2.4021480000 | 2.4724900000 |
| C | 4.6657910000 | -4.0999850000 | 0.5169440000 |
| H | 3.5550940000 | -3.0750400000 | -1.7472730000 |
| C | 1.9639880000 | -0.9908380000 | -2.3770030000 |
| C | 0.9135920000 | 4.1137150000 | -0.7199680000 |

| | | | |
|---|---|---|---|
| C | 1.9439640000 | 4.8575840000 | 0.1382760000 |
| H | -0.0592550000 | 4.5995990000 | -0.6160920000 |
| H | 1.1907270000 | 4.2001220000 | -1.7776100000 |
| C | 3.3997020000 | 4.4772000000 | -0.1415910000 |
| H | 1.7145160000 | 4.6930090000 | 1.1964410000 |
| H | 1.8247660000 | 5.9277990000 | -0.0515770000 |
| H | 4.0445040000 | 5.1873900000 | 0.3837570000 |
| C | 3.1915790000 | 1.9309930000 | -0.5546600000 |
| H | 3.7263320000 | 1.0025260000 | -0.3509180000 |
| C | 3.8127680000 | 3.0635310000 | 0.2744210000 |
| H | 3.3318740000 | 2.1445800000 | -1.6214240000 |
| H | 4.8986060000 | 2.9820050000 | 0.1750770000 |
| H | 3.6041160000 | 4.6075450000 | -1.2116520000 |
| H | 3.5805490000 | 2.9057550000 | 1.3331840000 |
| H | 1.1043690000 | -0.3237990000 | -2.3293800000 |
| H | 1.6812220000 | -1.8679650000 | -2.9621980000 |
| H | 2.7690250000 | -0.4744090000 | -2.9092790000 |
| H | 2.3874060000 | 0.8440860000 | 2.4519870000 |
| H | 2.7563360000 | -0.5445390000 | 3.4899830000 |
| H | 1.1321230000 | -0.3485400000 | 2.7980900000 |
| H | 5.4305350000 | -3.9459030000 | 1.2801000000 |
| H | 5.1586830000 | -4.3410110000 | -0.4256580000 |
| H | 4.0717840000 | -4.9681970000 | 0.8155870000 |
| C | -1.1636450000 | -1.6544070000 | -1.2181030000 |
| C | -1.8753680000 | -0.6567740000 | -2.0430560000 |
| H | -1.1648770000 | 0.0555230000 | -2.4760690000 |
| O | -2.8566790000 | 0.1594160000 | -1.3721250000 |
| H | -2.3939140000 | -1.1647780000 | -2.8607140000 |
| C | -0.6322310000 | -2.7868030000 | -1.1321610000 |
| C | -0.3463960000 | -4.0783920000 | -1.8021850000 |
| H | -0.6686360000 | -4.9188640000 | -1.1830990000 |
| H | 0.7344530000 | -4.1907040000 | -1.9354330000 |
| H | -0.8255740000 | -4.1707000000 | -2.7831430000 |
| H | -0.1882440000 | -2.4726840000 | 0.4947150000 |

Thermochemie

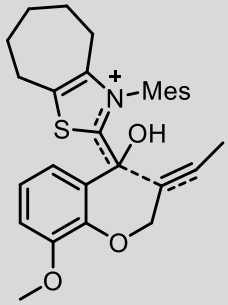
Zero-point correction= 0.558384 (Hartree/Particle)
Thermal correction to Energy= 0.591171
Thermal correction to Enthalpy= 0.592115
Thermal correction to Gibbs Free Energy= 0.494282
Sum of electronic and zero-point Energies= -1802.671243
Sum of electronic and thermal Energies= -1802.638456
Sum of electronic and thermal Enthalpies= -1802.637512
Sum of electronic and thermal Free Energies= -1802.735345

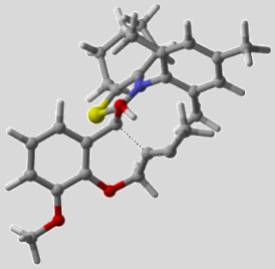
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 370.965 | 126.404 | 205.907 |

Imaginäre Frequenz

-434.1368

**TS-3b**
**(Z)**



67
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0454170000 | 0.3132290000 | 1.4068450000 |
| C | -4.0405250000 | 0.3949400000 | 2.3785420000 |
| C | -2.7411110000 | 0.0697000000 | 2.0538300000 |
| C | -2.4003570000 | -0.3465210000 | 0.7549790000 |
| C | -3.3969060000 | -0.4307510000 | -0.2145800000 |
| C | -4.7331730000 | -0.0969830000 | 0.1215110000 |
| H | -6.0632970000 | 0.5696410000 | 1.6677270000 |
| H | -4.2939800000 | 0.7139160000 | 3.3820530000 |
| H | -1.9531740000 | 0.1196080000 | 2.7966430000 |
| C | -0.9592760000 | -0.7147170000 | 0.4815890000 |
| O | -5.6305540000 | -0.2196590000 | -0.8886480000 |
| C | -6.9852500000 | 0.0722510000 | -0.5947530000 |
| H | -7.3690400000 | -0.5905010000 | 0.1861180000 |
| H | -7.5349480000 | -0.0963270000 | -1.5175960000 |
| H | -7.1051850000 | 1.1137710000 | -0.2827760000 |
| O | -0.4177820000 | -1.5273610000 | 1.4836170000 |
| N | 1.2197470000 | 0.4613500000 | 0.0541610000 |
| C | -0.1349170000 | 0.4112710000 | 0.1730750000 |
| S | -0.8138670000 | 1.9606610000 | -0.2053860000 |
| C | 0.7618510000 | 2.6320910000 | -0.5472080000 |
| C | 1.7251430000 | 1.7147960000 | -0.3397110000 |
| C | 2.0825340000 | -0.6951110000 | 0.1126370000 |
| C | 2.6171370000 | -1.0861530000 | 1.3407020000 |
| C | 3.5035830000 | -2.1618460000 | 1.3452710000 |
| C | 3.8702490000 | -2.8155780000 | 0.1682080000 |
| C | 3.3449850000 | -2.3623180000 | -1.0402510000 |
| C | 2.4466380000 | -1.2980380000 | -1.0933160000 |
| C | 2.2726130000 | -0.3419200000 | 2.6007370000 |
| H | 3.9252930000 | -2.4899180000 | 2.2904800000 |
| C | 4.7888010000 | -4.0085840000 | 0.2029210000 |
| H | 3.6350550000 | -2.8506970000 | -1.9657330000 |
| C | 1.9402430000 | -0.7776470000 | -2.4120110000 |
| C | 0.9335740000 | 4.0637850000 | -0.9637440000 |
| C | 1.8191250000 | 4.8717780000 | -0.0056620000 |
| H | -0.0499790000 | 4.5330620000 | -1.0347590000 |
| H | 1.3655980000 | 4.0949270000 | -1.9711950000 |
| C | 3.3077600000 | 4.5204430000 | -0.0717470000 |
| H | 1.4504960000 | 4.7429530000 | 1.0174240000 |
| H | 1.7050190000 | 5.9302830000 | -0.2549630000 |
| H | 3.8579850000 | 5.2531780000 | 0.5252470000 |
| C | 3.1999850000 | 1.9659010000 | -0.4655350000 |
| H | 3.7446350000 | 1.0552090000 | -0.2125070000 |
| C | 3.6932680000 | 3.1219400000 | 0.4184590000 |
| H | 3.4321560000 | 2.1908640000 | -1.5134350000 |
| H | 4.7842220000 | 3.0636200000 | 0.4585330000 |
| H | 3.6559870000 | 4.6413850000 | -1.1050790000 |
| H | 3.3302730000 | 2.9739190000 | 1.4411950000 |
| H | 2.4896500000 | 0.1233670000 | -2.7045870000 |
| H | 0.8808100000 | -0.5241220000 | -2.3611850000 |
| H | 2.0760410000 | -1.5253630000 | -3.1934440000 |

| | | | |
|---|---|---|---|
| H | 2.4893860000 | 0.7247210000 | 2.4908880000 |
| H | 2.8487820000 | -0.7245450000 | 3.4430320000 |
| H | 1.2086270000 | -0.4442480000 | 2.8208600000 |
| H | 5.4239210000 | -3.9942620000 | 1.0895750000 |
| H | 5.4251940000 | -4.0418800000 | -0.6827740000 |
| H | 4.2043570000 | -4.9331790000 | 0.2256390000 |
| C | -1.0490720000 | -1.8484390000 | -1.0060690000 |
| C | -1.8859440000 | -1.0747380000 | -1.9594230000 |
| H | -1.4311800000 | -0.1003330000 | -2.1777240000 |
| O | -3.2215060000 | -0.8312590000 | -1.4947150000 |
| H | -2.0087570000 | -1.6254540000 | -2.8893570000 |
| C | -0.4996240000 | -2.9978310000 | -1.0193880000 |
| C | 0.4143150000 | -3.9105860000 | -0.2848620000 |
| H | 1.0229070000 | -4.4957710000 | -0.9804610000 |
| H | -0.1753630000 | -4.6391850000 | 0.2833640000 |
| H | 1.1085300000 | -3.4111600000 | 0.4041120000 |
| H | -0.5390430000 | -2.4374720000 | 1.1834020000 |

Thermochemie

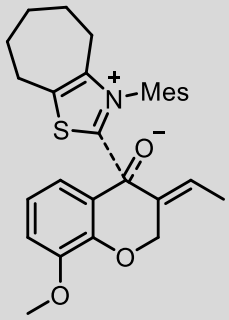
Zero-point correction= 0.559333 (Hartree/Particle)
Thermal correction to Energy= 0.592250
Thermal correction to Enthalpy= 0.593194
Thermal correction to Gibbs Free Energy= 0.495408
Sum of electronic and zero-point Energies= -1802.663062
Sum of electronic and thermal Energies= -1802.630145
Sum of electronic and thermal Enthalpies= -1802.629201
Sum of electronic and thermal Free Energies= -1802.726987

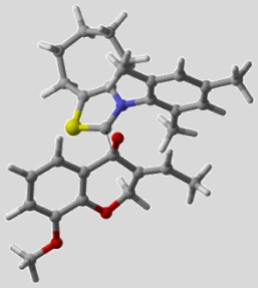
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 371.642 | 127.451 | 205.809 |

Imaginäre Frequenz

-546.9596

**TS-4b (E)**



67

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -4.9381520000 | 0.8990600000 | 1.2021170000 |
| C | -3.9469060000 | 1.0836510000 | 2.1738030000 |
| C | -2.7206190000 | 0.4624590000 | 2.0427170000 |
| C | -2.4486780000 | -0.3443020000 | 0.9326930000 |
| C | -3.4290520000 | -0.5290740000 | -0.0369400000 |
| C | -4.6899800000 | 0.0924140000 | 0.1007620000 |
| H | -5.8968510000 | 1.3861870000 | 1.3192310000 |
| H | -4.1572500000 | 1.7119240000 | 3.0309230000 |
| H | -1.9456750000 | 0.5727860000 | 2.7923930000 |
| C | -1.1079250000 | -1.0677620000 | 0.8452750000 |
| O | -5.5818450000 | -0.1611630000 | -0.8909350000 |
| C | -6.8533300000 | 0.4561580000 | -0.7939010000 |
| H | -7.3800090000 | 0.1328960000 | 0.1085130000 |
| H | -7.4097110000 | 0.1392300000 | -1.6727400000 |

| | | | |
|---|---|---|---|
| H | -6.7611330000 | 1.5460990000 | -0.7930270000 |
| O | -0.5368280000 | -1.3762250000 | 1.9159020000 |
| N | 1.2459200000 | 0.4863100000 | -0.1567310000 |
| C | -0.0732700000 | 0.4483560000 | 0.0266570000 |
| S | -0.6941420000 | 2.0108050000 | -0.2530820000 |
| C | 0.8634660000 | 2.6867160000 | -0.6290140000 |
| C | 1.8095100000 | 1.7253180000 | -0.5253580000 |
| C | 2.0665170000 | -0.6882660000 | 0.0576710000 |
| C | 2.5520590000 | -0.9232530000 | 1.3409580000 |
| C | 3.3473830000 | -2.0536600000 | 1.5292460000 |
| C | 3.6630250000 | -2.9103700000 | 0.4767450000 |
| C | 3.1708260000 | -2.6188620000 | -0.7969340000 |
| C | 2.3640280000 | -1.5091570000 | -1.0307400000 |
| C | 2.2218680000 | 0.0115990000 | 2.4710050000 |
| H | 3.7296630000 | -2.2646560000 | 2.5230150000 |
| C | 4.5371570000 | -4.1184330000 | 0.6926250000 |
| H | 3.4181540000 | -3.2743550000 | -1.6271400000 |
| C | 1.8151260000 | -1.2083080000 | -2.3984560000 |
| C | 1.0579500000 | 4.1290490000 | -0.9963680000 |
| C | 2.0939070000 | 4.8487480000 | -0.1235310000 |
| H | 0.0982110000 | 4.6444550000 | -0.9207690000 |
| H | 1.3624920000 | 4.1908440000 | -2.0480100000 |
| C | 3.5446760000 | 4.4340150000 | -0.3806620000 |
| H | 1.8446830000 | 4.6925210000 | 0.9314440000 |
| H | 2.0031100000 | 5.9210130000 | -0.3166880000 |
| H | 4.1973760000 | 5.1355410000 | 0.1464590000 |
| C | 3.2817790000 | 1.8893720000 | -0.7662180000 |
| H | 3.7850960000 | 0.9466910000 | -0.5444080000 |
| C | 3.9240790000 | 3.0164640000 | 0.0553500000 |
| H | 3.4419350000 | 2.0885870000 | -1.8329140000 |
| H | 5.0083350000 | 2.9091270000 | -0.0349360000 |
| H | 3.7658120000 | 4.5500460000 | -1.4489970000 |
| H | 3.6812300000 | 2.8777880000 | 1.1141650000 |
| H | 2.0495120000 | -0.1863650000 | -2.7093250000 |
| H | 0.7257760000 | -1.3096150000 | -2.4012410000 |
| H | 2.2262070000 | -1.8957430000 | -3.1377270000 |
| H | 1.1476210000 | -0.0273580000 | 2.6679160000 |
| H | 2.4889910000 | 1.0426750000 | 2.2212630000 |
| H | 2.7605680000 | -0.2736020000 | 3.3744920000 |
| H | 4.0860270000 | -5.0092060000 | 0.2507320000 |
| H | 4.6978350000 | -4.3041750000 | 1.7547830000 |
| H | 5.5134080000 | -3.9767810000 | 0.2215180000 |
| C | -1.0584160000 | -1.9938020000 | -0.3546120000 |
| C | -1.9012020000 | -1.5498690000 | -1.5127630000 |
| H | -1.5154620000 | -0.6107990000 | -1.9291860000 |
| O | -3.2636870000 | -1.3204390000 | -1.1309930000 |
| H | -1.9447780000 | -2.2890980000 | -2.3091090000 |
| C | -0.3090640000 | -3.0940900000 | -0.3047300000 |
| C | -0.1180580000 | -4.1278470000 | -1.3700810000 |
| H | -0.2839100000 | -5.1277380000 | -0.9607660000 |
| H | 0.9166110000 | -4.1032770000 | -1.7284080000 |
| H | -0.7778950000 | -3.9953890000 | -2.2270410000 |
| H | 0.2555370000 | -3.2326520000 | 0.6163170000 |

Thermochemie

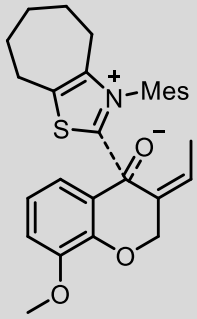
Zero-point correction= 0.560941 (Hartree/Particle)
Thermal correction to Energy= 0.593367
Thermal correction to Enthalpy= 0.594311
Thermal correction to Gibbs Free Energy= 0.497208
Sum of electronic and zero-point Energies= -1802.732488
Sum of electronic and thermal Energies= -1802.700062
Sum of electronic and thermal Enthalpies= -1802.699118

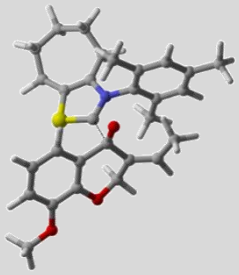
Sum of electronic and thermal Free Energies= -1802.796221

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 372.343 | 125.348 | 204.371 |

Imaginäre Frequenz
-172.9639

**TS-4b (Z)**



67
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -4.9621160000 | 0.7034780000 | 1.2159080000 |
| C | -3.9677580000 | 0.8186140000 | 2.1950510000 |
| C | -2.7347840000 | 0.2264380000 | 2.0063630000 |
| C | -2.4568640000 | -0.4794430000 | 0.8308750000 |
| C | -3.4398770000 | -0.5927160000 | -0.1471360000 |
| C | -4.7089180000 | -0.0036140000 | 0.0493660000 |
| H | -5.9266620000 | 1.1657430000 | 1.3773750000 |
| H | -4.1807300000 | 1.3697320000 | 3.1030760000 |
| H | -1.9564380000 | 0.2834960000 | 2.7583600000 |
| C | -1.0989110000 | -1.1768470000 | 0.6915670000 |
| O | -5.6035020000 | -0.1871700000 | -0.9555180000 |
| C | -6.8923180000 | 0.3766500000 | -0.7878400000 |
| H | -7.3924430000 | -0.0416190000 | 0.0903870000 |
| H | -7.4527430000 | 0.1179730000 | -1.6829760000 |
| H | -6.8360480000 | 1.4650050000 | -0.6930260000 |
| O | -0.5263000000 | -1.5349650000 | 1.7471420000 |
| N | 1.2119610000 | 0.4994280000 | -0.1823500000 |
| C | -0.1067180000 | 0.4074920000 | -0.0230570000 |
| S | -0.7741010000 | 1.9667660000 | -0.2008430000 |
| C | 0.7660760000 | 2.7150790000 | -0.5083840000 |
| C | 1.7408190000 | 1.7779640000 | -0.4572090000 |
| C | 2.0733120000 | -0.6576810000 | -0.0517570000 |
| C | 2.6085230000 | -0.9401340000 | 1.2030580000 |
| C | 3.4859300000 | -2.0198510000 | 1.2976190000 |
| C | 3.8183540000 | -2.7912190000 | 0.1849800000 |
| C | 3.2695420000 | -2.4572450000 | -1.0537140000 |
| C | 2.3925290000 | -1.3851720000 | -1.1977460000 |
| C | 2.2391640000 | -0.1067250000 | 2.3983940000 |
| H | 3.9137960000 | -2.2641270000 | 2.2649100000 |
| C | 4.7222400000 | -3.9885570000 | 0.3170530000 |
| H | 3.5304890000 | -3.0447820000 | -1.9291040000 |
| C | 1.8216990000 | -1.0018820000 | -2.5358830000 |
| C | 0.9129830000 | 4.1833390000 | -0.7851690000 |
| C | 1.9293060000 | 4.8849980000 | 0.1242950000 |
| H | -0.0627330000 | 4.6611570000 | -0.6741050000 |
| H | 1.2075880000 | 4.3193630000 | -1.8327050000 |
| C | 3.3917320000 | 4.5261960000 | -0.1516950000 |
| H | 1.6850450000 | 4.6681120000 | 1.1697720000 |
| H | 1.8073370000 | 5.9627560000 | -0.0137520000 |
| H | 4.0232780000 | 5.2183620000 | 0.4122700000 |

| | | | |
|---|---|---|---|
| C | 3.2097980000 | 1.9992560000 | -0.6722140000 |
| H | 3.7402780000 | 1.0625060000 | -0.4932550000 |
| C | 3.8102520000 | 3.1001820000 | 0.2129760000 |
| H | 3.3752760000 | 2.2561610000 | -1.7258150000 |
| H | 4.8979070000 | 3.0296440000 | 0.1277420000 |
| H | 3.6103370000 | 4.7027690000 | -1.2121870000 |
| H | 3.5631260000 | 2.8990720000 | 1.2608560000 |
| H | 2.1832480000 | -1.6734650000 | -3.3141260000 |
| H | 2.1017580000 | 0.0209190000 | -2.8056290000 |
| H | 0.7302360000 | -1.0484660000 | -2.5170610000 |
| H | 1.1707580000 | -0.2254330000 | 2.5997310000 |
| H | 2.4376780000 | 0.9541000000 | 2.2193100000 |
| H | 2.8058720000 | -0.4191990000 | 3.2753200000 |
| H | 4.1273210000 | -4.9053230000 | 0.3679220000 |
| H | 5.3260500000 | -3.9319560000 | 1.2234010000 |
| H | 5.3892770000 | -4.0756350000 | -0.5423140000 |
| C | -1.0685000000 | -2.0266710000 | -0.5612860000 |
| C | -1.9026280000 | -1.4852460000 | -1.6869610000 |
| H | -1.5150490000 | -0.5194540000 | -2.0347560000 |
| O | -3.2694960000 | -1.2818740000 | -1.3067310000 |
| H | -1.9288350000 | -2.1767620000 | -2.5280250000 |
| C | -0.4284040000 | -3.1919270000 | -0.6909890000 |
| C | 0.4554510000 | -3.8853070000 | 0.3041580000 |
| H | 1.1816750000 | -4.5131400000 | -0.2163150000 |
| H | -0.1441610000 | -4.5384840000 | 0.9471620000 |
| H | 0.9736010000 | -3.1748250000 | 0.9426690000 |
| H | -0.5693000000 | -3.7130550000 | -1.6380640000 |

Thermochemie

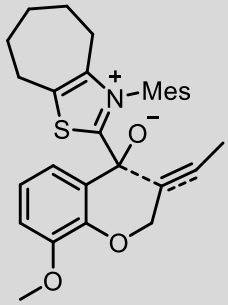
Zero-point correction= 0.561227 (Hartree/Particle)
Thermal correction to Energy= 0.593456
Thermal correction to Enthalpy= 0.594400
Thermal correction to Gibbs Free Energy= 0.497736
Sum of electronic and zero-point Energies= -1802.729492
Sum of electronic and thermal Energies= -1802.697263
Sum of electronic and thermal Enthalpies= -1802.696319
Sum of electronic and thermal Free Energies= -1802.792983

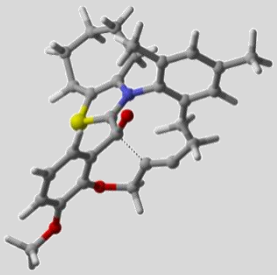
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 372.399 | 125.238 | 203.448 |

Imaginäre Frequenz

-179.2555

**TS-7b**



66

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.1198500000 | -0.3151500000 | 1.3025210000 |
| C | -4.2843950000 | -0.7424330000 | 2.3378590000 |
| C | -2.9299530000 | -0.9277320000 | 2.1256340000 |
| C | -2.3855420000 | -0.6691300000 | 0.8662570000 |

| | | | |
|---|---|---|---|
| C | -3.2172260000 | -0.2732230000 | -0.1759460000 |
| C | -4.5936150000 | -0.0873580000 | 0.0346150000 |
| H | -6.1760560000 | -0.1789110000 | 1.4916820000 |
| H | -4.7127570000 | -0.9294220000 | 3.3156100000 |
| H | -2.2605300000 | -1.2756000000 | 2.9020090000 |
| C | -0.8963220000 | -0.8895260000 | 0.6546280000 |
| O | -5.3149900000 | 0.3011930000 | -1.0481950000 |
| C | -6.7038500000 | 0.4696690000 | -0.8726720000 |
| H | -7.1813170000 | -0.4650270000 | -0.5603820000 |
| H | -7.0954690000 | 0.7707080000 | -1.8420440000 |
| H | -6.9193530000 | 1.2502430000 | -0.1354190000 |
| O | -0.2658180000 | -1.5705420000 | 1.5308460000 |
| N | 1.1503150000 | 0.4644550000 | 0.0665440000 |
| C | -0.1825750000 | 0.3609920000 | 0.2194030000 |
| S | -0.9153220000 | 1.8944120000 | 0.0058450000 |
| C | 0.6132650000 | 2.6574060000 | -0.3010300000 |
| C | 1.6163720000 | 1.7540060000 | -0.2263960000 |
| C | 2.0571810000 | -0.6657180000 | 0.0423490000 |
| C | 2.6813300000 | -1.0528410000 | 1.2324370000 |
| C | 3.6128030000 | -2.0808520000 | 1.1608480000 |
| C | 3.9369840000 | -2.6985690000 | -0.0498160000 |
| C | 3.3224390000 | -2.2495500000 | -1.2113850000 |
| C | 2.3727170000 | -1.2252100000 | -1.1920460000 |
| C | 2.3486800000 | -0.3758340000 | 2.5299920000 |
| H | 4.1010700000 | -2.4085620000 | 2.0734710000 |
| C | 4.9091680000 | -3.8482030000 | -0.0832730000 |
| H | 3.5748720000 | -2.7067180000 | -2.1640470000 |
| C | 1.7557950000 | -0.7600660000 | -2.4860590000 |
| C | 0.7114260000 | 4.1215680000 | -0.6181720000 |
| C | 1.6712180000 | 4.8893410000 | 0.2988330000 |
| H | -0.2854260000 | 4.5634100000 | -0.5490280000 |
| H | 1.0302540000 | 4.2422480000 | -1.6607300000 |
| C | 3.1525990000 | 4.5799890000 | 0.0700830000 |
| H | 1.4066930000 | 4.6883770000 | 1.3424710000 |
| H | 1.5121850000 | 5.9581850000 | 0.1305930000 |
| H | 3.7435360000 | 5.3009320000 | 0.6422180000 |
| C | 3.0774550000 | 2.0379060000 | -0.4243840000 |
| H | 3.6453770000 | 1.1287720000 | -0.2237740000 |
| C | 3.6101360000 | 3.1729460000 | 0.4612940000 |
| H | 3.2513580000 | 2.2868560000 | -1.4788640000 |
| H | 4.7020030000 | 3.1428850000 | 0.4096860000 |
| H | 3.3954520000 | 4.7540110000 | -0.9859030000 |
| H | 3.3398870000 | 2.9718880000 | 1.5035720000 |
| H | 2.5270590000 | -0.3633940000 | -3.1522490000 |
| H | 1.0011960000 | 0.0123190000 | -2.3339340000 |
| H | 1.2689310000 | -1.6002250000 | -2.9865070000 |
| H | 1.3135300000 | -0.6131680000 | 2.7889310000 |
| H | 2.4389040000 | 0.7116490000 | 2.4418230000 |
| H | 3.0163850000 | -0.7132740000 | 3.3227290000 |
| H | 5.3621320000 | -3.9568410000 | -1.0697260000 |
| H | 4.3947450000 | -4.7840530000 | 0.1537100000 |
| H | 5.7052450000 | -3.7140630000 | 0.6511180000 |
| C | -1.0295670000 | -1.7748700000 | -0.9930570000 |
| C | -1.9236500000 | -1.0852940000 | -1.9790940000 |
| H | -1.3370440000 | -0.6065930000 | -2.7673650000 |
| O | -2.7069200000 | -0.0248600000 | -1.4176830000 |
| H | -2.5985080000 | -1.8126340000 | -2.4389170000 |
| C | -0.4561330000 | -2.9088250000 | -1.0135680000 |
| C | 0.4119330000 | -3.8484060000 | -0.3045140000 |
| H | 1.2586580000 | -4.1581310000 | -0.9228640000 |
| H | -0.1447520000 | -4.7425030000 | -0.0133060000 |
| H | 0.7835750000 | -3.3516700000 | 0.6043320000 |

Thermochemie

| | |
|---|---|
| Zero-point correction= | 0.547759 (Hartree/Particle) |
| Thermal correction to Energy= | 0.579975 |
| Thermal correction to Enthalpy= | 0.580920 |
| Thermal correction to Gibbs Free Energy= | 0.484816 |
| Sum of electronic and zero-point Energies= | -1802.048125 |
| Sum of electronic and thermal Energies= | -1802.015909 |
| Sum of electronic and thermal Enthalpies= | -1802.014965 |
| Sum of electronic and thermal Free Energies= | -1802.111068 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 363.940 | 125.503 | 202.266 |

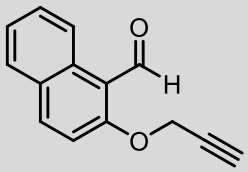
Imaginäre Frequenz

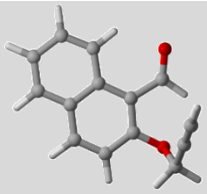
-711.5392

## *O*-propargylierte Aldehyde: Naph-Substituent

(u)M06-2X/6-311+G** SCRF=(PCM,Solvent=Tetrahydrofuran)

**19c**



26

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -0.8198000000 | -2.1728950000 | -0.0125820000 |
| C | -1.6680200000 | -1.0376160000 | 0.0882560000 |
| C | -1.1441900000 | 0.2612240000 | -0.1676020000 |
| C | 0.2468740000 | 0.3878720000 | -0.5189710000 |
| C | 1.0200710000 | -0.7569060000 | -0.6138710000 |
| C | 0.4939590000 | -2.0424200000 | -0.3570200000 |
| H | -1.2399200000 | -3.1548160000 | 0.1775630000 |
| C | -3.0324630000 | -1.1975930000 | 0.4349220000 |
| C | -2.0313430000 | 1.3656790000 | -0.0664400000 |
| C | 0.9233450000 | 1.6790550000 | -0.7846180000 |
| O | 2.3350950000 | -0.6701560000 | -1.0005130000 |
| O | 0.4320980000 | 2.7788670000 | -0.6452930000 |
| H | 1.9608470000 | 1.5820890000 | -1.1332000000 |
| C | 3.2832220000 | -0.9287080000 | 0.0384430000 |
| H | 3.0799750000 | -1.8937950000 | 0.5114670000 |
| C | 3.2737960000 | 0.1366760000 | 1.0469560000 |
| H | 4.2541580000 | -0.9804240000 | -0.4525840000 |
| C | 3.2391290000 | 1.0244040000 | 1.8537670000 |
| H | 3.2104910000 | 1.8123750000 | 2.5709300000 |
| C | -3.8622640000 | -0.1113780000 | 0.5280790000 |
| C | -3.3500110000 | 1.1775600000 | 0.2718990000 |
| H | -1.6601970000 | 2.3604870000 | -0.2559050000 |
| H | -4.0077370000 | 2.0362350000 | 0.3410310000 |
| H | -4.9046840000 | -0.2379910000 | 0.7938540000 |
| H | -3.4056900000 | -2.1982940000 | 0.6238700000 |
| H | 1.1413780000 | -2.9052950000 | -0.4578970000 |

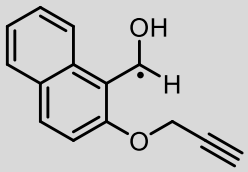
Thermochemie

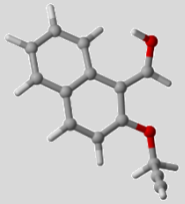
Zero-point correction= 0.199719 (Hartree/Particle)
Thermal correction to Energy= 0.213108
Thermal correction to Enthalpy= 0.214052
Thermal correction to Gibbs Free Energy= 0.158228
Sum of electronic and zero-point Energies= -689.580922
Sum of electronic and thermal Energies= -689.567533
Sum of electronic and thermal Enthalpies= -689.566589
Sum of electronic and thermal Free Energies= -689.622414

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 133.727 | 51.481 | 117.493 |

Volumen
Molar volume = 1907.363 bohr**3/mol (170.211 cm**3/mol)
Recommended a0 for SCRF calculation = 4.98 angstrom ( 9.41 bohr)

**25c**



27
XYZ-Matrix in Ångström

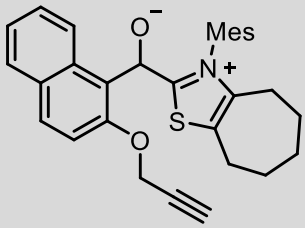
| | | | |
|---|---|---|---|
| C | -0.1558590000 | -1.9592960000 | -0.1039040000 |
| C | -1.3708730000 | -1.2371170000 | 0.0223060000 |
| C | -1.3599680000 | 0.1841110000 | -0.0577790000 |
| C | -0.0788060000 | 0.8819940000 | -0.1333570000 |
| C | 1.0832740000 | 0.0856780000 | -0.4015250000 |
| C | 1.0373720000 | -1.3033490000 | -0.3592720000 |
| C | -2.6059250000 | -1.9160840000 | 0.1612760000 |
| C | -2.6055700000 | 0.8489050000 | -0.1300680000 |
| C | 0.1102450000 | 2.2324160000 | 0.1039310000 |
| O | 2.2199790000 | 0.8011950000 | -0.6291250000 |
| O | -0.7979580000 | 3.0955190000 | 0.6061390000 |
| H | 1.0699860000 | 2.6977930000 | -0.0627470000 |
| C | 3.4334790000 | 0.1061100000 | -0.8650680000 |
| H | 3.3025650000 | -0.6399960000 | -1.6543940000 |
| C | 3.9735940000 | -0.5203930000 | 0.3476940000 |
| H | 4.1300410000 | 0.8617420000 | -1.2266690000 |
| C | 4.4304350000 | -1.0239660000 | 1.3363530000 |
| H | 4.8317210000 | -1.4709120000 | 2.2166450000 |
| H | -1.5384990000 | 2.6192020000 | 0.9999220000 |
| C | -3.7982240000 | -1.2332600000 | 0.1608950000 |
| C | -3.7971360000 | 0.1611860000 | -0.0188540000 |
| H | -2.5916480000 | -2.9976730000 | 0.2450840000 |
| H | -2.6493430000 | 1.9085390000 | -0.3503070000 |
| H | -4.7344350000 | 0.6996930000 | -0.0896330000 |
| H | -4.7354580000 | -1.7670910000 | 0.2623360000 |
| H | 1.9389310000 | -1.8861150000 | -0.4911220000 |
| H | -0.1762520000 | -3.0404970000 | -0.0409850000 |

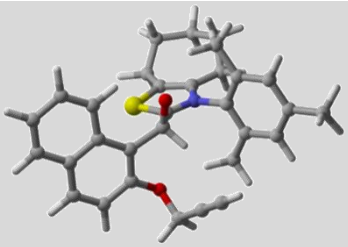
Thermochemie
Zero-point correction= 0.199719 (Hartree/Particle)
Thermal correction to Energy= 0.213108
Thermal correction to Enthalpy= 0.214052
Thermal correction to Gibbs Free Energy= 0.158228
Sum of electronic and zero-point Energies= -689.580922
Sum of electronic and thermal Energies= -689.567533

Sum of electronic and thermal Enthalpies= -689.566589
Sum of electronic and thermal Free Energies= -689.622414

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 133.727 | 51.481 | 117.493 |

**22c**



66
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -4.9049540000 | -0.1095160000 | -1.1870810000 |
| C | -4.6998470000 | 0.3545470000 | 0.1370760000 |
| C | -3.4077070000 | 0.2477450000 | 0.7344410000 |
| C | -2.3335290000 | -0.3481700000 | -0.0082450000 |
| C | -2.5915750000 | -0.7416740000 | -1.3031560000 |
| C | -3.8673630000 | -0.6348420000 | -1.9020070000 |
| H | -5.8893050000 | -0.0143180000 | -1.6323640000 |
| C | -5.7670160000 | 0.9500380000 | 0.8609390000 |
| C | -3.2403340000 | 0.7723190000 | 2.0502470000 |
| C | -0.9079370000 | -0.5830450000 | 0.5601590000 |
| O | -1.5371570000 | -1.1712670000 | -2.0924270000 |
| O | -0.7407820000 | -0.5557110000 | 1.8883690000 |
| C | -1.6095940000 | -2.5122410000 | -2.5682670000 |
| H | -2.6209970000 | -2.7503430000 | -2.9075290000 |
| C | -1.1834070000 | -3.4804910000 | -1.5497310000 |
| H | -0.9405220000 | -2.5659210000 | -3.4281430000 |
| C | -0.8145230000 | -4.2588570000 | -0.7134650000 |
| H | -0.4897920000 | -4.9410360000 | 0.0382380000 |
| N | 1.3488640000 | 0.3743820000 | -0.0687470000 |
| C | 0.0237870000 | 0.4831930000 | -0.0526780000 |
| S | -0.4527310000 | 2.0225550000 | -0.5831500000 |
| C | 1.1941250000 | 2.5246670000 | -0.8202970000 |
| C | 2.0407770000 | 1.5171860000 | -0.4995370000 |
| C | 2.0144590000 | -0.8516070000 | 0.3281810000 |
| C | 2.4580230000 | -0.9664720000 | 1.6463080000 |
| C | 3.0986810000 | -2.1508160000 | 2.0000530000 |
| C | 3.2879220000 | -3.1861120000 | 1.0827320000 |
| C | 2.8443280000 | -3.0131700000 | -0.2270180000 |
| C | 2.2064550000 | -1.8413210000 | -0.6332340000 |
| C | 2.2460130000 | 0.1529320000 | 2.6246230000 |
| H | 3.4522020000 | -2.2700670000 | 3.0194190000 |
| C | 3.9405730000 | -4.4746370000 | 1.5107840000 |
| H | 2.9968900000 | -3.8049040000 | -0.9538150000 |
| C | 1.7743570000 | -1.6333480000 | -2.0592500000 |
| C | 1.5319530000 | 3.8848190000 | -1.3583420000 |
| C | 2.5660860000 | 4.6459140000 | -0.5205250000 |
| H | 0.6151050000 | 4.4740120000 | -1.4240960000 |
| H | 1.9044140000 | 3.7737110000 | -2.3834260000 |
| C | 3.9868260000 | 4.0821530000 | -0.5948460000 |
| H | 2.2325600000 | 4.6774580000 | 0.5218770000 |
| H | 2.5841930000 | 5.6778510000 | -0.8803320000 |
| H | 4.6640710000 | 4.8056290000 | -0.1330310000 |
| C | 3.5377330000 | 1.5315690000 | -0.5997110000 |
| H | 3.9263360000 | 0.6061550000 | -0.1707510000 |

| | | | |
|---|---|---|---|
| C | 4.2005980000 | 2.7312170000 | 0.0916180000 |
| H | 3.8165460000 | 1.5259270000 | -1.6603120000 |
| H | 5.2740300000 | 2.5295390000 | 0.1286640000 |
| H | 4.2886660000 | 4.0041260000 | -1.6465110000 |
| H | 3.8547390000 | 2.7897020000 | 1.1288480000 |
| H | 2.4310880000 | -0.9115770000 | -2.5561470000 |
| H | 0.7563360000 | -1.2433820000 | -2.1119130000 |
| H | 1.8205390000 | -2.5718740000 | -2.6120920000 |
| H | 1.1717090000 | 0.3406500000 | 2.7091520000 |
| H | 2.7372470000 | 1.0698220000 | 2.2846280000 |
| H | 2.6519350000 | -0.1088170000 | 3.6014980000 |
| H | 4.7240300000 | -4.2923510000 | 2.2478960000 |
| H | 4.3773410000 | -4.9979850000 | 0.6594970000 |
| H | 3.2033660000 | -5.1387780000 | 1.9701580000 |
| H | -0.5705420000 | -1.5242360000 | 0.0846720000 |
| C | -5.5711990000 | 1.4410950000 | 2.1233210000 |
| C | -4.2898970000 | 1.3524400000 | 2.7158490000 |
| H | -2.2618030000 | 0.6756100000 | 2.4993760000 |
| H | -4.1374390000 | 1.7451070000 | 3.7148970000 |
| H | -6.3901240000 | 1.8974630000 | 2.6670900000 |
| H | -6.7404270000 | 1.0139390000 | 0.3858340000 |
| H | -4.0001120000 | -0.9499440000 | -2.9308050000 |

Thermochemie

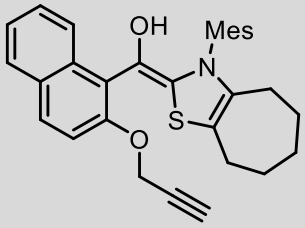
Zero-point correction= 0.545961 (Hartree/Particle)
Thermal correction to Energy= 0.578433
Thermal correction to Enthalpy= 0.579377
Thermal correction to Gibbs Free Energy= 0.479332
Sum of electronic and zero-point Energies= -1802.490189
Sum of electronic and thermal Energies= -1802.457717
Sum of electronic and thermal Enthalpies= -1802.456772
Sum of electronic and thermal Free Energies= -1802.556818

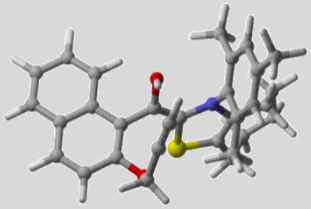
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 362.972 | 126.042 | 210.563 |

Volumen

Molar volume = 3941.243 bohr**3/mol (351.712 cm**3/mol)
Recommended a0 for SCRF calculation = 6.21 angstrom ( 11.73 bohr)

**23c**



66

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0447310000 | 0.2775080000 | -1.0594420000 |
| C | -4.7442970000 | 0.4879560000 | 0.3133870000 |
| C | -3.4036330000 | 0.3437770000 | 0.7595920000 |
| C | -2.3749100000 | -0.0238900000 | -0.1715620000 |
| C | -2.7244250000 | -0.2119080000 | -1.4911730000 |
| C | -4.0576340000 | -0.0571890000 | -1.9424250000 |
| H | -6.0678380000 | 0.3972760000 | -1.3987030000 |
| C | -5.7522550000 | 0.8560950000 | 1.2416420000 |
| C | -3.1120320000 | 0.5918840000 | 2.1268610000 |
| C | -0.9901140000 | -0.2320390000 | 0.3018760000 |
| O | -1.7618980000 | -0.5365610000 | -2.4248870000 |

| | | | |
|---|---|---|---|
| O | -0.8038850000 | -1.2291780000 | 1.2495890000 |
| C | -1.7527950000 | -1.9048540000 | -2.8118060000 |
| H | -2.7623460000 | -2.2369110000 | -3.0744290000 |
| C | -1.1946710000 | -2.7949600000 | -1.7811500000 |
| H | -1.1284450000 | -1.9608270000 | -3.7044470000 |
| C | -0.7140800000 | -3.5716060000 | -0.9995120000 |
| H | -0.2755540000 | -4.2604310000 | -0.3127140000 |
| H | -0.8588200000 | -2.0811180000 | 0.7957750000 |
| N | 1.3877930000 | 0.3827440000 | 0.2864280000 |
| C | 0.0419470000 | 0.5510280000 | -0.0648640000 |
| S | -0.1447820000 | 2.0142620000 | -1.0493880000 |
| C | 1.5843590000 | 2.3740130000 | -0.8845210000 |
| C | 2.2174450000 | 1.4293030000 | -0.1816100000 |
| C | 1.9238700000 | -0.9476130000 | 0.4224240000 |
| C | 2.2361170000 | -1.4287990000 | 1.6971870000 |
| C | 2.7518340000 | -2.7173030000 | 1.8077200000 |
| C | 2.9581880000 | -3.5214550000 | 0.6845230000 |
| C | 2.6386930000 | -3.0077060000 | -0.5694560000 |
| C | 2.1229290000 | -1.7190720000 | -0.7240590000 |
| C | 1.9880430000 | -0.5720680000 | 2.9070120000 |
| H | 2.9927560000 | -3.1067510000 | 2.7926950000 |
| C | 3.5394140000 | -4.9048370000 | 0.8308670000 |
| H | 2.7882700000 | -3.6223740000 | -1.4525570000 |
| C | 1.7950440000 | -1.1713020000 | -2.0874980000 |
| C | 2.1663770000 | 3.6310360000 | -1.4635050000 |
| C | 2.8456010000 | 4.5256040000 | -0.4183080000 |
| H | 1.3735650000 | 4.1948730000 | -1.9605450000 |
| H | 2.8949080000 | 3.3722030000 | -2.2424360000 |
| C | 4.1740150000 | 3.9802540000 | 0.1141210000 |
| H | 2.1519750000 | 4.6927290000 | 0.4125730000 |
| H | 3.0366020000 | 5.5006520000 | -0.8765180000 |
| H | 4.6432570000 | 4.7583760000 | 0.7235340000 |
| C | 3.6774980000 | 1.4446250000 | 0.1721150000 |
| H | 3.9106890000 | 0.5545620000 | 0.7595700000 |
| C | 4.0957690000 | 2.7001460000 | 0.9521620000 |
| H | 4.2741570000 | 1.3759040000 | -0.7458970000 |
| H | 5.0843550000 | 2.5160290000 | 1.3829640000 |
| H | 4.8491260000 | 3.8043770000 | -0.7332520000 |
| H | 3.4050590000 | 2.8460910000 | 1.7899500000 |
| H | 2.4585350000 | -0.3379710000 | -2.3398200000 |
| H | 0.7711780000 | -0.7895010000 | -2.1243680000 |
| H | 1.9086170000 | -1.9449630000 | -2.8479270000 |
| H | 0.9239360000 | -0.3347700000 | 2.9790750000 |
| H | 2.5282720000 | 0.3760960000 | 2.8364810000 |
| H | 2.3015300000 | -1.0847910000 | 3.8167820000 |
| H | 4.6294720000 | -4.8580560000 | 0.9063450000 |
| H | 3.2918090000 | -5.5296900000 | -0.0284290000 |
| H | 3.1686210000 | -5.3929070000 | 1.7339260000 |
| C | -5.4430320000 | 1.0800090000 | 2.5578910000 |
| C | -4.1064070000 | 0.9505500000 | 3.0010300000 |
| H | -3.8681510000 | 1.1402050000 | 4.0411850000 |
| H | -6.2182950000 | 1.3622110000 | 3.2602720000 |
| H | -2.0895810000 | 0.4907070000 | 2.4700500000 |
| H | -6.7719570000 | 0.9610820000 | 0.8864100000 |
| H | -4.2702620000 | -0.2069070000 | -2.9950460000 |

Thermochemie

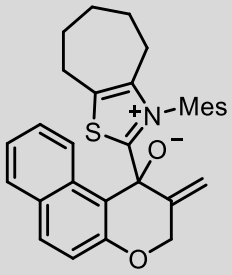
Zero-point correction= 0.544765 (Hartree/Particle)
Thermal correction to Energy= 0.577619
Thermal correction to Enthalpy= 0.578563
Thermal correction to Gibbs Free Energy= 0.480315
Sum of electronic and zero-point Energies= -1802.517488

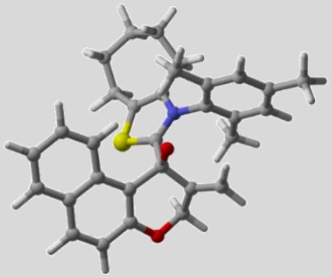
Sum of electronic and thermal Energies= -1802.484635
Sum of electronic and thermal Enthalpies= -1802.483691
Sum of electronic and thermal Free Energies= -1802.581938

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 362.461 | 127.916 | 206.780 |

Volumen
Molar volume = 4182.101 bohr**3/mol (373.206 cm**3/mol)
Recommended a0 for SCRF calculation = 6.32 angstrom ( 11.95 bohr)

**[24c + A]**



66
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.1927720000 | -0.7629440000 | -0.4386620000 |
| C | -4.5352200000 | -0.0974560000 | 0.6321020000 |
| C | -3.1268250000 | -0.2372520000 | 0.7790410000 |
| C | -2.3792490000 | -1.0293680000 | -0.1617580000 |
| C | -3.0696330000 | -1.6085600000 | -1.2084560000 |
| C | -4.4803340000 | -1.4949720000 | -1.3367030000 |
| H | -6.2690670000 | -0.6677170000 | -0.5363350000 |
| C | -5.2703940000 | 0.7054800000 | 1.5402510000 |
| C | -2.5080840000 | 0.4614130000 | 1.8548370000 |
| C | -0.8513650000 | -1.2900120000 | 0.0636200000 |
| O | -0.5213300000 | -1.5759960000 | 1.3082770000 |
| N | 1.1663820000 | 0.3443590000 | -0.2209310000 |
| C | -0.1210250000 | 0.0478710000 | -0.4020960000 |
| S | -0.9284210000 | 1.3744860000 | -1.0978570000 |
| C | 0.5096280000 | 2.3368080000 | -1.1323310000 |
| C | 1.5481240000 | 1.6376760000 | -0.6149650000 |
| C | 2.1597100000 | -0.6059800000 | 0.2472560000 |
| C | 2.4272720000 | -0.6933260000 | 1.6115030000 |
| C | 3.4195100000 | -1.5878930000 | 2.0073900000 |
| C | 4.1315320000 | -2.3538890000 | 1.0843630000 |
| C | 3.8616700000 | -2.1891290000 | -0.2737000000 |
| C | 2.8810900000 | -1.3054940000 | -0.7193760000 |
| C | 1.6751870000 | 0.1416880000 | 2.6066680000 |
| H | 3.6438040000 | -1.6835890000 | 3.0651990000 |
| C | 5.1664870000 | -3.3455520000 | 1.5472410000 |
| H | 4.4299760000 | -2.7548970000 | -1.0053180000 |
| C | 2.6287590000 | -1.0934140000 | -2.1880170000 |
| C | 0.5206610000 | 3.7386890000 | -1.6677200000 |
| C | 1.0553190000 | 4.7722240000 | -0.6681390000 |
| H | -0.4935450000 | 4.0108460000 | -1.9667660000 |
| H | 1.1309960000 | 3.7613540000 | -2.5781650000 |
| C | 2.5631750000 | 4.6942240000 | -0.4193500000 |
| H | 0.5150870000 | 4.6707250000 | 0.2789100000 |
| H | 0.8219300000 | 5.7644410000 | -1.0630010000 |
| H | 2.8583440000 | 5.5750030000 | 0.1574790000 |
| C | 2.9551110000 | 2.1349190000 | -0.4548840000 |
| H | 3.5495000000 | 1.3700370000 | 0.0464850000 |
| C | 3.0549090000 | 3.4526550000 | 0.3283270000 |

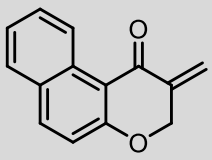
| | | | |
|---|---|---|---|
| H | 3.3940440000 | 2.2718660000 | -1.4506550000 |
| H | 4.1080760000 | 3.6001350000 | 0.5804890000 |
| H | 3.0882240000 | 4.7639790000 | -1.3799830000 |
| H | 2.5149790000 | 3.3525010000 | 1.2759190000 |
| H | 2.8560260000 | -0.0637960000 | -2.4813200000 |
| H | 1.5837940000 | -1.2868080000 | -2.4422530000 |
| H | 3.2535800000 | -1.7595840000 | -2.7823890000 |
| H | 0.6459100000 | -0.2230880000 | 2.6474020000 |
| H | 1.6552000000 | 1.1944370000 | 2.3082820000 |
| H | 2.1338950000 | 0.0716550000 | 3.5928050000 |
| H | 5.6329530000 | -3.0214910000 | 2.4785490000 |
| H | 5.9448800000 | -3.4834990000 | 0.7954880000 |
| H | 4.7033140000 | -4.3192790000 | 1.7292840000 |
| C | -0.4364060000 | -2.3525240000 | -0.9735550000 |
| C | -1.0759130000 | -2.2246310000 | -2.3171620000 |
| H | -0.8590580000 | -1.2508520000 | -2.7775190000 |
| O | -2.4962910000 | -2.3417240000 | -2.2037330000 |
| H | -0.7594480000 | -3.0143350000 | -2.9975950000 |
| C | 0.3770490000 | -3.3452500000 | -0.6403810000 |
| H | 0.7807120000 | -3.3853900000 | 0.3651720000 |
| H | 0.6543550000 | -4.1136700000 | -1.3552240000 |
| C | -4.6425810000 | 1.3676060000 | 2.5623660000 |
| C | -3.2436760000 | 1.2407410000 | 2.7128500000 |
| H | -1.4436540000 | 0.3428420000 | 2.0002470000 |
| H | -2.7439790000 | 1.7605790000 | 3.5227860000 |
| H | -5.2108090000 | 1.9817210000 | 3.2509080000 |
| H | -6.3438520000 | 0.7881880000 | 1.4036070000 |
| H | -4.9554300000 | -1.9989490000 | -2.1699500000 |

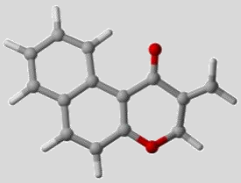
Thermochemie

Zero-point correction= 0.548336 (Hartree/Particle)
Thermal correction to Energy= 0.579084
Thermal correction to Enthalpy= 0.580028
Thermal correction to Gibbs Free Energy= 0.487871
Sum of electronic and zero-point Energies= -1802.550392
Sum of electronic and thermal Energies= -1802.519644
Sum of electronic and thermal Enthalpies= -1802.518700
Sum of electronic and thermal Free Energies= -1802.610857

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 363.381 | 123.263 | 193.961 |

**24c**



26

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -1.4779980000 | 2.1283990000 | -0.2197020000 |
| C | -1.9718730000 | 0.7990860000 | -0.0869780000 |
| C | -1.0565560000 | -0.2818900000 | 0.0379490000 |
| C | 0.3616510000 | -0.0008190000 | 0.0277140000 |
| C | 0.7776070000 | 1.3257360000 | -0.0412260000 |
| C | -0.1445990000 | 2.3918220000 | -0.1902340000 |
| H | -2.1912770000 | 2.9383780000 | -0.3287550000 |
| C | -3.3660380000 | 0.5609000000 | -0.0721550000 |
| C | -1.5975530000 | -1.5841870000 | 0.1947870000 |
| C | 1.3948500000 | -1.0574570000 | -0.0705360000 |

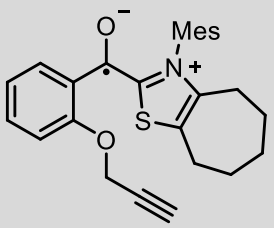
| | | | |
|---|---|---|---|
| O | 2.0704840000 | 1.7129230000 | -0.0045830000 |
| O | 1.1526360000 | -2.2297320000 | -0.2951160000 |
| C | 2.8096710000 | -0.5774480000 | 0.0461740000 |
| C | 2.9670460000 | 0.7930480000 | 0.6215560000 |
| H | 2.7346560000 | 0.7818510000 | 1.6935180000 |
| H | 3.9693770000 | 1.1892680000 | 0.4748040000 |
| C | 3.8225840000 | -1.3528900000 | -0.3279290000 |
| H | 4.8489390000 | -1.0088700000 | -0.2672290000 |
| H | 3.6360100000 | -2.3540250000 | -0.6986690000 |
| C | -3.8584020000 | -0.7110810000 | 0.0729200000 |
| C | -2.9589630000 | -1.7851470000 | 0.2135080000 |
| H | -0.9317320000 | -2.4252340000 | 0.3016250000 |
| H | -3.3439050000 | -2.7903940000 | 0.3404340000 |
| H | -4.9266110000 | -0.8897630000 | 0.0859270000 |
| H | -4.0372400000 | 1.4071690000 | -0.1716870000 |
| H | 0.2482650000 | 3.3976510000 | -0.2674540000 |

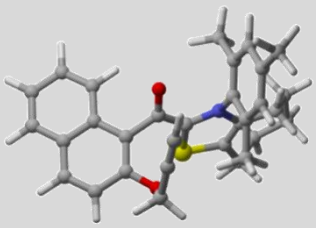
Thermochemie

Zero-point correction= 0.203674 (Hartree/Particle)
Thermal correction to Energy= 0.215396
Thermal correction to Enthalpy= 0.216340
Thermal correction to Gibbs Free Energy= 0.165580
Sum of electronic and zero-point Energies= -689.646965
Sum of electronic and thermal Energies= -689.635244
Sum of electronic and thermal Enthalpies= -689.634300
Sum of electronic and thermal Free Energies= -689.685060

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 135.163 | 47.893 | 106.834 |

**21c**



65

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.9856790000 | -0.3953430000 | -1.1255830000 |
| C | 4.7584100000 | -0.4385400000 | 0.2757240000 |
| C | 3.4455630000 | -0.2182190000 | 0.7748530000 |
| C | 2.3756730000 | 0.0423380000 | -0.1421410000 |
| C | 2.6482430000 | 0.0633900000 | -1.4912380000 |
| C | 3.9562450000 | -0.1544800000 | -1.9892160000 |
| H | 5.9884890000 | -0.5681600000 | -1.5009200000 |
| C | 5.8156210000 | -0.7077540000 | 1.1827240000 |
| C | 3.2355330000 | -0.2875560000 | 2.1786620000 |
| C | 1.0001940000 | 0.3467560000 | 0.3881390000 |
| O | 1.6353950000 | 0.2580240000 | -2.4067700000 |
| O | 0.8283940000 | 1.3180440000 | 1.1534920000 |
| C | 1.6484450000 | 1.5278720000 | -3.0593320000 |
| H | 2.6466320000 | 1.7489470000 | -3.4494950000 |
| C | 1.2022380000 | 2.6013700000 | -2.1653830000 |
| H | 0.9624370000 | 1.4351870000 | -3.9021910000 |
| C | 0.8097460000 | 3.4406860000 | -1.4026260000 |
| H | 0.4574020000 | 4.1713250000 | -0.7116160000 |
| N | -1.3849970000 | -0.3400320000 | 0.2516170000 |
| C | -0.0416190000 | -0.5429140000 | 0.0196390000 |

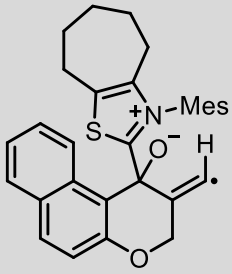
| | | | |
|---|---|---|---|
| S | 0.2127400000 | -2.1078410000 | -0.7008990000 |
| C | -1.5038430000 | -2.4517560000 | -0.6506900000 |
| C | -2.1943380000 | -1.4164730000 | -0.1276530000 |
| C | -1.9242720000 | 0.9895950000 | 0.4050540000 |
| C | -2.2129310000 | 1.4694290000 | 1.6828370000 |
| C | -2.7469170000 | 2.7492470000 | 1.7893470000 |
| C | -2.9848000000 | 3.5393650000 | 0.6615900000 |
| C | -2.6893810000 | 3.0178320000 | -0.5949370000 |
| C | -2.1602250000 | 1.7345120000 | -0.7483470000 |
| C | -1.9221120000 | 0.6225780000 | 2.8891330000 |
| H | -2.9770180000 | 3.1443040000 | 2.7745350000 |
| C | -3.5352240000 | 4.9341400000 | 0.8144380000 |
| H | -2.8763340000 | 3.6174780000 | -1.4808900000 |
| C | -1.8777410000 | 1.1589580000 | -2.1107400000 |
| C | -2.0442690000 | -3.7523040000 | -1.1702220000 |
| C | -2.9091880000 | -4.5133870000 | -0.1586460000 |
| H | -1.2071600000 | -4.3839810000 | -1.4758670000 |
| H | -2.6322300000 | -3.5599250000 | -2.0763640000 |
| C | -4.2743290000 | -3.8772370000 | 0.1131480000 |
| H | -2.3548680000 | -4.6195980000 | 0.7799440000 |
| H | -3.0714080000 | -5.5217460000 | -0.5497230000 |
| H | -4.8692500000 | -4.5818040000 | 0.7012830000 |
| C | -3.6834050000 | -1.3575140000 | 0.0569810000 |
| H | -3.9377160000 | -0.4240830000 | 0.5620370000 |
| C | -4.2538770000 | -2.5384070000 | 0.8550360000 |
| H | -4.1649420000 | -1.3189170000 | -0.9281280000 |
| H | -5.2820210000 | -2.2836670000 | 1.1266650000 |
| H | -4.8022840000 | -3.7473310000 | -0.8399510000 |
| H | -3.6953400000 | -2.6416010000 | 1.7918500000 |
| H | -2.5974660000 | 0.3695960000 | -2.3521050000 |
| H | -0.8787970000 | 0.7174290000 | -2.1543230000 |
| H | -1.9509350000 | 1.9331680000 | -2.8750920000 |
| H | -0.8454990000 | 0.4437410000 | 2.9559000000 |
| H | -2.4151010000 | -0.3512200000 | 2.8181930000 |
| H | -2.2570640000 | 1.1162820000 | 3.8013360000 |
| H | -4.3651020000 | 4.9516930000 | 1.5237100000 |
| H | -3.8887380000 | 5.3257370000 | -0.1400160000 |
| H | -2.7660720000 | 5.6122070000 | 1.1938640000 |
| C | 5.5833510000 | -0.7635240000 | 2.5316460000 |
| C | 4.2768050000 | -0.5542340000 | 3.0305070000 |
| H | 2.2405470000 | -0.1181400000 | 2.5704730000 |
| H | 4.0984830000 | -0.6041710000 | 4.0982530000 |
| H | 6.3955300000 | -0.9692740000 | 3.2186500000 |
| H | 6.8116940000 | -0.8700400000 | 0.7845470000 |
| H | 4.1153090000 | -0.1368600000 | -3.0614950000 |

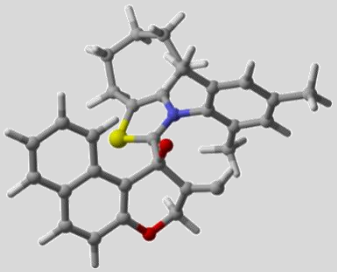
Thermochemie

Zero-point correction= 0.533060 (Hartree/Particle)
Thermal correction to Energy= 0.565646
Thermal correction to Enthalpy= 0.566590
Thermal correction to Gibbs Free Energy= 0.467095
Sum of electronic and zero-point Energies= -1801.925334
Sum of electronic and thermal Energies= -1801.892749
Sum of electronic and thermal Enthalpies= -1801.891805
Sum of electronic and thermal Free Energies= -1801.991300

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 354.948 | 125.800 | 209.405 |

**26c**



65

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.1735880000 | -0.7828960000 | -0.5557220000 |
| C | -4.5666570000 | -0.1389520000 | 0.5567960000 |
| C | -3.1635600000 | -0.2674500000 | 0.7565980000 |
| C | -2.3700890000 | -1.0293890000 | -0.1732420000 |
| C | -3.0129570000 | -1.5915480000 | -1.2592740000 |
| C | -4.4184110000 | -1.4863400000 | -1.4411200000 |
| H | -6.2458440000 | -0.6949080000 | -0.6949510000 |
| C | -5.3476090000 | 0.6317850000 | 1.4545790000 |
| C | -2.5968910000 | 0.4121140000 | 1.8728800000 |
| C | -0.8468780000 | -1.2622150000 | 0.1010160000 |
| O | -0.5380640000 | -1.5352080000 | 1.3509380000 |
| N | 1.1708280000 | 0.3514390000 | -0.1911120000 |
| C | -0.1208280000 | 0.0689550000 | -0.3578800000 |
| S | -0.9279510000 | 1.4102780000 | -1.0233750000 |
| C | 0.5188680000 | 2.3594840000 | -1.0675430000 |
| C | 1.5591310000 | 1.6448910000 | -0.5735130000 |
| C | 2.1593240000 | -0.6233470000 | 0.2326190000 |
| C | 2.4655250000 | -0.7149290000 | 1.5933500000 |
| C | 3.4448230000 | -1.6272810000 | 1.9651990000 |
| C | 4.1137010000 | -2.4150450000 | 1.0225100000 |
| C | 3.8017180000 | -2.2556280000 | -0.3224290000 |
| C | 2.8236390000 | -1.3527610000 | -0.7477730000 |
| C | 1.7570120000 | 0.1429320000 | 2.6014200000 |
| H | 3.6978960000 | -1.7249090000 | 3.0164310000 |
| C | 5.1477470000 | -3.4160420000 | 1.4667420000 |
| H | 4.3267240000 | -2.8438560000 | -1.0691440000 |
| C | 2.5288900000 | -1.2148740000 | -2.2188590000 |
| C | 0.5337560000 | 3.7613660000 | -1.6032220000 |
| C | 1.1141510000 | 4.7898790000 | -0.6249170000 |
| H | -0.4853300000 | 4.0472370000 | -1.8713890000 |
| H | 1.1155360000 | 3.7734880000 | -2.5323430000 |
| C | 2.6265060000 | 4.6860040000 | -0.4179550000 |
| H | 0.5992150000 | 4.7030990000 | 0.3376280000 |
| H | 0.8869410000 | 5.7837750000 | -1.0190840000 |
| H | 2.9532190000 | 5.5655950000 | 0.1435470000 |
| C | 2.9767280000 | 2.1177060000 | -0.4372230000 |
| H | 3.5603380000 | 1.3474880000 | 0.0683590000 |
| C | 3.1137480000 | 3.4420580000 | 0.3281790000 |
| H | 3.4067190000 | 2.2281570000 | -1.4401390000 |
| H | 4.1743170000 | 3.5736240000 | 0.5570290000 |
| H | 3.1268950000 | 4.7389750000 | -1.3927070000 |
| H | 2.5922610000 | 3.3595410000 | 1.2878560000 |
| H | 1.7901120000 | -0.4413150000 | -2.4323800000 |
| H | 2.1470820000 | -2.1613330000 | -2.6100780000 |
| H | 3.4428020000 | -0.9706140000 | -2.7648540000 |
| H | 0.7070460000 | -0.1598320000 | 2.6317780000 |
| H | 1.8041400000 | 1.2009970000 | 2.3250750000 |
| H | 2.2041860000 | 0.0257850000 | 3.5883560000 |
| H | 5.8138840000 | -2.9844270000 | 2.2161420000 |
| H | 5.7490480000 | -3.7618120000 | 0.6254320000 |
| H | 4.6656730000 | -4.2868250000 | 1.9187380000 |

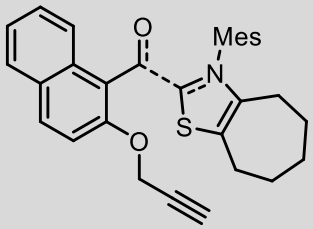
| | | | |
|---|---|---|---|
| C | -0.3929940000 | -2.3438610000 | -0.9302920000 |
| C | -0.9781750000 | -2.2112090000 | -2.3019340000 |
| H | -0.7156600000 | -1.2420420000 | -2.7468290000 |
| O | -2.4005840000 | -2.3026090000 | -2.2473880000 |
| H | -0.6454350000 | -3.0072310000 | -2.9655180000 |
| C | 0.3949660000 | -3.3182410000 | -0.5634160000 |
| H | 0.9127950000 | -3.5785900000 | 0.3484040000 |
| C | -4.7697360000 | 1.2735120000 | 2.5183220000 |
| C | -3.3765780000 | 1.1592760000 | 2.7206290000 |
| H | -1.5376450000 | 0.3023900000 | 2.0567940000 |
| H | -2.9156210000 | 1.6635600000 | 3.5626130000 |
| H | -5.3723470000 | 1.8632270000 | 3.1989710000 |
| H | -6.4155540000 | 0.7056870000 | 1.2767750000 |
| H | -4.8544950000 | -1.9746370000 | -2.3042830000 |

Thermochemie

Zero-point correction= 0.534755 (Hartree/Particle)
Thermal correction to Energy= 0.565642
Thermal correction to Enthalpy= 0.566586
Thermal correction to Gibbs Free Energy= 0.473141
Sum of electronic and zero-point Energies= -1801.879712
Sum of electronic and thermal Energies= -1801.848826
Sum of electronic and thermal Enthalpies= -1801.847881
Sum of electronic and thermal Free Energies= -1801.941326

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 354.946 | 123.302 | 196.671 |

**TS-1c**

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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.7613720000 | -1.6580750000 | 0.8561560000 |
| C | 4.2830620000 | -1.4583890000 | 2.1522290000 |
| C | 3.1163090000 | -0.7452650000 | 2.3731640000 |
| C | 2.4011900000 | -0.2162150000 | 1.2968190000 |
| C | 2.8696970000 | -0.4173290000 | 0.0030580000 |
| C | 4.0527190000 | -1.1422500000 | -0.2253170000 |
| H | 5.6742000000 | -2.2173360000 | 0.7013320000 |
| H | 4.8399430000 | -1.8658690000 | 2.9877660000 |
| H | 2.7371800000 | -0.5716740000 | 3.3726960000 |
| C | 1.1591460000 | 0.6038030000 | 1.5640200000 |
| O | 2.1331480000 | 0.0046660000 | -1.0768450000 |
| O | 4.4104780000 | -1.2899140000 | -1.5275340000 |
| C | 5.6008400000 | -2.0113770000 | -1.8012810000 |
| H | 6.4676350000 | -1.5244980000 | -1.3461120000 |
| H | 5.7095540000 | -2.0123610000 | -2.8830330000 |
| H | 5.5257910000 | -3.0404870000 | -1.4398430000 |
| O | 0.8200220000 | 0.8565280000 | 2.7277320000 |
| C | 2.6737620000 | 1.1125260000 | -1.8074820000 |
| H | 3.7641040000 | 1.0557190000 | -1.8261900000 |
| C | 2.2156370000 | 2.3851760000 | -1.2422190000 |
| H | 2.3100530000 | 1.0031690000 | -2.8306410000 |
| C | 1.7750950000 | 3.3850160000 | -0.7382710000 |
| C | 1.2212780000 | 4.5683120000 | -0.0865840000 |

| | | | |
|---|---|---|---|
| N | -1.3548500000 | -0.3992250000 | 0.0962830000 |
| C | -0.2146810000 | -0.8001430000 | 0.6609950000 |
| S | -0.1783680000 | -2.5028160000 | 0.5856490000 |
| C | -1.7222730000 | -2.6275800000 | -0.2162030000 |
| C | -2.2249260000 | -1.3866560000 | -0.4062720000 |
| C | -1.6559190000 | 1.0145580000 | 0.0332520000 |
| C | -2.2026070000 | 1.6231650000 | 1.1654510000 |
| C | -2.4504150000 | 2.9915970000 | 1.1020850000 |
| C | -2.1646410000 | 3.7358000000 | -0.0450820000 |
| C | -1.6277730000 | 3.0829750000 | -1.1514940000 |
| C | -1.3627620000 | 1.7129600000 | -1.1350880000 |
| C | -2.4880140000 | 0.8178270000 | 2.4036880000 |
| H | -2.8711080000 | 3.4903950000 | 1.9701570000 |
| C | -2.4068860000 | 5.2229520000 | -0.0632490000 |
| H | -1.3918850000 | 3.6502020000 | -2.0471330000 |
| C | -0.7859570000 | 1.0087390000 | -2.3326230000 |
| C | -2.3505210000 | -3.9345190000 | -0.6032960000 |
| C | -3.7611560000 | -4.1262720000 | -0.0317220000 |
| H | -1.7070360000 | -4.7502780000 | -0.2674760000 |
| H | -2.3914270000 | -4.0003080000 | -1.6972580000 |
| C | -4.8360620000 | -3.2474380000 | -0.6772270000 |
| H | -3.7374540000 | -3.9513590000 | 1.0491710000 |
| H | -4.0411350000 | -5.1730600000 | -0.1787380000 |
| H | -5.8128040000 | -3.5935740000 | -0.3273810000 |
| C | -3.5374170000 | -1.0409550000 | -1.0454380000 |
| H | -3.6808430000 | 0.0403730000 | -0.9972570000 |
| C | -4.7376390000 | -1.7450980000 | -0.3965370000 |
| H | -3.4960950000 | -1.3066820000 | -2.1088480000 |
| H | -5.6451760000 | -1.2671980000 | -0.7751430000 |
| H | -4.8230590000 | -3.4084090000 | -1.7624710000 |
| H | -4.7158440000 | -1.5714390000 | 0.6846350000 |
| H | -1.5592450000 | 0.4341370000 | -2.8534750000 |
| H | 0.0006670000 | 0.3138880000 | -2.0308480000 |
| H | -0.3696810000 | 1.7325270000 | -3.0344090000 |
| H | -1.5459740000 | 0.4919400000 | 2.8537030000 |
| H | -3.0769040000 | -0.0730000000 | 2.1679340000 |
| H | -3.0374280000 | 1.4152300000 | 3.1310890000 |
| H | -1.7142100000 | 5.7321070000 | 0.6131610000 |
| H | -3.4199830000 | 5.4590480000 | 0.2690840000 |
| H | -2.2672380000 | 5.6345240000 | -1.0636220000 |
| H | 0.8922740000 | 1.2795120000 | 0.7419660000 |
| H | 0.5903220000 | 5.1325970000 | -0.7765170000 |
| H | 2.0152250000 | 5.2223510000 | 0.2773320000 |
| H | 0.6034750000 | 4.2621510000 | 0.7619850000 |

Thermochemie

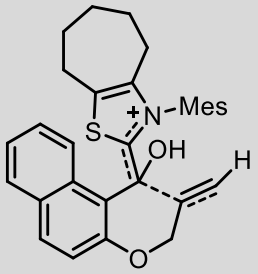
Zero-point correction= 0.543915 (Hartree/Particle)
Thermal correction to Energy= 0.576391
Thermal correction to Enthalpy= 0.577335
Thermal correction to Gibbs Free Energy= 0.477759
Sum of electronic and zero-point Energies= -1802.478350
Sum of electronic and thermal Energies= -1802.445875
Sum of electronic and thermal Enthalpies= -1802.444930
Sum of electronic and thermal Free Energies= -1802.544506

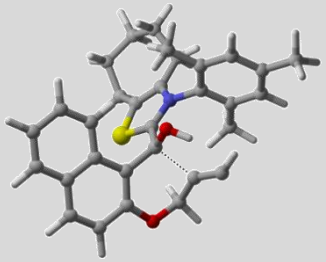
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 361.691 | 125.422 | 209.575 |

Imaginäre Frequenz

-143.6982

**TS-3c**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.2181290000 | -0.4809000000 | -0.4781900000 |
| C | -4.5483340000 | -0.0442980000 | 0.6981690000 |
| C | -3.1383320000 | -0.1945260000 | 0.7810480000 |
| C | -2.4038570000 | -0.7914880000 | -0.3072460000 |
| C | -3.1038830000 | -1.1604090000 | -1.4391510000 |
| C | -4.5184220000 | -1.0136850000 | -1.5146830000 |
| H | -6.2956560000 | -0.3726380000 | -0.5413290000 |
| C | -5.2634960000 | 0.5445830000 | 1.7695890000 |
| C | -2.4924080000 | 0.2781350000 | 1.9546840000 |
| C | -0.9183090000 | -0.9995910000 | -0.1504060000 |
| O | -0.5622950000 | -1.7306030000 | 0.9804010000 |
| H | -0.2218480000 | -2.5845610000 | 0.6610430000 |
| N | 1.1832640000 | 0.3593420000 | -0.0822800000 |
| C | -0.1349520000 | 0.1700420000 | -0.3558470000 |
| S | -0.7897030000 | 1.5961230000 | -1.0938790000 |
| C | 0.7549470000 | 2.4119930000 | -1.0239000000 |
| C | 1.6827760000 | 1.6248460000 | -0.4485030000 |
| C | 2.0755700000 | -0.7064400000 | 0.3120330000 |
| C | 2.2715760000 | -0.9798990000 | 1.6665340000 |
| C | 3.1535330000 | -2.0062770000 | 1.9967900000 |
| C | 3.8324140000 | -2.7344350000 | 1.0188160000 |
| C | 3.6409690000 | -2.3958550000 | -0.3196050000 |
| C | 2.7722680000 | -1.3738200000 | -0.6977730000 |
| C | 1.5526580000 | -0.2019550000 | 2.7329680000 |
| H | 3.3197560000 | -2.2373850000 | 3.0446890000 |
| C | 4.7453820000 | -3.8697300000 | 1.4019860000 |
| H | 4.1803200000 | -2.9370110000 | -1.0910930000 |
| C | 2.6276920000 | -0.9745290000 | -2.1418150000 |
| C | 0.9269030000 | 3.8109790000 | -1.5399110000 |
| C | 1.4510870000 | 4.7925740000 | -0.4838360000 |
| H | -0.0317270000 | 4.1679960000 | -1.9224180000 |
| H | 1.6146520000 | 3.7947970000 | -2.3938420000 |
| C | 2.9183490000 | 4.5881400000 | -0.0987360000 |
| H | 0.8197460000 | 4.7309200000 | 0.4088770000 |
| H | 1.3389060000 | 5.8038830000 | -0.8841440000 |
| H | 3.2271620000 | 5.4315500000 | 0.5251780000 |
| C | 3.1080490000 | 2.0100750000 | -0.1762480000 |
| H | 3.6084810000 | 1.1894380000 | 0.3399380000 |
| C | 3.2420530000 | 3.2949090000 | 0.6544760000 |
| H | 3.6281820000 | 2.1434760000 | -1.1326320000 |
| H | 4.2762910000 | 3.3536320000 | 1.0038810000 |
| H | 3.5344870000 | 4.6330010000 | -1.0054100000 |
| H | 2.6104550000 | 3.2161700000 | 1.5460320000 |
| H | 3.2133090000 | -0.0727670000 | -2.3496800000 |
| H | 1.5880640000 | -0.7639330000 | -2.3985560000 |
| H | 2.9860970000 | -1.7697090000 | -2.7952510000 |
| H | 0.5419230000 | -0.5970780000 | 2.8563590000 |
| H | 1.4671440000 | 0.8547280000 | 2.4684680000 |
| H | 2.0773080000 | -0.2825770000 | 3.6851690000 |
| H | 5.2044900000 | -3.6950920000 | 2.3761320000 |

| | | | |
|---|---|---|---|
| H | 5.5356800000 | -4.0063140000 | 0.6626350000 |
| H | 4.1830320000 | -4.8056070000 | 1.4634110000 |
| C | -0.4571590000 | -2.2949440000 | -1.5792460000 |
| C | -1.1571790000 | -1.6944570000 | -2.7357560000 |
| H | -0.8297160000 | -0.6626140000 | -2.9060170000 |
| O | -2.5764890000 | -1.6927390000 | -2.5701030000 |
| H | -0.9762350000 | -2.2794540000 | -3.6358730000 |
| C | 0.2052730000 | -3.3295220000 | -1.2927690000 |
| H | 0.7471590000 | -3.7805050000 | -0.4759990000 |
| C | -4.6106250000 | 0.9876840000 | 2.8911410000 |
| C | -3.2077180000 | 0.8546180000 | 2.9754610000 |
| H | -5.0067560000 | -1.3413310000 | -2.4245090000 |
| H | -1.4189650000 | 0.1781700000 | 2.0448840000 |
| H | -2.6884420000 | 1.2104120000 | 3.8580570000 |
| H | -5.1621800000 | 1.4403700000 | 3.7064110000 |
| H | -6.3406110000 | 0.6424860000 | 1.6807930000 |

Thermochemie

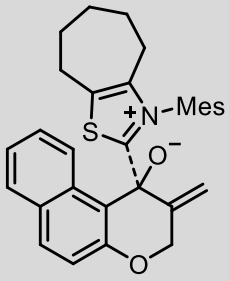
Zero-point correction= 0.544704 (Hartree/Particle)
Thermal correction to Energy= 0.576164
Thermal correction to Enthalpy= 0.577108
Thermal correction to Gibbs Free Energy= 0.482241
Sum of electronic and zero-point Energies= -1802.482996
Sum of electronic and thermal Energies= -1802.451536
Sum of electronic and thermal Enthalpies= -1802.450592
Sum of electronic and thermal Free Energies= -1802.545459

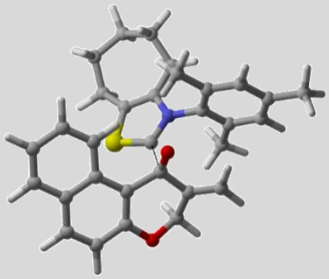
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 361.548 | 124.920 | 199.665 |

Imaginäre Frequenz

-611.2985

**TS-4c**



66

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.1758870000 | -0.6420010000 | -0.5250610000 |
| C | -4.5189920000 | 0.0259380000 | 0.5447260000 |
| C | -3.1389070000 | -0.2254710000 | 0.7800650000 |
| C | -2.4252750000 | -1.1353340000 | -0.0711120000 |
| C | -3.1025280000 | -1.7088440000 | -1.1302940000 |
| C | -4.4868320000 | -1.4814970000 | -1.3459350000 |
| H | -6.2326030000 | -0.4592290000 | -0.6884400000 |
| C | -5.2228770000 | 0.9438980000 | 1.3637870000 |
| C | -2.5098300000 | 0.4841340000 | 1.8405460000 |
| C | -0.9892830000 | -1.5610720000 | 0.2385410000 |
| O | -0.6419920000 | -1.7095000000 | 1.4319210000 |
| N | 1.2116730000 | 0.4081250000 | -0.2788530000 |
| C | -0.0658800000 | 0.0856780000 | -0.4792270000 |
| S | -0.8595780000 | 1.4435360000 | -1.1347020000 |
| C | 0.5737110000 | 2.4289250000 | -1.1280940000 |
| C | 1.6078480000 | 1.7158310000 | -0.6238320000 |

| | | | |
|---|---|---|---|
| C | 2.1679620000 | -0.5760060000 | 0.1866800000 |
| C | 2.3973160000 | -0.7110950000 | 1.5535280000 |
| C | 3.3304950000 | -1.6662960000 | 1.9549090000 |
| C | 4.0200890000 | -2.4522050000 | 1.0324740000 |
| C | 3.7779870000 | -2.2584770000 | -0.3277100000 |
| C | 2.8522420000 | -1.3193020000 | -0.7748230000 |
| C | 1.6587140000 | 0.1359500000 | 2.5511190000 |
| H | 3.5258200000 | -1.7937300000 | 3.0152430000 |
| C | 4.9960020000 | -3.5023990000 | 1.4956990000 |
| H | 4.3194400000 | -2.8524440000 | -1.0575520000 |
| C | 2.5861780000 | -1.1119790000 | -2.2410200000 |
| C | 0.5882470000 | 3.8452090000 | -1.6250080000 |
| C | 1.1359400000 | 4.8513780000 | -0.6052650000 |
| H | -0.4272300000 | 4.1302550000 | -1.9077470000 |
| H | 1.1907220000 | 3.8916680000 | -2.5401560000 |
| C | 2.6436920000 | 4.7540350000 | -0.3608290000 |
| H | 0.5977500000 | 4.7342480000 | 0.3412960000 |
| H | 0.9116130000 | 5.8549160000 | -0.9767320000 |
| H | 2.9493980000 | 5.6244150000 | 0.2265340000 |
| C | 3.0176660000 | 2.1932950000 | -0.4329010000 |
| H | 3.5912400000 | 1.4122090000 | 0.0694310000 |
| C | 3.1237110000 | 3.4977240000 | 0.3701420000 |
| H | 3.4796010000 | 2.3370340000 | -1.4174770000 |
| H | 4.1762970000 | 3.6350510000 | 0.6314110000 |
| H | 3.1675670000 | 4.8306060000 | -1.3217450000 |
| H | 2.5765160000 | 3.3872210000 | 1.3125990000 |
| H | 2.7820470000 | -0.0775380000 | -2.5385820000 |
| H | 1.5398210000 | -1.3267390000 | -2.4764600000 |
| H | 3.2164740000 | -1.7665480000 | -2.8424840000 |
| H | 0.6230600000 | -0.2078820000 | 2.6059750000 |
| H | 1.6555230000 | 1.1895120000 | 2.2578980000 |
| H | 2.1139000000 | 0.0521850000 | 3.5379880000 |
| H | 5.7814310000 | -3.6632080000 | 0.7558360000 |
| H | 4.4840420000 | -4.4562410000 | 1.6501510000 |
| H | 5.4601200000 | -3.2188790000 | 2.4412870000 |
| C | -0.4606310000 | -2.5242490000 | -0.8064820000 |
| C | -1.1042770000 | -2.4135270000 | -2.1509400000 |
| H | -0.8982420000 | -1.4378700000 | -2.6092980000 |
| O | -2.5252690000 | -2.5450420000 | -2.0374780000 |
| H | -0.7762070000 | -3.2035180000 | -2.8248370000 |
| C | 0.4628170000 | -3.4276580000 | -0.5014130000 |
| H | 0.8840180000 | -3.4529130000 | 0.4980530000 |
| H | 0.8297850000 | -4.1336990000 | -1.2394700000 |
| C | -4.5876670000 | 1.6111450000 | 2.3783470000 |
| C | -3.2137730000 | 1.3775760000 | 2.6095070000 |
| H | -1.4633330000 | 0.3033600000 | 2.0371780000 |
| H | -2.7080660000 | 1.9095610000 | 3.4076050000 |
| H | -5.1310150000 | 2.3147430000 | 2.9977400000 |
| H | -6.2760170000 | 1.1129500000 | 1.1642370000 |
| H | -4.9617100000 | -1.9864340000 | -2.1785420000 |

Thermochemie

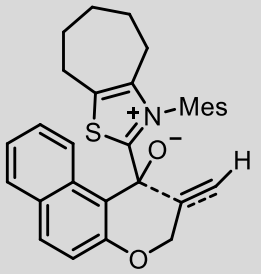
Zero-point correction= 0.547337 (Hartree/Particle)
Thermal correction to Energy= 0.578057
Thermal correction to Enthalpy= 0.579001
Thermal correction to Gibbs Free Energy= 0.486057
Sum of electronic and zero-point Energies= -1802.544740
Sum of electronic and thermal Energies= -1802.514020
Sum of electronic and thermal Enthalpies= -1802.513076
Sum of electronic and thermal Free Energies= -1802.606020

| | E (Thermal) | CV | S |
|---|---|---|---|

| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 362.736 | 122.330 | 195.618 |

Imaginäre Frequenz
-174.8773

**TS-7c**




65
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.2048120000 | -0.6133350000 | -0.4870240000 |
| C | -4.5455040000 | -0.1379050000 | 0.6782860000 |
| C | -3.1394780000 | -0.3074440000 | 0.7940240000 |
| C | -2.3922010000 | -0.9335900000 | -0.2707340000 |
| C | -3.0826600000 | -1.3232330000 | -1.4011200000 |
| C | -4.4956400000 | -1.1841610000 | -1.4943190000 |
| H | -6.2811610000 | -0.5025220000 | -0.5653910000 |
| C | -5.2737910000 | 0.5028700000 | 1.7098770000 |
| C | -2.5156610000 | 0.1934990000 | 1.9696700000 |
| C | -0.8865930000 | -1.1506150000 | -0.0203370000 |
| O | -0.5338690000 | -1.7312500000 | 1.0471910000 |
| N | 1.1801620000 | 0.3407970000 | -0.1303080000 |
| C | -0.1191550000 | 0.0965630000 | -0.3767060000 |
| S | -0.8552490000 | 1.4763030000 | -1.0825450000 |
| C | 0.6362040000 | 2.3670360000 | -1.0502630000 |
| C | 1.6193640000 | 1.6213530000 | -0.4996380000 |
| C | 2.1245100000 | -0.6723580000 | 0.2973850000 |
| C | 2.2855750000 | -0.9484610000 | 1.6546470000 |
| C | 3.2356170000 | -1.9059830000 | 2.0001570000 |
| C | 4.0029070000 | -2.5655340000 | 1.0417340000 |
| C | 3.8319460000 | -2.2277660000 | -0.2986870000 |
| C | 2.9004060000 | -1.2717740000 | -0.6961990000 |
| C | 1.4647710000 | -0.2695570000 | 2.7129410000 |
| H | 3.3740680000 | -2.1452490000 | 3.0501400000 |
| C | 4.9829600000 | -3.6340720000 | 1.4496080000 |
| H | 4.4328450000 | -2.7203690000 | -1.0567920000 |
| C | 2.7676360000 | -0.8835310000 | -2.1455420000 |
| C | 0.7323010000 | 3.7821620000 | -1.5409360000 |
| C | 1.2075270000 | 4.7685560000 | -0.4654330000 |
| H | -0.2454680000 | 4.0951570000 | -1.9141200000 |
| H | 1.4167000000 | 3.8192050000 | -2.3972470000 |
| C | 2.6875020000 | 4.6411420000 | -0.0956270000 |
| H | 0.5880180000 | 4.6480450000 | 0.4295430000 |
| H | 1.0331840000 | 5.7817260000 | -0.8383390000 |
| H | 2.9518660000 | 5.4853510000 | 0.5473360000 |
| C | 3.0250720000 | 2.0807920000 | -0.2441470000 |
| H | 3.5802650000 | 1.2767700000 | 0.2410650000 |
| C | 3.0957100000 | 3.3497660000 | 0.6190410000 |
| H | 3.5181060000 | 2.2700280000 | -1.2054550000 |
| H | 4.1287290000 | 3.4606790000 | 0.9594750000 |
| H | 3.2919950000 | 4.7481620000 | -1.0053910000 |
| H | 2.4823550000 | 3.2083750000 | 1.5154100000 |
| H | 1.7274030000 | -0.7000970000 | -2.4189350000 |
| H | 3.1453240000 | -1.6810130000 | -2.7855580000 |

| | | | |
|---|---|---|---|
| H | 3.3441040000 | 0.0233160000 | -2.3581990000 |
| H | 0.5424980000 | -0.8390010000 | 2.8510760000 |
| H | 1.1880570000 | 0.7471170000 | 2.4218770000 |
| H | 2.0154350000 | -0.2250170000 | 3.6534960000 |
| H | 4.4701020000 | -4.5908340000 | 1.5802000000 |
| H | 5.4649380000 | -3.3858960000 | 2.3966830000 |
| H | 5.7569580000 | -3.7710620000 | 0.6932560000 |
| C | -0.3763440000 | -2.1846910000 | -1.5389270000 |
| C | -1.1514900000 | -1.7512850000 | -2.7267440000 |
| H | -0.9353930000 | -0.7050160000 | -2.9800310000 |
| O | -2.5504280000 | -1.8794540000 | -2.5209480000 |
| H | -0.9238490000 | -2.3763780000 | -3.5888620000 |
| C | 0.4273440000 | -3.1248890000 | -1.2686400000 |
| H | 0.9881290000 | -3.5093630000 | -0.4328610000 |
| C | -4.6407400000 | 0.9800280000 | 2.8268810000 |
| C | -3.2443740000 | 0.8216710000 | 2.9484820000 |
| H | -1.4530890000 | 0.0467400000 | 2.1013110000 |
| H | -2.7396560000 | 1.1911530000 | 3.8340100000 |
| H | -5.2030900000 | 1.4711900000 | 3.6120710000 |
| H | -6.3472790000 | 0.6108730000 | 1.5926640000 |
| H | -4.9683240000 | -1.5443980000 | -2.3997590000 |

Thermochemie

Zero-point correction= 0.532002 (Hartree/Particle)
Thermal correction to Energy= 0.563210
Thermal correction to Enthalpy= 0.564154
Thermal correction to Gibbs Free Energy= 0.469034
Sum of electronic and zero-point Energies= -1801.850547
Sum of electronic and thermal Energies= -1801.819339
Sum of electronic and thermal Enthalpies= -1801.818395
Sum of electronic and thermal Free Energies= -1801.913515

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 353.420 | 123.515 | 200.198 |

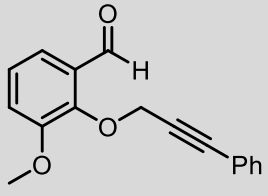
Imaginäre Frequenz

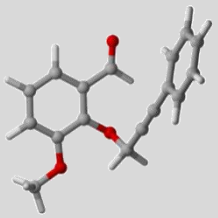
-773.7210

## *O*-propargylierte Aldehyde: Ph-Substituent

(u)M06-2X/6-311+G** SCRF=(PCM,Solvent=Tetrahydrofuran)

**19d**



34

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -3.4102180000 | 0.6794590000 | 1.3188470000 |
| C | -2.7106650000 | 1.8717260000 | 1.5310360000 |
| C | -1.6526290000 | 2.2220510000 | 0.7156800000 |
| C | -1.2785610000 | 1.3749200000 | -0.3349480000 |
| C | -1.9744320000 | 0.1897910000 | -0.5571000000 |
| C | -3.0483780000 | -0.1694240000 | 0.2787600000 |
| H | -4.2378230000 | 0.4279290000 | 1.9685120000 |

| | | | |
|---|---|---|---|
| H | -3.0107410000 | 2.5194220000 | 2.3453750000 |
| H | -1.0996490000 | 3.1407920000 | 0.8666530000 |
| C | -0.1434250000 | 1.7396560000 | -1.2174770000 |
| O | -1.6435700000 | -0.6245900000 | -1.6066690000 |
| O | -3.6549690000 | -1.3422510000 | -0.0153790000 |
| C | -4.7588860000 | -1.7312730000 | 0.7901540000 |
| H | -4.4547470000 | -1.8617420000 | 1.8319350000 |
| H | -5.1028050000 | -2.6804820000 | 0.3878560000 |
| H | -5.5628230000 | -0.9933910000 | 0.7277930000 |
| O | 0.5671730000 | 2.6986110000 | -1.0168580000 |
| H | 0.0246280000 | 1.0835980000 | -2.0843700000 |
| C | -0.9217570000 | -1.8065310000 | -1.2322410000 |
| H | -1.4690390000 | -2.3466890000 | -0.4559030000 |
| C | 0.4322540000 | -1.4760130000 | -0.7790580000 |
| H | -0.8874260000 | -2.4240850000 | -2.1294600000 |
| C | 1.5346040000 | -1.1501420000 | -0.4176710000 |
| C | 2.8457520000 | -0.7441370000 | -0.0011860000 |
| C | 3.3611750000 | 0.4853720000 | -0.4302200000 |
| C | 4.6296820000 | 0.8843580000 | -0.0286290000 |
| C | 5.3939670000 | 0.0641930000 | 0.7975820000 |
| C | 4.8848460000 | -1.1594660000 | 1.2252450000 |
| C | 3.6156430000 | -1.5651660000 | 0.8319300000 |
| H | 2.7615440000 | 1.1230670000 | -1.0690770000 |
| H | 5.0214190000 | 1.8375780000 | -0.3628800000 |
| H | 6.3834360000 | 0.3777520000 | 1.1079660000 |
| H | 5.4772840000 | -1.7994070000 | 1.8682550000 |
| H | 3.2138340000 | -2.5147540000 | 1.1643840000 |

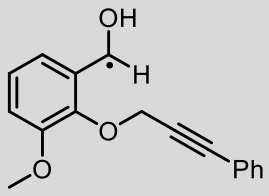
Thermochemie

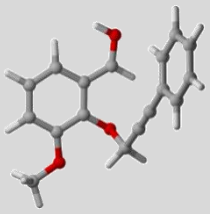
Zero-point correction= 0.268740 (Hartree/Particle)
Thermal correction to Energy= 0.286491
Thermal correction to Enthalpy= 0.287435
Thermal correction to Gibbs Free Energy= 0.220356
Sum of electronic and zero-point Energies= -881.433515
Sum of electronic and thermal Energies= -881.415764
Sum of electronic and thermal Enthalpies= -881.414819
Sum of electronic and thermal Free Energies= -881.481898

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 179.776 | 66.792 | 141.179 |

Volumen

**25d**



35

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -3.3492680000 | 0.5777320000 | 1.3910540000 |
| C | -2.6815720000 | 1.7904600000 | 1.5874370000 |
| C | -1.6769460000 | 2.2061140000 | 0.7392910000 |
| C | -1.2841700000 | 1.3991810000 | -0.3619840000 |
| C | -1.9644050000 | 0.1709130000 | -0.5504690000 |
| C | -2.9891000000 | -0.2299730000 | 0.3090600000 |
| H | -4.1383050000 | 0.2830520000 | 2.0679940000 |
| H | -2.9687740000 | 2.4178290000 | 2.4228310000 |

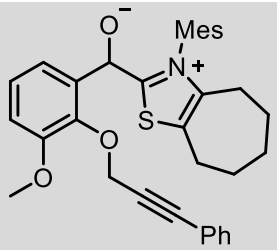
| | | | |
|---|---|---|---|
| H | -1.2051900000 | 3.1645660000 | 0.9236310000 |
| C | -0.2627880000 | 1.7618110000 | -1.2625700000 |
| O | -1.6403050000 | -0.6090430000 | -1.6342920000 |
| O | -3.5769100000 | -1.4172000000 | 0.0110160000 |
| C | -4.6181020000 | -1.8682090000 | 0.8638540000 |
| H | -4.2531360000 | -2.0124500000 | 1.8841690000 |
| H | -4.9474390000 | -2.8206890000 | 0.4561300000 |
| H | -5.4536280000 | -1.1634960000 | 0.8668060000 |
| O | 0.4895610000 | 2.8776570000 | -1.1487560000 |
| H | -0.0111510000 | 1.1634090000 | -2.1236810000 |
| C | -0.9268070000 | -1.8076980000 | -1.3139320000 |
| H | -1.4867010000 | -2.3908540000 | -0.5791050000 |
| C | 0.4218270000 | -1.5112820000 | -0.8212240000 |
| H | -0.8755070000 | -2.3765320000 | -2.2428340000 |
| C | 1.5195460000 | -1.2033290000 | -0.4327220000 |
| H | 0.2883760000 | 3.3535240000 | -0.3356840000 |
| C | 2.8189550000 | -0.7855250000 | 0.0063160000 |
| C | 3.7096370000 | -1.6959500000 | 0.5871750000 |
| C | 4.9685460000 | -1.2723810000 | 0.9953170000 |
| C | 5.3487910000 | 0.0570880000 | 0.8310690000 |
| C | 4.4639420000 | 0.9663630000 | 0.2564020000 |
| C | 3.2037730000 | 0.5517270000 | -0.1559580000 |
| H | 3.4091090000 | -2.7291380000 | 0.7123900000 |
| H | 5.6544110000 | -1.9824650000 | 1.4418830000 |
| H | 6.3312060000 | 0.3836610000 | 1.1504020000 |
| H | 4.7563710000 | 2.0015770000 | 0.1270290000 |
| H | 2.5104390000 | 1.2544390000 | -0.6044000000 |

Thermochemie

| | |
|---|---|
| Zero-point correction= | 0.278811 (Hartree/Particle) |
| Thermal correction to Energy= | 0.297063 |
| Thermal correction to Enthalpy= | 0.298008 |
| Thermal correction to Gibbs Free Energy= | 0.229673 |
| Sum of electronic and zero-point Energies= | -881.986333 |
| Sum of electronic and thermal Energies= | -881.968080 |
| Sum of electronic and thermal Enthalpies= | -881.967136 |
| Sum of electronic and thermal Free Energies= | -882.035471 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 186.410 | 69.538 | 143.823 |

**22d**

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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -3.2645400000 | -4.0338710000 | 1.1183830000 |
| C | -2.8772670000 | -3.4159880000 | 2.3072700000 |
| C | -1.9923000000 | -2.3479410000 | 2.2969410000 |
| C | -1.4742780000 | -1.8751540000 | 1.0913890000 |
| C | -1.8564460000 | -2.4913190000 | -0.0951460000 |
| C | -2.7580450000 | -3.5687810000 | -0.0931010000 |
| H | -3.9558810000 | -4.8652790000 | 1.1443830000 |
| H | -3.2751640000 | -3.7853330000 | 3.2455410000 |
| H | -1.6643900000 | -1.8588650000 | 3.2058990000 |

| | | | |
|---|---|---|---|
| C | -0.4795300000 | -0.7004090000 | 1.1121200000 |
| O | -1.4094420000 | -1.9966820000 | -1.3044720000 |
| O | -3.0763450000 | -4.0796870000 | -1.3122130000 |
| C | -3.9905330000 | -5.1637950000 | -1.3493300000 |
| H | -3.5957980000 | -6.0285260000 | -0.8089960000 |
| H | -4.1148450000 | -5.4157580000 | -2.3997220000 |
| H | -4.9563410000 | -4.8751270000 | -0.9256130000 |
| O | -0.0220500000 | -0.3573130000 | 2.3259540000 |
| C | -0.4527340000 | -2.8220430000 | -1.9797350000 |
| H | -0.7739490000 | -3.8654330000 | -1.9568290000 |
| C | 0.8822080000 | -2.6620020000 | -1.3938110000 |
| H | -0.4503950000 | -2.4872400000 | -3.0185380000 |
| C | 1.9289150000 | -2.4182900000 | -0.8487670000 |
| N | -0.4944970000 | 1.5622410000 | -0.0090120000 |
| C | -1.1606410000 | 0.5288630000 | 0.4957470000 |
| S | -2.8226130000 | 0.8610820000 | 0.5593650000 |
| C | -2.5963150000 | 2.4492470000 | -0.1092330000 |
| C | -1.2834820000 | 2.6693890000 | -0.3593740000 |
| C | 0.9442930000 | 1.5303060000 | -0.1980510000 |
| C | 1.7564330000 | 2.0574040000 | 0.8062020000 |
| C | 3.1313320000 | 2.0448030000 | 0.5823140000 |
| C | 3.6806070000 | 1.5256300000 | -0.5898790000 |
| C | 2.8243580000 | 1.0184040000 | -1.5660930000 |
| C | 1.4412680000 | 1.0205250000 | -1.3972090000 |
| C | 1.1541630000 | 2.6043200000 | 2.0692120000 |
| H | 3.7903220000 | 2.4355900000 | 1.3516130000 |
| C | 5.1703860000 | 1.5303250000 | -0.8102270000 |
| H | 3.2398190000 | 0.6034190000 | -2.4797010000 |
| C | 0.5126650000 | 0.5321650000 | -2.4756220000 |
| C | -3.7558700000 | 3.3627680000 | -0.3809460000 |
| C | -3.5953920000 | 4.7645650000 | 0.2194510000 |
| H | -4.6659790000 | 2.9035560000 | 0.0103420000 |
| H | -3.8903990000 | 3.4453710000 | -1.4659550000 |
| C | -2.5382030000 | 5.6342990000 | -0.4644110000 |
| H | -3.3702230000 | 4.6757370000 | 1.2873450000 |
| H | -4.5621340000 | 5.2684250000 | 0.1384240000 |
| H | -2.6453510000 | 6.6558570000 | -0.0895010000 |
| C | -0.6782820000 | 3.9033800000 | -0.9603340000 |
| H | 0.4087080000 | 3.8052660000 | -0.9427610000 |
| C | -1.0848330000 | 5.2038360000 | -0.2532980000 |
| H | -0.9720880000 | 3.9585820000 | -2.0156490000 |
| H | -0.4327890000 | 5.9951510000 | -0.6316580000 |
| H | -2.7482330000 | 5.6762110000 | -1.5402640000 |
| H | -0.8812780000 | 5.1129790000 | 0.8187920000 |
| H | 0.0205930000 | 1.3784310000 | -2.9670410000 |
| H | -0.2678130000 | -0.1128540000 | -2.0676600000 |
| H | 1.0666680000 | -0.0251370000 | -3.2314680000 |
| H | 0.6011430000 | 1.8023650000 | 2.5683190000 |
| H | 0.4587370000 | 3.4209340000 | 1.8510460000 |
| H | 1.9310420000 | 2.9858960000 | 2.7315260000 |
| H | 5.4701510000 | 2.4126520000 | -1.3833840000 |
| H | 5.4813410000 | 0.6442720000 | -1.3657670000 |
| H | 5.7067040000 | 1.5449810000 | 0.1395100000 |
| H | 0.3045580000 | -0.9540270000 | 0.3754300000 |
| C | 3.1272000000 | -2.0660040000 | -0.1438420000 |
| C | 4.3843760000 | -2.3656680000 | -0.6836310000 |
| C | 5.5387550000 | -2.0035900000 | -0.0018920000 |
| C | 5.4488650000 | -1.3352070000 | 1.2171880000 |
| C | 4.1996200000 | -1.0308890000 | 1.7506500000 |
| C | 3.0353210000 | -1.3931540000 | 1.0823370000 |
| H | 4.4463360000 | -2.8821930000 | -1.6343580000 |
| H | 6.5088460000 | -2.2390570000 | -0.4240020000 |

| | | | |
|---|---|---|---|
| H | 6.3505310000 | -1.0496000000 | 1.7467110000 |
| H | 4.1254330000 | -0.5031600000 | 2.6947370000 |
| H | 2.0656670000 | -1.1383920000 | 1.5066880000 |

Thermochemie

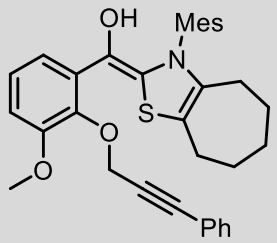
Zero-point correction= 0.614861 (Hartree/Particle)
Thermal correction to Energy= 0.651082
Thermal correction to Enthalpy= 0.652026
Thermal correction to Gibbs Free Energy= 0.546389
Sum of electronic and zero-point Energies= -1994.354651
Sum of electronic and thermal Energies= -1994.318430
Sum of electronic and thermal Enthalpies= -1994.317486
Sum of electronic and thermal Free Energies= -1994.423123

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 408.560 | 141.016 | 222.332 |

Volumen

Molar volume = 4856.613 bohr**3/mol (433.399 cm**3/mol)
Recommended a0 for SCRF calculation = 6.62 angstrom ( 12.51 bohr)

**23d**

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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -2.8652770000 | 4.2153240000 | 1.2277050000 |
| C | -2.5527340000 | 3.4773720000 | 2.3726470000 |
| C | -1.7025300000 | 2.3898090000 | 2.3051590000 |
| C | -1.1341490000 | 2.0023790000 | 1.0799220000 |
| C | -1.4700270000 | 2.7215730000 | -0.0672620000 |
| C | -2.3268700000 | 3.8365660000 | 0.0034410000 |
| H | -3.5249820000 | 5.0689250000 | 1.3022820000 |
| H | -2.9791960000 | 3.7746350000 | 3.3233580000 |
| H | -1.4585900000 | 1.8210550000 | 3.1942720000 |
| C | -0.2475150000 | 0.8253120000 | 1.0322660000 |
| O | -0.9861850000 | 2.3395070000 | -1.2961780000 |
| O | -2.5787170000 | 4.4566470000 | -1.1771600000 |
| C | -3.4617710000 | 5.5671310000 | -1.1581920000 |
| H | -4.4530380000 | 5.2724840000 | -0.8030180000 |
| H | -3.5297140000 | 5.9137870000 | -2.1863440000 |
| H | -3.0679530000 | 6.3685460000 | -0.5274870000 |
| O | -0.7193800000 | -0.3112900000 | 1.6781160000 |
| C | -1.9439790000 | 1.6452710000 | -2.0985490000 |
| H | -2.8132500000 | 2.2849090000 | -2.2758260000 |
| C | -2.3691540000 | 0.3778270000 | -1.4915050000 |
| H | -1.4495070000 | 1.4584700000 | -3.0525390000 |
| C | -2.7418500000 | -0.6464900000 | -0.9763220000 |
| H | -1.1475930000 | -0.8904280000 | 1.0329810000 |
| N | 1.8344500000 | -0.2928080000 | 0.4063910000 |
| C | 1.0057080000 | 0.8322870000 | 0.5335740000 |
| S | 1.8733000000 | 2.2849430000 | 0.0081850000 |
| C | 3.3437400000 | 1.3327020000 | -0.2690570000 |
| C | 3.1410680000 | 0.0320320000 | -0.0339090000 |
| C | 1.2452570000 | -1.5450350000 | -0.0004520000 |

| | | | |
|---|---|---|---|
| C | 1.1822090000 | -2.6007930000 | 0.9143730000 |
| C | 0.6040820000 | -3.7994360000 | 0.5007960000 |
| C | 0.1004150000 | -3.9628130000 | -0.7905640000 |
| C | 0.1819450000 | -2.8909190000 | -1.6761320000 |
| C | 0.7546660000 | -1.6740610000 | -1.3043950000 |
| C | 1.7112970000 | -2.4277270000 | 2.3112620000 |
| H | 0.5429640000 | -4.6248090000 | 1.2040610000 |
| C | -0.4840130000 | -5.2815540000 | -1.2252180000 |
| H | -0.2075300000 | -3.0006760000 | -2.6844780000 |
| C | 0.8632570000 | -0.5382910000 | -2.2870130000 |
| C | 4.6136950000 | 2.0028130000 | -0.7072420000 |
| C | 5.8045840000 | 1.7259150000 | 0.2187760000 |
| H | 4.4457690000 | 3.0808840000 | -0.7613740000 |
| H | 4.8667200000 | 1.6790680000 | -1.7249810000 |
| C | 6.3538050000 | 0.2991790000 | 0.1377090000 |
| H | 5.5162890000 | 1.9549560000 | 1.2503910000 |
| H | 6.6099780000 | 2.4164880000 | -0.0485090000 |
| H | 7.2895370000 | 0.2609810000 | 0.7033100000 |
| C | 4.1721820000 | -1.0520810000 | -0.1770820000 |
| H | 3.7244340000 | -2.0057160000 | 0.1085190000 |
| C | 5.4358440000 | -0.8091080000 | 0.6606510000 |
| H | 4.4523060000 | -1.1476710000 | -1.2337550000 |
| H | 6.0078510000 | -1.7413890000 | 0.6819490000 |
| H | 6.6150430000 | 0.0789550000 | -0.9053020000 |
| H | 5.1430570000 | -0.5918520000 | 1.6939490000 |
| H | 1.9123990000 | -0.3242150000 | -2.5150610000 |
| H | 0.4293930000 | 0.3795190000 | -1.8829420000 |
| H | 0.3524440000 | -0.7888900000 | -3.2175670000 |
| H | 1.1601380000 | -1.6344990000 | 2.8205480000 |
| H | 2.7646720000 | -2.1342070000 | 2.3004610000 |
| H | 1.6138270000 | -3.3538940000 | 2.8781880000 |
| H | 0.3051250000 | -5.9550530000 | -1.5719200000 |
| H | -1.1916480000 | -5.1477740000 | -2.0454990000 |
| H | -1.0021070000 | -5.7723970000 | -0.3993200000 |
| C | -3.1841600000 | -1.8458090000 | -0.3240950000 |
| C | -3.5884980000 | -1.7985320000 | 1.0178200000 |
| C | -4.0020800000 | -2.9578650000 | 1.6616190000 |
| C | -4.0294950000 | -4.1682710000 | 0.9741340000 |
| C | -3.6406700000 | -4.2178170000 | -0.3624740000 |
| C | -3.2134890000 | -3.0660980000 | -1.0102310000 |
| H | -3.5698960000 | -0.8513080000 | 1.5449930000 |
| H | -4.3073130000 | -2.9145320000 | 2.7002290000 |
| H | -4.3560310000 | -5.0705040000 | 1.4775400000 |
| H | -3.6645160000 | -5.1580930000 | -0.9004810000 |
| H | -2.9017460000 | -3.0988330000 | -2.0475060000 |

Thermochemie

Zero-point correction= 0.614257 (Hartree/Particle)
Thermal correction to Energy= 0.650991
Thermal correction to Enthalpy= 0.651935
Thermal correction to Gibbs Free Energy= 0.544887
Sum of electronic and zero-point Energies= -1994.369223
Sum of electronic and thermal Energies= -1994.332489
Sum of electronic and thermal Enthalpies= -1994.331545
Sum of electronic and thermal Free Energies= -1994.438594

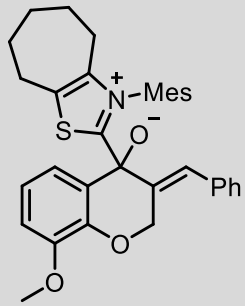
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 408.503 | 142.922 | 225.303 |

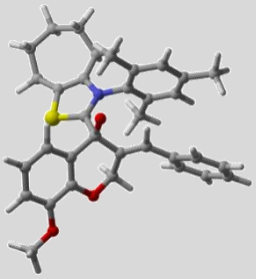
Volumen

Molar volume = 4734.905 bohr**3/mol (422.538 cm**3/mol)

Recommended a0 for SCRF calculation = 6.57 angstrom ( 12.41 bohr)

**[24d + A]**
**(E)**



74
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0741330000 | -1.6813860000 | 1.0458890000 |
| C | -4.5676200000 | -0.7032500000 | 1.9106570000 |
| C | -3.2394010000 | -0.3344670000 | 1.8398200000 |
| C | -2.3824210000 | -0.9133910000 | 0.8945970000 |
| C | -2.8823850000 | -1.8881160000 | 0.0395970000 |
| C | -4.2385420000 | -2.2809510000 | 0.1166760000 |
| H | -6.1142260000 | -1.9696890000 | 1.1150500000 |
| H | -5.2260010000 | -0.2509110000 | 2.6425570000 |
| H | -2.8181630000 | 0.3912560000 | 2.5251320000 |
| C | -0.8833220000 | -0.5086510000 | 0.9159840000 |
| O | -4.6185610000 | -3.2487990000 | -0.7577610000 |
| C | -5.9628310000 | -3.6903590000 | -0.6901890000 |
| H | -6.1869760000 | -4.1156880000 | 0.2923360000 |
| H | -6.0662400000 | -4.4596720000 | -1.4517080000 |
| H | -6.6574500000 | -2.8720170000 | -0.9010620000 |
| O | -0.4152510000 | -0.3054260000 | 2.1347810000 |
| N | 0.3115290000 | 1.6171620000 | -0.0147630000 |
| C | -0.7875300000 | 0.8738190000 | 0.1380110000 |
| S | -2.1454890000 | 1.7256750000 | -0.4309120000 |
| C | -1.1968040000 | 3.1054670000 | -0.8743850000 |
| C | 0.1063630000 | 2.8864550000 | -0.5786930000 |
| C | 1.6460420000 | 1.1425710000 | 0.3058990000 |
| C | 2.1497840000 | 1.3375030000 | 1.5887650000 |
| C | 3.4147780000 | 0.8121110000 | 1.8571610000 |
| C | 4.1587730000 | 0.1469820000 | 0.8840960000 |
| C | 3.6453770000 | 0.0611700000 | -0.4104940000 |
| C | 2.3873410000 | 0.5625930000 | -0.7246150000 |
| C | 1.3672020000 | 2.0861680000 | 2.6289960000 |
| H | 3.8253340000 | 0.9276920000 | 2.8554950000 |
| C | 5.4839450000 | -0.4859680000 | 1.2155560000 |
| H | 4.2253310000 | -0.4286380000 | -1.1870400000 |
| C | 1.8434330000 | 0.4877860000 | -2.1248850000 |
| C | -1.8085130000 | 4.3303380000 | -1.4887960000 |
| C | -1.4876360000 | 5.6230710000 | -0.7278890000 |
| H | -2.8908800000 | 4.1958550000 | -1.5402340000 |
| H | -1.4552980000 | 4.4185500000 | -2.5227500000 |
| C | -0.0380850000 | 6.0957510000 | -0.8610370000 |
| H | -1.7403620000 | 5.4906360000 | 0.3292700000 |
| H | -2.1437840000 | 6.4060740000 | -1.1166380000 |
| H | 0.0311550000 | 7.1038800000 | -0.4433460000 |
| C | 1.2386720000 | 3.8443770000 | -0.8052270000 |
| H | 2.1578730000 | 3.4087520000 | -0.4108970000 |
| C | 1.0146310000 | 5.2252030000 | -0.1704810000 |
| H | 1.3845340000 | 3.9654950000 | -1.8855590000 |
| H | 1.9705020000 | 5.7541810000 | -0.2009440000 |
| H | 0.2133150000 | 6.1847510000 | -1.9251950000 |
| H | 0.7563810000 | 5.1005700000 | 0.8863630000 |

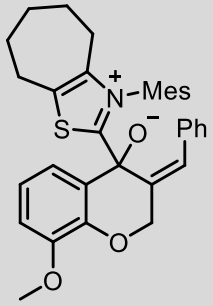
| | | | |
|---|---|---|---|
| H | 1.6845550000 | 1.4882940000 | -2.5386690000 |
| H | 0.8804620000 | -0.0282400000 | -2.1524580000 |
| H | 2.5376670000 | -0.0417990000 | -2.7769370000 |
| H | 0.4897910000 | 1.4930840000 | 2.8986170000 |
| H | 1.0260350000 | 3.0511570000 | 2.2413090000 |
| H | 1.9808140000 | 2.2705500000 | 3.5108210000 |
| H | 6.2088160000 | -0.3262080000 | 0.4153470000 |
| H | 5.3592850000 | -1.5664550000 | 1.3364000000 |
| H | 5.8940850000 | -0.0873190000 | 2.1441490000 |
| C | -0.1272130000 | -1.5413420000 | 0.0488520000 |
| C | -0.8559260000 | -1.9799700000 | -1.1858460000 |
| H | -1.0313400000 | -1.1332090000 | -1.8644950000 |
| O | -2.1329760000 | -2.5494220000 | -0.8798380000 |
| H | -0.3292710000 | -2.7609890000 | -1.7280340000 |
| C | 1.0572100000 | -1.9724970000 | 0.4854370000 |
| H | 1.3520990000 | -1.5640180000 | 1.4521440000 |
| C | 2.0302840000 | -2.8832410000 | -0.1417970000 |
| C | 2.8564500000 | -3.6449970000 | 0.6959540000 |
| C | 3.8340820000 | -4.4828710000 | 0.1735590000 |
| C | 4.0206150000 | -4.5635600000 | -1.2043790000 |
| C | 3.2252740000 | -3.7944480000 | -2.0492980000 |
| C | 2.2437290000 | -2.9602840000 | -1.5238570000 |
| H | 2.7235530000 | -3.5716870000 | 1.7704740000 |
| H | 4.4559880000 | -5.0682140000 | 0.8411400000 |
| H | 4.7860920000 | -5.2112230000 | -1.6151070000 |
| H | 3.3776940000 | -3.8332530000 | -3.1218090000 |
| H | 1.6703100000 | -2.3330160000 | -2.1950900000 |

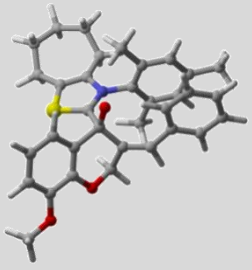
Thermochemie

Zero-point correction= 0.616282 (Hartree/Particle)
Thermal correction to Energy= 0.651559
Thermal correction to Enthalpy= 0.652503
Thermal correction to Gibbs Free Energy= 0.548998
Sum of electronic and zero-point Energies= -1994.397004
Sum of electronic and thermal Energies= -1994.361727
Sum of electronic and thermal Enthalpies= -1994.360783
Sum of electronic and thermal Free Energies= -1994.464288

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 408.859 | 139.027 | 217.845 |

**[24d + A]**
**(Z)**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 5.2908260000 | -1.0346510000 | -1.1208670000 |
| C | 4.4664990000 | -0.5128710000 | -2.1242870000 |
| C | 3.1049180000 | -0.4044950000 | -1.9201700000 |
| C | 2.5278350000 | -0.7897070000 | -0.7037860000 |
| C | 3.3452930000 | -1.3156710000 | 0.2903050000 |
| C | 4.7367720000 | -1.4451220000 | 0.0821480000 |
| H | 6.3547360000 | -1.1238840000 | -1.2941510000 |

| | | | |
|---|---|---|---|
| H | 4.9059570000 | -0.2073340000 | -3.0662820000 |
| H | 2.4411620000 | -0.0418480000 | -2.6951720000 |
| C | 0.9704950000 | -0.6784130000 | -0.5719820000 |
| O | 5.4365350000 | -1.9814060000 | 1.1161360000 |
| C | 6.8348830000 | -2.1291020000 | 0.9448260000 |
| H | 7.0606690000 | -2.7942550000 | 0.1064370000 |
| H | 7.2066550000 | -2.5676900000 | 1.8678520000 |
| H | 7.3153040000 | -1.1598800000 | 0.7817610000 |
| O | 0.3598930000 | -0.8177490000 | -1.7351470000 |
| N | -0.5169800000 | 1.3309610000 | 0.1513070000 |
| C | 0.6807260000 | 0.8045450000 | -0.1041750000 |
| S | 1.8667680000 | 2.0243450000 | -0.1153930000 |
| C | 0.7059960000 | 3.2635380000 | 0.2262050000 |
| C | -0.5316030000 | 2.7259980000 | 0.3340900000 |
| C | -1.7461510000 | 0.5660300000 | 0.2830630000 |
| C | -2.5587410000 | 0.4252120000 | -0.8420560000 |
| C | -3.7815020000 | -0.2220840000 | -0.6722020000 |
| C | -4.1922280000 | -0.7027960000 | 0.5685210000 |
| C | -3.3574560000 | -0.5101820000 | 1.6676300000 |
| C | -2.1293510000 | 0.1365730000 | 1.5543770000 |
| C | -2.1312010000 | 0.9642990000 | -2.1774030000 |
| H | -4.4226300000 | -0.3608480000 | -1.5370660000 |
| C | -5.5244880000 | -1.3854880000 | 0.7341130000 |
| H | -3.6692420000 | -0.8698470000 | 2.6443100000 |
| C | -1.2727270000 | 0.3352080000 | 2.7771250000 |
| C | 1.1058260000 | 4.7011520000 | 0.3899660000 |
| C | 0.3218610000 | 5.6677040000 | -0.5061700000 |
| H | 2.1735010000 | 4.7960330000 | 0.1818180000 |
| H | 0.9667630000 | 4.9848400000 | 1.4399360000 |
| C | -1.1383530000 | 5.8699650000 | -0.0960140000 |
| H | 0.3729400000 | 5.3196320000 | -1.5430580000 |
| H | 0.8286120000 | 6.6355360000 | -0.4691410000 |
| H | -1.5432590000 | 6.7031540000 | -0.6769900000 |
| C | -1.7951160000 | 3.4752550000 | 0.6425790000 |
| H | -2.6393280000 | 2.7870160000 | 0.5964460000 |
| C | -2.0577780000 | 4.6633250000 | -0.2946190000 |
| H | -1.7400040000 | 3.8347770000 | 1.6775000000 |
| H | -3.0884440000 | 4.9855360000 | -0.1258450000 |
| H | -1.1755730000 | 6.1798000000 | 0.9557070000 |
| H | -1.9999260000 | 4.3238120000 | -1.3340550000 |
| H | -0.4982840000 | 1.0905400000 | 2.6324110000 |
| H | -0.7813060000 | -0.6032290000 | 3.0485120000 |
| H | -1.8900690000 | 0.6391300000 | 3.6240440000 |
| H | -1.1905350000 | 0.4857550000 | -2.4661500000 |
| H | -1.9656040000 | 2.0456620000 | -2.1282890000 |
| H | -2.8964890000 | 0.7725590000 | -2.9297850000 |
| H | -6.2719450000 | -0.6823720000 | 1.1130910000 |
| H | -5.4497350000 | -2.2107650000 | 1.4443590000 |
| H | -5.8813600000 | -1.7833860000 | -0.2167360000 |
| C | 0.5986990000 | -1.5930860000 | 0.6095440000 |
| C | 1.5316310000 | -1.3884720000 | 1.7783120000 |
| H | 1.5421600000 | -0.3334650000 | 2.0851840000 |
| O | 2.8805680000 | -1.7606420000 | 1.4861930000 |
| H | 1.2425280000 | -1.9938110000 | 2.6359410000 |
| C | -0.3828970000 | -2.4980840000 | 0.7550630000 |
| H | -0.3686750000 | -2.9954930000 | 1.7258090000 |
| C | -1.5379780000 | -2.9616200000 | -0.0421890000 |
| C | -2.5156660000 | -3.6793350000 | 0.6665690000 |
| C | -3.6568970000 | -4.1635620000 | 0.0412160000 |
| C | -3.8386770000 | -3.9560080000 | -1.3231950000 |
| C | -2.8661460000 | -3.2686410000 | -2.0440430000 |
| C | -1.7272770000 | -2.7731400000 | -1.4172430000 |

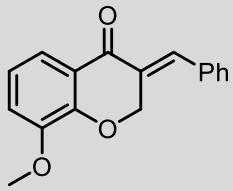
| | | | |
|---|---|---|---|
| H | -2.3806870000 | -3.8474230000 | 1.7308710000 |
| H | -4.4011440000 | -4.7029960000 | 0.6162210000 |
| H | -4.7258250000 | -4.3336540000 | -1.8193340000 |
| H | -2.9973540000 | -3.1091690000 | -3.1090310000 |
| H | -0.9791300000 | -2.2079610000 | -1.9589450000 |

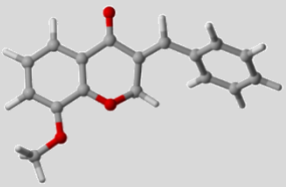
Thermochemie

Zero-point correction= 0.616237 (Hartree/Particle)
Thermal correction to Energy= 0.651330
Thermal correction to Enthalpy= 0.652275
Thermal correction to Gibbs Free Energy= 0.550375
Sum of electronic and zero-point Energies= -1994.392158
Sum of electronic and thermal Energies= -1994.357065
Sum of electronic and thermal Enthalpies= -1994.356120
Sum of electronic and thermal Free Energies= -1994.458020

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 408.716 | 138.976 | 214.465 |

**24d (E)**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -4.3278110000 | 0.1154720000 | 0.0516390000 |
| C | -4.1433310000 | 1.4946740000 | -0.1275940000 |
| C | -2.8738850000 | 2.0210640000 | -0.2152130000 |
| C | -1.7605380000 | 1.1695910000 | -0.1407410000 |
| C | -1.9380280000 | -0.2040770000 | 0.0127200000 |
| C | -3.2395140000 | -0.7400950000 | 0.1278960000 |
| H | -5.3328570000 | -0.2778050000 | 0.1254410000 |
| H | -5.0113230000 | 2.1390650000 | -0.1876820000 |
| H | -2.7036570000 | 3.0838930000 | -0.3317330000 |
| C | -0.3867930000 | 1.7278840000 | -0.1232150000 |
| O | -0.9060180000 | -1.0726600000 | 0.0983230000 |
| O | -3.3098010000 | -2.0794800000 | 0.3012480000 |
| C | -4.6022950000 | -2.6550600000 | 0.4114110000 |
| H | -5.1353120000 | -2.2549520000 | 1.2782240000 |
| H | -4.4438420000 | -3.7225010000 | 0.5415740000 |
| H | -5.1869290000 | -2.4778110000 | -0.4955230000 |
| O | -0.1808860000 | 2.9240410000 | -0.0406950000 |
| C | 0.7143950000 | 0.7219360000 | -0.1844230000 |
| C | 0.2947060000 | -0.6699990000 | -0.5668810000 |
| H | 0.1151760000 | -0.7366980000 | -1.6475660000 |
| H | 1.0413450000 | -1.4094670000 | -0.2854990000 |
| C | 1.9628420000 | 1.1196980000 | 0.1023390000 |
| H | 2.0779610000 | 2.1544210000 | 0.4177130000 |
| C | 3.1877110000 | 0.3111350000 | 0.0565290000 |
| C | 3.4129310000 | -0.6467900000 | -0.9399400000 |
| C | 4.5847640000 | -1.3949620000 | -0.9484880000 |
| C | 5.5467720000 | -1.1979930000 | 0.0377000000 |
| C | 5.3437770000 | -0.2319070000 | 1.0211920000 |
| C | 4.1803380000 | 0.5261530000 | 1.0218980000 |
| H | 2.6872310000 | -0.7808950000 | -1.7339360000 |
| H | 4.7487490000 | -2.1274710000 | -1.7297740000 |
| H | 6.4575680000 | -1.7848560000 | 0.0325900000 |
| H | 6.0963330000 | -0.0657920000 | 1.7828110000 |

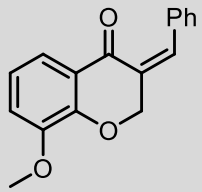
| | | | |
|---|---|---|---|
| H | 4.0269510000 | 1.2853220000 | 1.7813720000 |

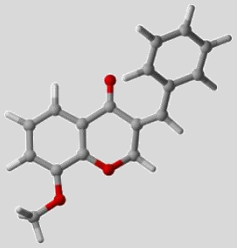
Thermochemie

Zero-point correction= 0.271761 (Hartree/Particle)
Thermal correction to Energy= 0.287985
Thermal correction to Enthalpy= 0.288929
Thermal correction to Gibbs Free Energy= 0.226876
Sum of electronic and zero-point Energies= -881.492877
Sum of electronic and thermal Energies= -881.476653
Sum of electronic and thermal Enthalpies= -881.475709
Sum of electronic and thermal Free Energies= -881.537763

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 180.713 | 63.605 | 130.603 |

**24d (Z)**



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XYZ-Matrix in Ångström

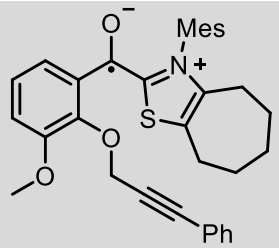
| | | | |
|---|---|---|---|
| C | -3.8482610000 | 1.2723250000 | 0.1808690000 |
| C | -3.0161230000 | 2.3049200000 | -0.2781680000 |
| C | -1.7160240000 | 2.0390470000 | -0.6429100000 |
| C | -1.2199600000 | 0.7276310000 | -0.5604590000 |
| C | -2.0497480000 | -0.3068680000 | -0.1240080000 |
| C | -3.3794740000 | -0.0290260000 | 0.2642700000 |
| H | -4.8672300000 | 1.5010400000 | 0.4634170000 |
| H | -3.4086820000 | 3.3121970000 | -0.3361720000 |
| H | -1.0478350000 | 2.8207660000 | -0.9814580000 |
| C | 0.2170690000 | 0.4606250000 | -0.8357350000 |
| O | -1.6485940000 | -1.5946160000 | -0.0379470000 |
| O | -4.0981240000 | -1.0940140000 | 0.6862720000 |
| C | -5.4423550000 | -0.8606960000 | 1.0765590000 |
| H | -5.4899810000 | -0.1660450000 | 1.9196220000 |
| H | -5.8377400000 | -1.8272480000 | 1.3780940000 |
| H | -6.0286760000 | -0.4680240000 | 0.2412020000 |
| O | 0.9707800000 | 1.3249190000 | -1.2328510000 |
| C | 0.6244160000 | -0.9545400000 | -0.5844850000 |
| C | -0.5035360000 | -1.9161680000 | -0.8353990000 |
| H | -0.8134390000 | -1.8774370000 | -1.8871420000 |
| H | -0.2308020000 | -2.9373500000 | -0.5783510000 |
| C | 1.8375730000 | -1.3798380000 | -0.2093010000 |
| H | 1.9689880000 | -2.4586730000 | -0.1337910000 |
| C | 3.0398100000 | -0.5966470000 | 0.1310500000 |
| C | 2.9804380000 | 0.5942360000 | 0.8619220000 |
| C | 4.1446710000 | 1.2756620000 | 1.1893300000 |
| C | 5.3850320000 | 0.7809360000 | 0.7896210000 |
| C | 5.4560060000 | -0.4124650000 | 0.0782650000 |
| C | 4.2905130000 | -1.1040000000 | -0.2343230000 |
| H | 2.0210040000 | 0.9794090000 | 1.1854170000 |
| H | 4.0866130000 | 2.1939490000 | 1.7616630000 |
| H | 6.2910700000 | 1.3182750000 | 1.0435520000 |
| H | 6.4169730000 | -0.8098410000 | -0.2260000000 |
| H | 4.3469420000 | -2.0421240000 | -0.7764340000 |

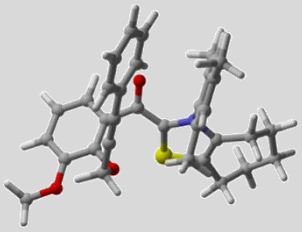
Thermochemie

| | |
|---|---|
| Zero-point correction= | 0.271171 (Hartree/Particle) |
| Thermal correction to Energy= | 0.287534 |
| Thermal correction to Enthalpy= | 0.288478 |
| Thermal correction to Gibbs Free Energy= | 0.225512 |
| Sum of electronic and zero-point Energies= | -881.487816 |
| Sum of electronic and thermal Energies= | -881.471453 |
| Sum of electronic and thermal Enthalpies= | -881.470509 |
| Sum of electronic and thermal Free Energies= | -881.533475 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 180.430 | 63.854 | 132.523 |

**21d**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -0.7809830000 | 5.0891570000 | 1.3041080000 |
| C | -0.7006070000 | 4.3389330000 | 2.4791340000 |
| C | -0.4181170000 | 2.9860210000 | 2.4341380000 |
| C | -0.1978370000 | 2.3505960000 | 1.2051800000 |
| C | -0.2910030000 | 3.0905890000 | 0.0293710000 |
| C | -0.5787380000 | 4.4691330000 | 0.0760740000 |
| H | -0.9999840000 | 6.1468200000 | 1.3580690000 |
| H | -0.8616450000 | 4.8299100000 | 3.4312180000 |
| H | -0.3624750000 | 2.3971260000 | 3.3414310000 |
| C | 0.0770310000 | 0.8741410000 | 1.2085150000 |
| O | -0.0827000000 | 2.4990040000 | -1.1930560000 |
| O | -0.6392340000 | 5.0967190000 | -1.1248850000 |
| C | -0.9429800000 | 6.4831700000 | -1.1268020000 |
| H | -1.9248070000 | 6.6687690000 | -0.6834870000 |
| H | -0.9499890000 | 6.7863800000 | -2.1706090000 |
| H | -0.1809530000 | 7.0502930000 | -0.5860000000 |
| O | -0.6859970000 | 0.1082080000 | 1.8338530000 |
| C | -1.2690160000 | 2.2930910000 | -1.9662030000 |
| H | -1.8131480000 | 3.2346030000 | -2.0733130000 |
| C | -2.1384640000 | 1.2601620000 | -1.3949980000 |
| H | -0.9200460000 | 1.9833460000 | -2.9526120000 |
| C | -2.8536160000 | 0.4034560000 | -0.9394730000 |
| N | 1.5604770000 | -0.9020730000 | 0.3101940000 |
| C | 1.2540080000 | 0.4196860000 | 0.5578260000 |
| S | 2.5920070000 | 1.4419830000 | 0.1169050000 |
| C | 3.5423370000 | 0.0520190000 | -0.3633970000 |
| C | 2.8476450000 | -1.0936370000 | -0.2044920000 |
| C | 0.5204750000 | -1.8789560000 | 0.0840580000 |
| C | 0.2024690000 | -2.7920370000 | 1.0867080000 |
| C | -0.7815240000 | -3.7419190000 | 0.8131840000 |
| C | -1.4369340000 | -3.7815400000 | -0.4165720000 |
| C | -1.0795850000 | -2.8558190000 | -1.3961570000 |
| C | -0.0959140000 | -1.8961240000 | -1.1706290000 |
| C | 0.8995050000 | -2.7292640000 | 2.4164270000 |
| H | -1.0521120000 | -4.4553150000 | 1.5858250000 |
| C | -2.5346640000 | -4.7766420000 | -0.6871920000 |
| H | -1.5871030000 | -2.8733250000 | -2.3566400000 |

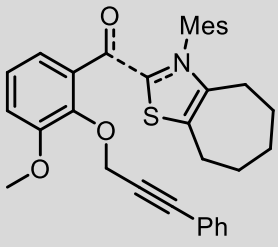
| | | | |
|---|---|---|---|
| C | 0.3185670000 | -0.9300350000 | -2.2494510000 |
| C | 4.9421180000 | 0.2110270000 | -0.8814510000 |
| C | 5.9817600000 | -0.6063640000 | -0.1038950000 |
| H | 5.2139190000 | 1.2681560000 | -0.8462120000 |
| H | 4.9699890000 | -0.0805180000 | -1.9385640000 |
| C | 5.9092050000 | -2.1168590000 | -0.3421310000 |
| H | 5.8788280000 | -0.3928250000 | 0.9652100000 |
| H | 6.9742720000 | -0.2594500000 | -0.4045300000 |
| H | 6.7872390000 | -2.5776940000 | 0.1192660000 |
| C | 3.3519370000 | -2.4720110000 | -0.5212600000 |
| H | 2.5841310000 | -3.1990340000 | -0.2516060000 |
| C | 4.6628390000 | -2.8235600000 | 0.1976650000 |
| H | 3.4976980000 | -2.5599060000 | -1.6048620000 |
| H | 4.8132550000 | -3.9020470000 | 0.0994770000 |
| H | 5.9890150000 | -2.3114390000 | -1.4189280000 |
| H | 4.5521390000 | -2.6149620000 | 1.2673210000 |
| H | 1.3006940000 | -1.2015860000 | -2.6509210000 |
| H | 0.3915540000 | 0.0897930000 | -1.8646280000 |
| H | -0.4005570000 | -0.9431000000 | -3.0690370000 |
| H | 0.7028530000 | -1.7626310000 | 2.8865240000 |
| H | 1.9827660000 | -2.8262340000 | 2.2980950000 |
| H | 0.5513680000 | -3.5249890000 | 3.0750720000 |
| H | -2.7260440000 | -5.4020160000 | 0.1858000000 |
| H | -2.2764790000 | -5.4270510000 | -1.5266210000 |
| H | -3.4611490000 | -4.2546530000 | -0.9414640000 |
| C | -3.7161140000 | -0.6105170000 | -0.4030150000 |
| C | -4.9662780000 | -0.8542830000 | -0.9870490000 |
| C | -5.8000590000 | -1.8350510000 | -0.4631930000 |
| C | -5.3960410000 | -2.5776760000 | 0.6442380000 |
| C | -4.1504770000 | -2.3408750000 | 1.2207210000 |
| C | -3.3072560000 | -1.3647870000 | 0.7034210000 |
| H | -5.2764910000 | -0.2708960000 | -1.8459150000 |
| H | -6.7661680000 | -2.0178140000 | -0.9185680000 |
| H | -6.0479910000 | -3.3415500000 | 1.0517850000 |
| H | -3.8261470000 | -2.9268590000 | 2.0734260000 |
| H | -2.3305520000 | -1.1773350000 | 1.1364250000 |

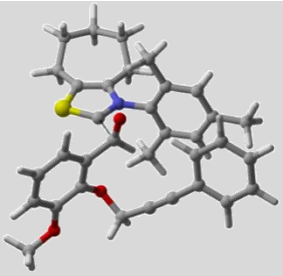
Thermochemie

Zero-point correction= 0.602951 (Hartree/Particle)
Thermal correction to Energy= 0.639449
Thermal correction to Enthalpy= 0.640393
Thermal correction to Gibbs Free Energy= 0.533059
Sum of electronic and zero-point Energies= -1993.780937
Sum of electronic and thermal Energies= -1993.744439
Sum of electronic and thermal Enthalpies= -1993.743495
Sum of electronic and thermal Free Energies= -1993.850829

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 401.260 | 140.943 | 225.903 |

**TS-1d**



XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -0.3877150000 | 5.1499290000 | 1.0846020000 |
| C | -0.2971460000 | 4.4802130000 | 2.3061560000 |
| C | -0.3288200000 | 3.0966950000 | 2.3584900000 |
| C | -0.4481010000 | 2.3526190000 | 1.1828530000 |
| C | -0.5350210000 | 3.0139530000 | -0.0369410000 |
| C | -0.5041280000 | 4.4185070000 | -0.0940730000 |
| H | -0.3614790000 | 6.2309660000 | 1.0629960000 |
| H | -0.2074820000 | 5.0582040000 | 3.2183460000 |
| H | -0.2734750000 | 2.5626170000 | 3.2990220000 |
| C | -0.5335300000 | 0.8485510000 | 1.2591210000 |
| O | -0.5631430000 | 2.3054220000 | -1.2148510000 |
| O | -0.5859570000 | 4.9588330000 | -1.3370730000 |
| C | -0.5453460000 | 6.3732290000 | -1.4406880000 |
| H | -1.3849760000 | 6.8300710000 | -0.9099270000 |
| H | -0.6192910000 | 6.5981460000 | -2.5018190000 |
| H | 0.3960920000 | 6.7667490000 | -1.0481010000 |
| O | -0.6275760000 | 0.2789250000 | 2.3520080000 |
| C | -1.8213590000 | 2.2838040000 | -1.8954280000 |
| H | -2.3008860000 | 3.2637600000 | -1.8361910000 |
| C | -2.6923550000 | 1.2353470000 | -1.3523450000 |
| H | -1.5936470000 | 2.0769820000 | -2.9425240000 |
| C | -3.3349760000 | 0.3417410000 | -0.8613520000 |
| N | 1.7169930000 | -0.7606730000 | -0.0579480000 |
| C | 1.4494180000 | 0.4547190000 | 0.4237300000 |
| S | 2.9274510000 | 1.2980950000 | 0.5200570000 |
| C | 3.8758970000 | -0.0274840000 | -0.1032360000 |
| C | 3.0570190000 | -1.0721090000 | -0.3649110000 |
| C | 0.6320900000 | -1.7002310000 | -0.2474450000 |
| C | 0.3256070000 | -2.5788690000 | 0.7885040000 |
| C | -0.7506070000 | -3.4470500000 | 0.6013190000 |
| C | -1.5006830000 | -3.4357200000 | -0.5728150000 |
| C | -1.1506960000 | -2.5423410000 | -1.5862090000 |
| C | -0.0838700000 | -1.6600980000 | -1.4454510000 |
| C | 1.1224550000 | -2.5602500000 | 2.0634280000 |
| H | -1.0199070000 | -4.1295020000 | 1.4015940000 |
| C | -2.6916910000 | -4.3390200000 | -0.7517860000 |
| H | -1.7383780000 | -2.5172860000 | -2.4995690000 |
| C | 0.2835600000 | -0.6773040000 | -2.5234710000 |
| C | 5.3590970000 | 0.0603930000 | -0.3171330000 |
| C | 6.1489890000 | -1.0872900000 | 0.3230610000 |
| H | 5.7165910000 | 1.0119470000 | 0.0821310000 |
| H | 5.5619670000 | 0.0802630000 | -1.3947970000 |
| C | 5.9661660000 | -2.4459130000 | -0.3579590000 |
| H | 5.8783410000 | -1.1637480000 | 1.3816620000 |
| H | 7.2091760000 | -0.8221140000 | 0.2843860000 |
| H | 6.7176690000 | -3.1320990000 | 0.0426890000 |
| C | 3.4419500000 | -2.4079910000 | -0.9307090000 |
| H | 2.5647500000 | -3.0582600000 | -0.9221040000 |
| C | 4.5919010000 | -3.0971580000 | -0.1841800000 |
| H | 3.7225090000 | -2.2783420000 | -1.9833350000 |
| H | 4.6499010000 | -4.1253150000 | -0.5513340000 |
| H | 6.1819880000 | -2.3424100000 | -1.4287260000 |
| H | 4.3483720000 | -3.1559980000 | 0.8821020000 |
| H | 1.3055490000 | -0.8462100000 | -2.8769240000 |
| H | 0.2360520000 | 0.3448920000 | -2.1385160000 |
| H | -0.3942550000 | -0.7692900000 | -3.3724060000 |
| H | 1.0267590000 | -1.5817200000 | 2.5407840000 |
| H | 2.1838610000 | -2.7394460000 | 1.8689290000 |
| H | 0.7643900000 | -3.3246290000 | 2.7528630000 |
| H | -2.5318280000 | -5.0372470000 | -1.5774790000 |
| H | -3.5814140000 | -3.7457460000 | -0.9814270000 |

| | | | |
|---|---|---|---|
| H | -2.8927820000 | -4.9142190000 | 0.1527250000 |
| H | -0.9179180000 | 0.3777020000 | 0.3472640000 |
| C | -4.0474250000 | -0.7206800000 | -0.2114220000 |
| C | -5.2600560000 | -1.1986510000 | -0.7235970000 |
| C | -5.9401880000 | -2.2168640000 | -0.0651740000 |
| C | -5.4162780000 | -2.7683340000 | 1.1015090000 |
| C | -4.2050880000 | -2.3015780000 | 1.6068120000 |
| C | -3.5185890000 | -1.2823250000 | 0.9587750000 |
| H | -5.6645070000 | -0.7644430000 | -1.6302270000 |
| H | -6.8799880000 | -2.5798660000 | -0.4643450000 |
| H | -5.9479810000 | -3.5627640000 | 1.6121760000 |
| H | -3.7887310000 | -2.7340260000 | 2.5092900000 |
| H | -2.5726740000 | -0.9225330000 | 1.3526230000 |

Thermochemie

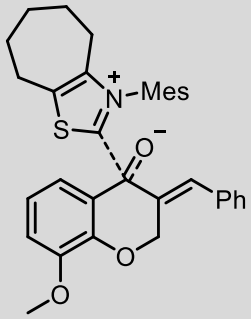
Zero-point correction= 0.613652 (Hartree/Particle)
Thermal correction to Energy= 0.649847
Thermal correction to Enthalpy= 0.650791
Thermal correction to Gibbs Free Energy= 0.544675
Sum of electronic and zero-point Energies= -1994.337513
Sum of electronic and thermal Energies= -1994.301318
Sum of electronic and thermal Enthalpies= -1994.300374
Sum of electronic and thermal Free Energies= -1994.406491

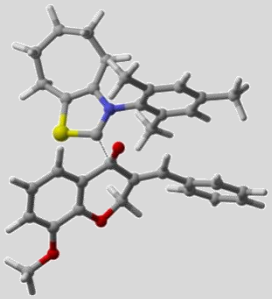
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 407.785 | 140.501 | 223.341 |

Imaginäre Frequenz

-112.7821

**TS-4c (E)**



74

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -4.7877900000 | -2.3263880000 | 1.0203780000 |
| C | -4.4036800000 | -1.2844680000 | 1.8738500000 |
| C | -3.0978420000 | -0.8376200000 | 1.8815550000 |
| C | -2.1479950000 | -1.4083230000 | 1.0267920000 |
| C | -2.5244210000 | -2.4390430000 | 0.1760410000 |
| C | -3.8558440000 | -2.9118940000 | 0.1759660000 |
| H | -5.8126420000 | -2.6722990000 | 1.0282300000 |
| H | -5.1405200000 | -0.8409380000 | 2.5325120000 |
| H | -2.7721680000 | -0.0488460000 | 2.5495170000 |
| C | -0.6974600000 | -0.9557950000 | 1.1135440000 |
| O | -4.1154070000 | -3.9350980000 | -0.6770750000 |
| C | -5.4343500000 | -4.4526010000 | -0.6884560000 |
| H | -5.7112560000 | -4.8439710000 | 0.2945410000 |
| H | -5.4332170000 | -5.2616820000 | -1.4149070000 |
| H | -6.1543070000 | -3.6878760000 | -0.9943210000 |
| O | -0.2736420000 | -0.5751040000 | 2.2296130000 |
| N | 0.0296590000 | 1.6639200000 | -0.0862230000 |
| C | -0.8736810000 | 0.6853450000 | -0.0130650000 |

| | | | |
|---|---|---|---|
| S | -2.3439270000 | 1.2726640000 | -0.6435500000 |
| C | -1.6926400000 | 2.8427100000 | -1.0098620000 |
| C | -0.3936380000 | 2.8905820000 | -0.6329450000 |
| C | 1.4037370000 | 1.4347320000 | 0.3126230000 |
| C | 1.7860530000 | 1.7186180000 | 1.6197510000 |
| C | 3.1045470000 | 1.4304810000 | 1.9755180000 |
| C | 4.0118530000 | 0.8973710000 | 1.0608430000 |
| C | 3.5941090000 | 0.6812390000 | -0.2531450000 |
| C | 2.2872030000 | 0.9450070000 | -0.6501030000 |
| C | 0.8096290000 | 2.3176350000 | 2.5927660000 |
| H | 3.4262830000 | 1.6270180000 | 2.9935090000 |
| C | 5.4156580000 | 0.5392820000 | 1.4734000000 |
| H | 4.2929450000 | 0.2713110000 | -0.9772120000 |
| C | 1.8213760000 | 0.7019700000 | -2.0590490000 |
| C | -2.5065280000 | 3.9308160000 | -1.6476330000 |
| C | -2.5042020000 | 5.2453180000 | -0.8581470000 |
| H | -3.5334600000 | 3.5790160000 | -1.7661290000 |
| H | -2.1215020000 | 4.1141590000 | -2.6578930000 |
| C | -1.1754990000 | 6.0047070000 | -0.8881770000 |
| H | -2.7922710000 | 5.0424350000 | 0.1788490000 |
| H | -3.2784610000 | 5.8895070000 | -1.2834350000 |
| H | -1.3419460000 | 6.9980200000 | -0.4619120000 |
| C | 0.5341310000 | 4.0638370000 | -0.7534750000 |
| H | 1.4862530000 | 3.8113950000 | -0.2827230000 |
| C | -0.0166560000 | 5.3541670000 | -0.1286110000 |
| H | 0.7465260000 | 4.2401860000 | -1.8150610000 |
| H | 0.8076100000 | 6.0705640000 | -0.0803480000 |
| H | -0.8762860000 | 6.1633670000 | -1.9317220000 |
| H | -0.3215970000 | 5.1539840000 | 0.9041750000 |
| H | 1.4554140000 | 1.6256600000 | -2.5177690000 |
| H | 0.9939670000 | -0.0133650000 | -2.0721680000 |
| H | 2.6318020000 | 0.3073540000 | -2.6714990000 |
| H | -0.0175760000 | 1.6227020000 | 2.7522070000 |
| H | 0.4034970000 | 3.2578080000 | 2.2071930000 |
| H | 1.2946090000 | 2.5196020000 | 3.5477910000 |
| H | 6.1450850000 | 0.9311880000 | 0.7615110000 |
| H | 5.5346810000 | -0.5478910000 | 1.4991600000 |
| H | 5.6507670000 | 0.9314410000 | 2.4632200000 |
| C | 0.2069870000 | -1.7478100000 | 0.1813170000 |
| C | -0.4770670000 | -2.3497150000 | -1.0110100000 |
| H | -0.7718520000 | -1.5701790000 | -1.7267490000 |
| O | -1.6577540000 | -3.0771790000 | -0.6533170000 |
| H | 0.1508990000 | -3.0781710000 | -1.5172780000 |
| C | 1.4990080000 | -1.8543940000 | 0.5059530000 |
| H | 1.7749490000 | -1.3745380000 | 1.4446660000 |
| C | 2.6116900000 | -2.4916050000 | -0.2162750000 |
| C | 3.6996250000 | -2.9551690000 | 0.5372980000 |
| C | 4.8086860000 | -3.5252080000 | -0.0741660000 |
| C | 4.8633130000 | -3.6293060000 | -1.4623810000 |
| C | 3.8032210000 | -3.1514820000 | -2.2267940000 |
| C | 2.6908730000 | -2.5853760000 | -1.6117910000 |
| H | 3.6670060000 | -2.8594310000 | 1.6178550000 |
| H | 5.6345360000 | -3.8808380000 | 0.5311120000 |
| H | 5.7294410000 | -4.0678020000 | -1.9436110000 |
| H | 3.8455080000 | -3.2079110000 | -3.3084570000 |
| H | 1.9024790000 | -2.1777050000 | -2.2313280000 |

Thermochemie

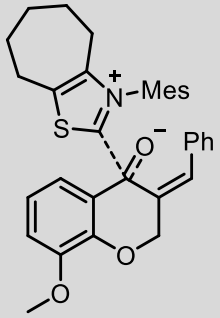
Zero-point correction= 0.614544 (Hartree/Particle)
Thermal correction to Energy= 0.649800
Thermal correction to Enthalpy= 0.650744
Thermal correction to Gibbs Free Energy= 0.547068

Sum of electronic and zero-point Energies= -1994.392266
Sum of electronic and thermal Energies= -1994.357010
Sum of electronic and thermal Enthalpies= -1994.356066
Sum of electronic and thermal Free Energies= -1994.459742

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 407.756 | 138.323 | 218.204 |

Imaginäre Frequenz
-178.2179

**TS-4d**
**(Z)**




74
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.2896320000 | -1.0088930000 | 1.1273500000 |
| C | -4.4563910000 | -0.4218990000 | 2.0875290000 |
| C | -3.0871980000 | -0.4143070000 | 1.9106110000 |
| C | -2.5161890000 | -0.9736380000 | 0.7617090000 |
| C | -3.3414170000 | -1.5504530000 | -0.1968450000 |
| C | -4.7407310000 | -1.5793210000 | -0.0117980000 |
| H | -6.3600610000 | -1.0155530000 | 1.2822520000 |
| H | -4.8976620000 | 0.0157910000 | 2.9746830000 |
| H | -2.4218960000 | 0.0069180000 | 2.6546170000 |
| C | -0.9895590000 | -1.0424530000 | 0.6591810000 |
| O | -5.4504720000 | -2.1824190000 | -0.9990660000 |
| C | -6.8562930000 | -2.2555740000 | -0.8373640000 |
| H | -7.1191640000 | -2.8213110000 | 0.0609970000 |
| H | -7.2330310000 | -2.7729520000 | -1.7164130000 |
| H | -7.2989240000 | -1.2567500000 | -0.7835130000 |
| O | -0.3590530000 | -1.0624320000 | 1.7371730000 |
| N | 0.4800020000 | 1.4310120000 | -0.2370480000 |
| C | -0.6953280000 | 0.8187020000 | -0.0980260000 |
| S | -1.9203230000 | 2.0040280000 | -0.1424270000 |
| C | -0.8032860000 | 3.3171630000 | -0.3667570000 |
| C | 0.4609040000 | 2.8349500000 | -0.3849900000 |
| C | 1.7314380000 | 0.6998830000 | -0.2871640000 |
| C | 2.4762330000 | 0.5695410000 | 0.8831540000 |
| C | 3.7226310000 | -0.0479820000 | 0.7868430000 |
| C | 4.2160880000 | -0.5195200000 | -0.4272750000 |
| C | 3.4310160000 | -0.3708420000 | -1.5705740000 |
| C | 2.1844220000 | 0.2478630000 | -1.5271690000 |
| C | 1.9502730000 | 1.0914720000 | 2.1913250000 |
| H | 4.3169390000 | -0.1691340000 | 1.6874320000 |
| C | 5.5847170000 | -1.1427880000 | -0.5123320000 |
| H | 3.8006460000 | -0.7409550000 | -2.5225560000 |
| C | 1.3572350000 | 0.4254060000 | -2.7716800000 |
| C | -1.2506660000 | 4.7418910000 | -0.5222710000 |
| C | -0.5833950000 | 5.7125600000 | 0.4593370000 |
| H | -2.3344820000 | 4.7857520000 | -0.3961220000 |
| H | -1.0439190000 | 5.0663370000 | -1.5492440000 |
| C | 0.8972840000 | 5.9807630000 | 0.1800750000 |

| | | | |
|---|---|---|---|
| H | -0.7065580000 | 5.3333500000 | 1.4793430000 |
| H | -1.1224980000 | 6.6621800000 | 0.4051150000 |
| H | 1.2166340000 | 6.8157650000 | 0.8099960000 |
| C | 1.7197220000 | 3.6359030000 | -0.5522860000 |
| H | 2.5798060000 | 2.9744880000 | -0.4365530000 |
| C | 1.8463060000 | 4.8071540000 | 0.4323660000 |
| H | 1.7583800000 | 4.0209200000 | -1.5788230000 |
| H | 2.8730280000 | 5.1769330000 | 0.3673900000 |
| H | 1.0109160000 | 6.3169140000 | -0.8580470000 |
| H | 1.7089230000 | 4.4371970000 | 1.4539200000 |
| H | 0.9838960000 | 1.4488380000 | -2.8645730000 |
| H | 0.4887580000 | -0.2386820000 | -2.7567060000 |
| H | 1.9464500000 | 0.1911360000 | -3.6581950000 |
| H | 1.0181240000 | 0.5777190000 | 2.4400300000 |
| H | 1.7426920000 | 2.1643740000 | 2.1321380000 |
| H | 2.6759680000 | 0.9277020000 | 2.9881970000 |
| H | 6.3383090000 | -0.3816030000 | -0.7355780000 |
| H | 5.6228240000 | -1.8959490000 | -1.3009520000 |
| H | 5.8545180000 | -1.6206560000 | 0.4303170000 |
| C | -0.5621610000 | -1.8123850000 | -0.5723480000 |
| C | -1.5584050000 | -1.6758790000 | -1.6980270000 |
| H | -1.6584470000 | -0.6273440000 | -2.0036250000 |
| O | -2.8625040000 | -2.1343660000 | -1.3263680000 |
| H | -1.2704260000 | -2.2726000000 | -2.5615690000 |
| C | 0.5242270000 | -2.5754750000 | -0.7899650000 |
| H | 0.5497100000 | -3.0050930000 | -1.7916550000 |
| C | 1.7225340000 | -2.9801550000 | -0.0284750000 |
| C | 2.7183480000 | -3.6371230000 | -0.7722110000 |
| C | 3.8895520000 | -4.0884570000 | -0.1805440000 |
| C | 4.0907230000 | -3.9035540000 | 1.1847150000 |
| C | 3.1103680000 | -3.2655660000 | 1.9378180000 |
| C | 1.9397610000 | -2.8033720000 | 1.3440110000 |
| H | 2.5677530000 | -3.7899450000 | -1.8364490000 |
| H | 4.6426150000 | -4.5848390000 | -0.7820590000 |
| H | 5.0018950000 | -4.2561040000 | 1.6550290000 |
| H | 3.2586990000 | -3.1177600000 | 3.0019920000 |
| H | 1.1921980000 | -2.2845670000 | 1.9259010000 |

Thermochemie

Zero-point correction= 0.615063 (Hartree/Particle)
Thermal correction to Energy= 0.650086
Thermal correction to Enthalpy= 0.651030
Thermal correction to Gibbs Free Energy= 0.548448
Sum of electronic and zero-point Energies= -1994.385479
Sum of electronic and thermal Energies= -1994.350456
Sum of electronic and thermal Enthalpies= -1994.349512
Sum of electronic and thermal Free Energies= -1994.452094

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 407.935 | 138.093 | 215.901 |

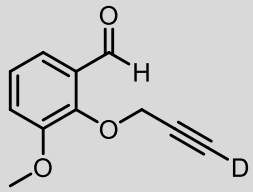
Imaginäre Frequenz

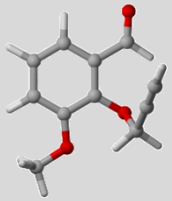
-169.3226

## *O*-propargylierte Aldehyde: D-Substituent

| (u)M06-2X/6-311+G** SCRF=(PCM,Solvent=Tetrahydrofuran) |
|---|

**19e**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.7485080000 | -1.4569120000 | 0.5012870000 |
| C | 0.7644790000 | -2.4307060000 | 0.7007430000 |
| C | -0.5420630000 | -2.1993040000 | 0.3187530000 |
| C | -0.8853380000 | -0.9762950000 | -0.2703860000 |
| C | 0.0895810000 | -0.0042050000 | -0.4779370000 |
| C | 1.4213380000 | -0.2410110000 | -0.0885630000 |
| H | 2.7669060000 | -1.6614950000 | 0.8035710000 |
| H | 1.0416950000 | -3.3719890000 | 1.1589080000 |
| H | -1.3164630000 | -2.9419150000 | 0.4658420000 |
| C | -2.2897830000 | -0.7147900000 | -0.6733810000 |
| O | -0.2316380000 | 1.1744310000 | -1.0976100000 |
| O | 2.2937450000 | 0.7628060000 | -0.3364890000 |
| C | 3.6518960000 | 0.5595860000 | 0.0286490000 |
| H | 3.7467380000 | 0.4047360000 | 1.1065260000 |
| H | 4.1770340000 | 1.4667700000 | -0.2582600000 |
| H | 4.0740720000 | -0.2943340000 | -0.5072650000 |
| O | -3.1884830000 | -1.4995610000 | -0.4735940000 |
| H | -2.4785510000 | 0.2461780000 | -1.1737910000 |
| C | -0.2763710000 | 2.3121040000 | -0.2279200000 |
| H | 0.6713270000 | 2.4128050000 | 0.3059010000 |
| C | -1.3927790000 | 2.2168940000 | 0.7188980000 |
| H | -0.4053100000 | 3.1751810000 | -0.8801780000 |
| C | -2.3125830000 | 2.1089260000 | 1.4827130000 |
| H | -3.1277580000 | 2.0169410000 | 2.1631520000 |

Thermochemie

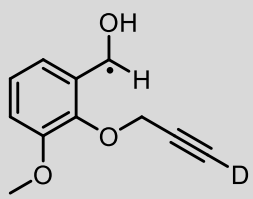
Zero-point correction= 0.183143 (Hartree/Particle)
Thermal correction to Energy= 0.196545
Thermal correction to Enthalpy= 0.197489
Thermal correction to Gibbs Free Energy= 0.142426
Sum of electronic and zero-point Energies= -650.495647
Sum of electronic and thermal Energies= -650.482245
Sum of electronic and thermal Enthalpies= -650.481301
Sum of electronic and thermal Free Energies= -650.536364

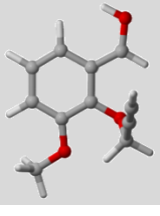
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 123.334 | 49.378 | 115.890 |

Volumen

Molar volume = 1705.805 bohr**3/mol (152.224 cm**3/mol)
Recommended a0 for SCRF calculation = 4.82 angstrom ( 9.10 bohr)

**25e**



25

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.6020710000 | -1.6027720000 | 0.5398490000 |

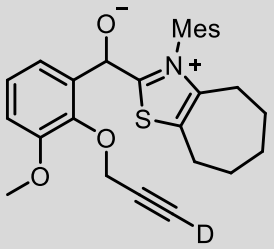
| | | | |
|---|---|---|---|
| C | 0.5193580000 | -2.4580940000 | 0.7660050000 |
| C | -0.7598260000 | -2.1204800000 | 0.3776110000 |
| C | -1.0144770000 | -0.8749420000 | -0.2569010000 |
| C | 0.0882460000 | -0.0125040000 | -0.4760730000 |
| C | 1.3807040000 | -0.3771400000 | -0.0942360000 |
| H | 2.5951370000 | -1.8992920000 | 0.8455820000 |
| H | 0.6956400000 | -3.4108240000 | 1.2510480000 |
| H | -1.5608760000 | -2.8274450000 | 0.5615370000 |
| C | -2.2949330000 | -0.4655030000 | -0.6770750000 |
| O | -0.1298280000 | 1.1736560000 | -1.1349890000 |
| O | 2.3571250000 | 0.5211760000 | -0.3849150000 |
| C | 3.6910580000 | 0.1801880000 | -0.0397710000 |
| H | 3.7932330000 | 0.0382620000 | 1.0392900000 |
| H | 4.3051000000 | 1.0197640000 | -0.3560920000 |
| H | 4.0098080000 | -0.7249110000 | -0.5632750000 |
| O | -3.4208070000 | -1.1854390000 | -0.4941940000 |
| H | -2.4645030000 | 0.4710160000 | -1.1835460000 |
| C | 0.0245520000 | 2.3494530000 | -0.3376400000 |
| H | 1.0342790000 | 2.3935470000 | 0.0755510000 |
| C | -0.9653680000 | 2.4227860000 | 0.7437860000 |
| H | -0.1098040000 | 3.1865790000 | -1.0226870000 |
| C | -1.7737410000 | 2.4818650000 | 1.6294650000 |
| H | -2.4921170000 | 2.5335190000 | 2.4147040000 |
| H | -3.2436770000 | -1.9925030000 | 0.0005560000 |

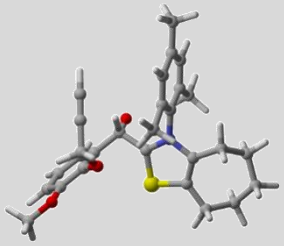
Thermochemie

Zero-point correction= 0.193202 (Hartree/Particle)
Thermal correction to Energy= 0.207219
Thermal correction to Enthalpy= 0.208164
Thermal correction to Gibbs Free Energy= 0.151337
Sum of electronic and zero-point Energies= -651.048138
Sum of electronic and thermal Energies= -651.034121
Sum of electronic and thermal Enthalpies= -651.033177
Sum of electronic and thermal Free Energies= -651.090004

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 130.032 | 52.316 | 119.602 |

**22e**



64

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.9575520000 | -0.7901780000 | 1.0829830000 |
| C | 4.2929190000 | -0.7335880000 | 2.3072950000 |
| C | 2.9630150000 | -0.3447070000 | 2.3757040000 |
| C | 2.2736630000 | 0.0101860000 | 1.2171680000 |
| C | 2.9384460000 | -0.0313850000 | -0.0032190000 |
| C | 4.2775920000 | -0.4488550000 | -0.0838880000 |
| H | 5.9909590000 | -1.1076270000 | 1.0457670000 |
| H | 4.8300050000 | -1.0014960000 | 3.2098100000 |
| H | 2.4213390000 | -0.2911690000 | 3.3116820000 |
| C | 0.8004630000 | 0.4485670000 | 1.3274450000 |
| O | 2.2473700000 | 0.2581010000 | -1.1640980000 |
| O | 4.8144250000 | -0.4982130000 | -1.3325230000 |

| | | | |
|---|---|---|---|
| C | 6.1687150000 | -0.9051170000 | -1.4482680000 |
| H | 6.8298860000 | -0.2234750000 | -0.9063120000 |
| H | 6.4020810000 | -0.8735470000 | -2.5096970000 |
| H | 6.3041500000 | -1.9232240000 | -1.0735910000 |
| O | 0.3115530000 | 0.4950950000 | 2.5748960000 |
| C | 2.6636880000 | 1.4456640000 | -1.8407070000 |
| H | 3.7510730000 | 1.4706770000 | -1.9302490000 |
| C | 2.1761760000 | 2.6602770000 | -1.1757110000 |
| H | 2.2392100000 | 1.3809430000 | -2.8437650000 |
| C | 1.7598320000 | 3.6475490000 | -0.6339780000 |
| H | 1.3874380000 | 4.5176640000 | -0.1443520000 |
| N | -1.2744190000 | -0.2837460000 | 0.0699780000 |
| C | -0.0627920000 | -0.5550130000 | 0.5448280000 |
| S | 0.2750280000 | -2.2125690000 | 0.4016060000 |
| C | -1.2755410000 | -2.5339650000 | -0.3151320000 |
| C | -1.9879230000 | -1.3878010000 | -0.4248030000 |
| C | -1.8066790000 | 1.0643050000 | 0.0627940000 |
| C | -2.5771520000 | 1.4770170000 | 1.1516010000 |
| C | -3.0728540000 | 2.7773300000 | 1.1204670000 |
| C | -2.8183430000 | 3.6358950000 | 0.0486880000 |
| C | -2.0612670000 | 3.1677090000 | -1.0230410000 |
| C | -1.5499760000 | 1.8702500000 | -1.0436470000 |
| C | -2.8517780000 | 0.5400980000 | 2.2936240000 |
| H | -3.6685190000 | 3.1302980000 | 1.9567690000 |
| C | -3.3804680000 | 5.0337020000 | 0.0469470000 |
| H | -1.8601420000 | 3.8229030000 | -1.8649310000 |
| C | -0.7874060000 | 1.3421160000 | -2.2274450000 |
| C | -1.6667970000 | -3.9133260000 | -0.7602130000 |
| C | -3.0251440000 | -4.3772440000 | -0.2213770000 |
| H | -0.8927150000 | -4.6165670000 | -0.4460170000 |
| H | -1.6829040000 | -3.9372850000 | -1.8561250000 |
| C | -4.2312420000 | -3.6602940000 | -0.8319100000 |
| H | -3.0385500000 | -4.2653460000 | 0.8678380000 |
| H | -3.1147730000 | -5.4459330000 | -0.4329100000 |
| H | -5.1342860000 | -4.1992240000 | -0.5324560000 |
| C | -3.3581170000 | -1.2297590000 | -1.0148760000 |
| H | -3.6896330000 | -0.2011840000 | -0.8607380000 |
| C | -4.4022270000 | -2.1927120000 | -0.4331080000 |
| H | -3.2917970000 | -1.3795580000 | -2.0993970000 |
| H | -5.3822860000 | -1.8535650000 | -0.7781620000 |
| H | -4.1769490000 | -3.7325350000 | -1.9253410000 |
| H | -4.4046730000 | -2.1071840000 | 0.6586350000 |
| H | -1.4266490000 | 0.6856500000 | -2.8274550000 |
| H | 0.0807000000 | 0.7605270000 | -1.9130880000 |
| H | -0.4524600000 | 2.1624270000 | -2.8626790000 |
| H | -1.8985970000 | 0.2410000000 | 2.7410260000 |
| H | -3.3690130000 | -0.3585980000 | 1.9427490000 |
| H | -3.4775240000 | 1.0231520000 | 3.0437910000 |
| H | -4.4525430000 | 5.0148090000 | -0.1666650000 |
| H | -2.8973870000 | 5.6523270000 | -0.7098380000 |
| H | -3.2478040000 | 5.5084650000 | 1.0208130000 |
| H | 0.7179120000 | 1.3938250000 | 0.7538050000 |

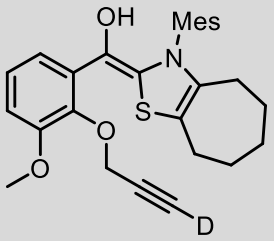
Thermochemie

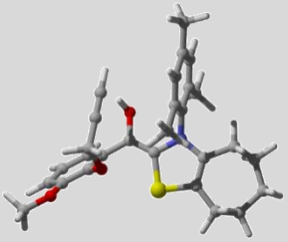
Zero-point correction= 0.528843 (Hartree/Particle)
Thermal correction to Energy= 0.561339
Thermal correction to Enthalpy= 0.562283
Thermal correction to Gibbs Free Energy= 0.462908
Sum of electronic and zero-point Energies= -1763.408555
Sum of electronic and thermal Energies= -1763.376060
Sum of electronic and thermal Enthalpies= -1763.375116
Sum of electronic and thermal Free Energies= -1763.474491

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 352.245 | 123.902 | 209.153 |

Volumen
Molar volume = 4101.568 bohr**3/mol (366.020 cm**3/mol)
Recommended a0 for SCRF calculation = 6.28 angstrom ( 11.87 bohr)

**23e**



64
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 5.0419500000 | -0.6133430000 | 1.3219130000 |
| C | 4.2773440000 | -0.4489450000 | 2.4799980000 |
| C | 2.9209440000 | -0.1949690000 | 2.4041570000 |
| C | 2.2820430000 | -0.1000070000 | 1.1563740000 |
| C | 3.0499020000 | -0.2388530000 | 0.0015570000 |
| C | 4.4306600000 | -0.5046710000 | 0.0782230000 |
| H | 6.1002590000 | -0.8200990000 | 1.4026160000 |
| H | 4.7604110000 | -0.5321480000 | 3.4463460000 |
| H | 2.3294060000 | -0.0700560000 | 3.3029910000 |
| C | 0.8391840000 | 0.2022370000 | 1.1006080000 |
| O | 2.4727640000 | -0.1097770000 | -1.2394240000 |
| O | 5.0710240000 | -0.6164750000 | -1.1123650000 |
| C | 6.4675930000 | -0.8666970000 | -1.0846460000 |
| H | 6.9999950000 | -0.0583610000 | -0.5761460000 |
| H | 6.7838000000 | -0.9152740000 | -2.1236900000 |
| H | 6.6836610000 | -1.8181510000 | -0.5915190000 |
| O | 0.4215350000 | 1.2994360000 | 1.8397120000 |
| C | 2.7160810000 | 1.1512840000 | -1.8567740000 |
| H | 3.7900540000 | 1.3537180000 | -1.8908010000 |
| C | 2.0151320000 | 2.2606050000 | -1.1902010000 |
| H | 2.3477370000 | 1.0582310000 | -2.8793980000 |
| C | 1.4414600000 | 3.1955190000 | -0.6986710000 |
| H | 0.9262170000 | 4.0286220000 | -0.2767600000 |
| H | 0.7252850000 | 2.0964350000 | 1.3848440000 |
| N | -1.4468380000 | -0.2944800000 | 0.3683680000 |
| C | -0.0792570000 | -0.5771530000 | 0.4955230000 |
| S | 0.2697380000 | -2.1751100000 | -0.1898130000 |
| C | -1.4513100000 | -2.4291640000 | -0.5334780000 |
| C | -2.1820600000 | -1.3599830000 | -0.2017750000 |
| C | -1.8689380000 | 1.0647120000 | 0.1465870000 |
| C | -2.5449870000 | 1.7430860000 | 1.1650240000 |
| C | -2.9443230000 | 3.0559390000 | 0.9307970000 |
| C | -2.6832350000 | 3.6953410000 | -0.2833960000 |
| C | -2.0126210000 | 2.9868590000 | -1.2775880000 |
| C | -1.6021820000 | 1.6662010000 | -1.0857810000 |
| C | -2.8076490000 | 1.0640290000 | 2.4802840000 |
| H | -3.4660600000 | 3.5963130000 | 1.7155540000 |
| C | -3.1479260000 | 5.1095870000 | -0.5207690000 |
| H | -1.8009660000 | 3.4698180000 | -2.2273710000 |
| C | -0.9055640000 | 0.9002190000 | -2.1788310000 |
| C | -1.9401000000 | -3.7314580000 | -1.0980990000 |
| C | -2.9950450000 | -4.4172310000 | -0.2197280000 |

| | | | |
|---|---|---|---|
| H | -1.0900830000 | -4.4046430000 | -1.2304820000 |
| H | -2.3600160000 | -3.5639490000 | -2.0982230000 |
| C | -4.3672120000 | -3.7375770000 | -0.2283320000 |
| H | -2.6177900000 | -4.4815670000 | 0.8064510000 |
| H | -3.1220620000 | -5.4429660000 | -0.5786840000 |
| H | -5.0738810000 | -4.3876540000 | 0.2962200000 |
| C | -3.6731010000 | -1.2507070000 | -0.3508290000 |
| H | -3.9949960000 | -0.2686640000 | 0.0006110000 |
| C | -4.4406750000 | -2.3449860000 | 0.4056850000 |
| H | -3.9342530000 | -1.2988790000 | -1.4153570000 |
| H | -5.4928420000 | -2.0482220000 | 0.4496510000 |
| H | -4.7220130000 | -3.6710150000 | -1.2647400000 |
| H | -4.0787170000 | -2.3871860000 | 1.4388970000 |
| H | -1.5400120000 | 0.0852480000 | -2.5418010000 |
| H | 0.0214590000 | 0.4499100000 | -1.8151340000 |
| H | -0.6711230000 | 1.5561360000 | -3.0179960000 |
| H | -1.8604230000 | 0.8086050000 | 2.9605780000 |
| H | -3.3608430000 | 0.1316390000 | 2.3385820000 |
| H | -3.3819740000 | 1.7117280000 | 3.1433380000 |
| H | -4.1891750000 | 5.1205870000 | -0.8553040000 |
| H | -2.5476620000 | 5.5985290000 | -1.2894050000 |
| H | -3.0905660000 | 5.7017130000 | 0.3941660000 |

Thermochemie

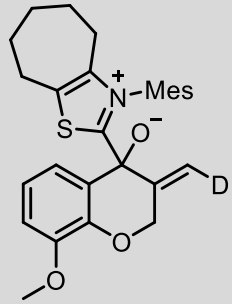
Zero-point correction= 0.528293 (Hartree/Particle)
Thermal correction to Energy= 0.561089
Thermal correction to Enthalpy= 0.562033
Thermal correction to Gibbs Free Energy= 0.464652
Sum of electronic and zero-point Energies= -1763.427892
Sum of electronic and thermal Energies= -1763.395097
Sum of electronic and thermal Enthalpies= -1763.394152
Sum of electronic and thermal Free Energies= -1763.491533

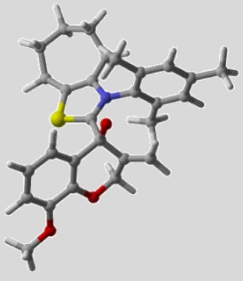
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 352.089 | 125.830 | 204.956 |

Volumen

Molar volume = 3901.102 bohr**3/mol (348.130 cm**3/mol)
Recommended a0 for SCRF calculation = 6.19 angstrom ( 11.69 bohr)

**[24e + A]**



64

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0346550000 | 0.4910720000 | 1.1790910000 |
| C | -4.0851080000 | 0.6616600000 | 2.1931480000 |
| C | -2.7938670000 | 0.2034440000 | 2.0184450000 |
| C | -2.4098060000 | -0.4185950000 | 0.8252560000 |
| C | -3.3543150000 | -0.6003970000 | -0.1806540000 |
| C | -4.6800720000 | -0.1443010000 | -0.0016490000 |
| H | -6.0449270000 | 0.8483090000 | 1.3262530000 |
| H | -4.3766230000 | 1.1475020000 | 3.1165450000 |

| | | | |
|---|---|---|---|
| H | -2.0455890000 | 0.2941970000 | 2.7967820000 |
| C | -0.9416150000 | -0.9284870000 | 0.7019770000 |
| O | -5.5253520000 | -0.3783980000 | -1.0395180000 |
| C | -6.8701790000 | 0.0394920000 | -0.8881460000 |
| H | -7.3436790000 | -0.4595270000 | -0.0377660000 |
| H | -7.3789580000 | -0.2453660000 | -1.8060430000 |
| H | -6.9337230000 | 1.1237080000 | -0.7570890000 |
| O | -0.4007680000 | -1.2933970000 | 1.8502950000 |
| N | 1.1964050000 | 0.3209240000 | -0.0824660000 |
| C | -0.1167400000 | 0.2966690000 | 0.1421910000 |
| S | -0.7725140000 | 1.8521410000 | -0.0681170000 |
| C | 0.7677370000 | 2.5336320000 | -0.4686930000 |
| C | 1.7261410000 | 1.5773590000 | -0.4245700000 |
| C | 2.0522010000 | -0.8492940000 | 0.0007360000 |
| C | 2.6787260000 | -1.1134670000 | 1.2213220000 |
| C | 3.5323520000 | -2.2100720000 | 1.2754170000 |
| C | 3.7765680000 | -3.0078640000 | 0.1549580000 |
| C | 3.1675510000 | -2.6714110000 | -1.0502320000 |
| C | 2.2991880000 | -1.5835270000 | -1.1554640000 |
| C | 2.4392270000 | -0.2341970000 | 2.4146380000 |
| H | 4.0266680000 | -2.4425170000 | 2.2134520000 |
| C | 4.6777600000 | -4.2107700000 | 0.2533610000 |
| H | 3.3741030000 | -3.2618240000 | -1.9379890000 |
| C | 1.6648890000 | -1.2545180000 | -2.4805270000 |
| C | 0.9198830000 | 3.9851510000 | -0.8205600000 |
| C | 1.9917490000 | 4.7129070000 | -0.0005940000 |
| H | -0.0430430000 | 4.4816160000 | -0.6831560000 |
| H | 1.1606960000 | 4.0641490000 | -1.8872990000 |
| C | 3.4299120000 | 4.3154980000 | -0.3393920000 |
| H | 1.8021200000 | 4.5498360000 | 1.0654720000 |
| H | 1.8753060000 | 5.7839780000 | -0.1848310000 |
| H | 4.1034320000 | 5.0230240000 | 0.1518790000 |
| C | 3.1862370000 | 1.7647960000 | -0.7186930000 |
| H | 3.7125590000 | 0.8321200000 | -0.5129160000 |
| C | 3.8425960000 | 2.9023280000 | 0.0768260000 |
| H | 3.3021940000 | 1.9588250000 | -1.7920210000 |
| H | 4.9230320000 | 2.8060700000 | -0.0574120000 |
| H | 3.5911300000 | 4.4337380000 | -1.4180470000 |
| H | 3.6442730000 | 2.7598130000 | 1.1443200000 |
| H | 1.3122860000 | -0.2229380000 | -2.5328150000 |
| H | 0.8108620000 | -1.9137050000 | -2.6603370000 |
| H | 2.3805270000 | -1.4118050000 | -3.2887680000 |
| H | 1.3809250000 | -0.2968970000 | 2.6827900000 |
| H | 2.6788260000 | 0.8096730000 | 2.1879680000 |
| H | 3.0557390000 | -0.5512200000 | 3.2555030000 |
| H | 5.4564630000 | -4.0595240000 | 1.0023250000 |
| H | 5.1518620000 | -4.4275720000 | -0.7048070000 |
| H | 4.1018940000 | -5.0925520000 | 0.5476610000 |
| C | -0.9924120000 | -1.9820800000 | -0.4144750000 |
| C | -1.7443260000 | -1.5609910000 | -1.6404220000 |
| H | -1.2785020000 | -0.6767370000 | -2.0960550000 |
| O | -3.1092980000 | -1.2311640000 | -1.3601930000 |
| H | -1.7781640000 | -2.3571100000 | -2.3842060000 |
| C | -0.4497500000 | -3.1816670000 | -0.2586380000 |
| H | 0.0949380000 | -3.4044410000 | 0.6526940000 |
| H | -0.5271250000 | -3.9441010000 | -1.0275700000 |

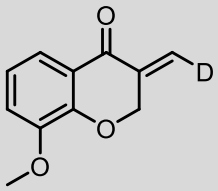
Thermochemie

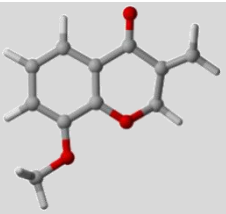
Zero-point correction= 0.531396 (Hartree/Particle)
Thermal correction to Energy= 0.562131
Thermal correction to Enthalpy= 0.563075
Thermal correction to Gibbs Free Energy= 0.470761

Sum of electronic and zero-point Energies= -1763.461748
Sum of electronic and thermal Energies= -1763.431014
Sum of electronic and thermal Enthalpies= -1763.430070
Sum of electronic and thermal Free Energies= -1763.522383

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 352.742 | 121.183 | 194.291 |

**24e**



24

XYZ-Matrix in Ångström

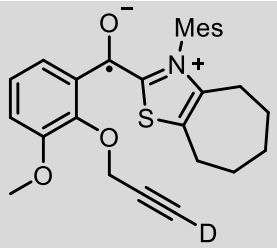
| | | | |
|---|---|---|---|
| C | 2.2570000000 | 1.1655470000 | 0.0045420000 |
| C | 1.4186880000 | 2.2879610000 | 0.0854720000 |
| C | 0.0515480000 | 2.1327700000 | 0.1167740000 |
| C | -0.5067200000 | 0.8446370000 | 0.0823530000 |
| C | 0.3230450000 | -0.2768940000 | 0.0240190000 |
| C | 1.7253130000 | -0.1137720000 | -0.0315290000 |
| H | 3.3288460000 | 1.3087680000 | -0.0237670000 |
| H | 1.8608840000 | 3.2756590000 | 0.1166550000 |
| H | -0.6174810000 | 2.9830930000 | 0.1562730000 |
| C | -1.9772210000 | 0.6707390000 | -0.0019740000 |
| O | -0.1427940000 | -1.5456470000 | -0.0137540000 |
| O | 2.4442680000 | -1.2561820000 | -0.1110890000 |
| C | 3.8558920000 | -1.1338070000 | -0.1895660000 |
| H | 4.1495950000 | -0.5652520000 | -1.0761060000 |
| H | 4.2400880000 | -2.1479140000 | -0.2625320000 |
| H | 4.2573290000 | -0.6534360000 | 0.7069260000 |
| O | -2.7397080000 | 1.6088610000 | -0.1189390000 |
| C | -2.4390630000 | -0.7508030000 | 0.0151640000 |
| C | -1.4399660000 | -1.7285010000 | 0.5604710000 |
| H | -1.3444810000 | -1.5950930000 | 1.6452160000 |
| H | -1.7250020000 | -2.7573410000 | 0.3509620000 |
| C | -3.6543790000 | -1.0786690000 | -0.4126020000 |
| H | -3.9894610000 | -2.1097560000 | -0.4294440000 |
| H | -4.3392630000 | -0.3102370000 | -0.7526710000 |

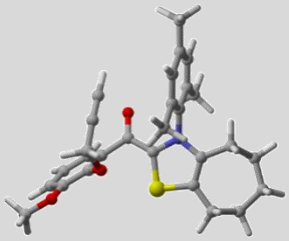
Thermochemie

Zero-point correction= 0.186564 (Hartree/Particle)
Thermal correction to Energy= 0.198362
Thermal correction to Enthalpy= 0.199306
Thermal correction to Gibbs Free Energy= 0.148607
Sum of electronic and zero-point Energies= -650.558425
Sum of electronic and thermal Energies= -650.546626
Sum of electronic and thermal Enthalpies= -650.545682
Sum of electronic and thermal Free Energies= -650.596381

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 124.474 | 45.907 | 106.706 |

**21e**



63

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 5.0582480000 | -0.4298890000 | 1.2704140000 |
| C | 4.3310690000 | -0.2315560000 | 2.4456000000 |
| C | 2.9730790000 | 0.0260960000 | 2.3998970000 |
| C | 2.3030510000 | 0.0778260000 | 1.1709310000 |
| C | 3.0249760000 | -0.1123870000 | -0.0045510000 |
| C | 4.4100770000 | -0.3655690000 | 0.0418670000 |
| H | 6.1195890000 | -0.6300600000 | 1.3244430000 |
| H | 4.8437290000 | -0.2813910000 | 3.3987110000 |
| H | 2.4075960000 | 0.1936450000 | 3.3084630000 |
| C | 0.8340870000 | 0.3985540000 | 1.1833460000 |
| O | 2.4078290000 | -0.0707980000 | -1.2331030000 |
| O | 5.0158490000 | -0.5241030000 | -1.1609390000 |
| C | 6.4164320000 | -0.7539110000 | -1.1654760000 |
| H | 6.9506050000 | 0.0798400000 | -0.7018590000 |
| H | 6.7029540000 | -0.8355340000 | -2.2109720000 |
| H | 6.6613160000 | -1.6836620000 | -0.6451700000 |
| O | 0.4308680000 | 1.4054540000 | 1.7999520000 |
| C | 2.6216270000 | 1.1445230000 | -1.9565750000 |
| H | 3.6918120000 | 1.3526430000 | -2.0336900000 |
| C | 1.9142640000 | 2.2683460000 | -1.3345370000 |
| H | 2.2299360000 | 0.9631970000 | -2.9583470000 |
| C | 1.2962730000 | 3.1380560000 | -0.7843160000 |
| H | 0.7375640000 | 3.8944680000 | -0.2832860000 |
| N | -1.3881120000 | -0.3025420000 | 0.3269250000 |
| C | -0.0435870000 | -0.5187130000 | 0.5470160000 |
| S | 0.3876790000 | -2.1398820000 | 0.0817320000 |
| C | -1.2675170000 | -2.4890210000 | -0.3752810000 |
| C | -2.0625140000 | -1.4141130000 | -0.1895830000 |
| C | -1.9035050000 | 1.0334420000 | 0.1482800000 |
| C | -2.5867280000 | 1.6528040000 | 1.1958100000 |
| C | -3.0821120000 | 2.9346120000 | 0.9797330000 |
| C | -2.9031500000 | 3.5936020000 | -0.2393820000 |
| C | -2.2280340000 | 2.9334750000 | -1.2628530000 |
| C | -1.7212390000 | 1.6437180000 | -1.0922040000 |
| C | -2.7525270000 | 0.9487710000 | 2.5125880000 |
| H | -3.6142360000 | 3.4360520000 | 1.7828870000 |
| C | -3.4106630000 | 4.9999900000 | -0.4291560000 |
| H | -2.0888300000 | 3.4291490000 | -2.2192100000 |
| C | -1.0318060000 | 0.9213780000 | -2.2201800000 |
| C | -1.6511090000 | -3.8369010000 | -0.9136390000 |
| C | -2.8013570000 | -4.5047740000 | -0.1502050000 |
| H | -0.7751680000 | -4.4888750000 | -0.8879080000 |
| H | -1.9290430000 | -3.7358270000 | -1.9701450000 |
| C | -4.1704440000 | -3.8556110000 | -0.3674100000 |
| H | -2.5625560000 | -4.5192690000 | 0.9185890000 |
| H | -2.8596290000 | -5.5464870000 | -0.4781750000 |
| H | -4.9302770000 | -4.5060430000 | 0.0752460000 |
| C | -3.5347220000 | -1.3499040000 | -0.4782910000 |
| H | -3.9112350000 | -0.3738270000 | -0.1673110000 |
| C | -4.3453790000 | -2.4522760000 | 0.2179500000 |
| H | -3.6922200000 | -1.4133980000 | -1.5620280000 |
| H | -5.4017800000 | -2.1800330000 | 0.1434160000 |

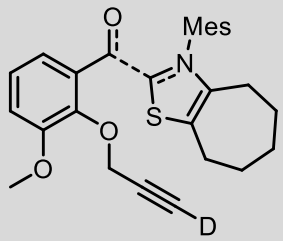
| | | | |
|---|---|---|---|
| H | -4.3825750000 | -3.8213290000 | -1.4433860000 |
| H | -4.0948000000 | -2.4620620000 | 1.2844470000 |
| H | -1.7026020000 | 0.1793520000 | -2.6661100000 |
| H | -0.1398490000 | 0.3948750000 | -1.8719350000 |
| H | -0.7356310000 | 1.6257740000 | -2.9981180000 |
| H | -1.7702190000 | 0.7849520000 | 2.9629180000 |
| H | -3.2249710000 | -0.0290490000 | 2.3824160000 |
| H | -3.3629370000 | 1.5408370000 | 3.1946160000 |
| H | -4.3731840000 | 5.1414590000 | 0.0655190000 |
| H | -3.5265360000 | 5.2375880000 | -1.4873490000 |
| H | -2.7100220000 | 5.7211030000 | 0.0011000000 |

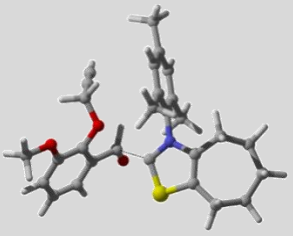
Thermochemie

Zero-point correction= 0.517164 (Hartree/Particle)
Thermal correction to Energy= 0.549394
Thermal correction to Enthalpy= 0.550338
Thermal correction to Gibbs Free Energy= 0.453421
Sum of electronic and zero-point Energies= -1762.836821
Sum of electronic and thermal Energies= -1762.804592
Sum of electronic and thermal Enthalpies= -1762.803648
Sum of electronic and thermal Free Energies= -1762.900565

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 344.750 | 123.551 | 203.979 |

**TS-1e**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 4.3973750000 | -2.4111020000 | 0.0088670000 |
| C | 3.9515630000 | -2.8181580000 | 1.2671140000 |
| C | 2.8884630000 | -2.1770340000 | 1.8824470000 |
| C | 2.2541800000 | -1.1068540000 | 1.2483780000 |
| C | 2.6969660000 | -0.6943550000 | -0.0028360000 |
| C | 3.7650840000 | -1.3518820000 | -0.6373160000 |
| H | 5.2239530000 | -2.9279810000 | -0.4600270000 |
| H | 4.4493780000 | -3.6448590000 | 1.7601110000 |
| H | 2.5344920000 | -2.4772360000 | 2.8608720000 |
| C | 1.1275640000 | -0.3873630000 | 1.9506970000 |
| O | 2.0138020000 | 0.2892300000 | -0.6745840000 |
| O | 4.0917600000 | -0.8947600000 | -1.8745250000 |
| C | 5.1601460000 | -1.5382880000 | -2.5508490000 |
| H | 6.0925630000 | -1.4469860000 | -1.9872700000 |
| H | 5.2604030000 | -1.0296450000 | -3.5065070000 |
| H | 4.9348420000 | -2.5944990000 | -2.7210310000 |
| O | 0.7801760000 | -0.7383000000 | 3.0855400000 |
| C | 2.7144060000 | 1.5153860000 | -0.8736800000 |
| H | 3.7528110000 | 1.3236560000 | -1.1515930000 |
| C | 2.6521780000 | 2.3762240000 | 0.3130410000 |
| H | 2.2195830000 | 2.0115660000 | -1.7101600000 |
| C | 2.5932180000 | 3.0802660000 | 1.2840910000 |
| H | 2.5349190000 | 3.7008030000 | 2.1483390000 |
| N | -1.3443690000 | -0.1480660000 | 0.0003860000 |
| C | -0.4452280000 | -0.9524960000 | 0.5730110000 |

| | | | |
|---|---|---|---|
| S | -1.0532110000 | -2.5436680000 | 0.4835720000 |
| C | -2.5191700000 | -2.0746780000 | -0.3335110000 |
| C | -2.5182860000 | -0.7349820000 | -0.5144230000 |
| C | -1.1044480000 | 1.2778980000 | -0.0412000000 |
| C | -1.3428700000 | 2.0224240000 | 1.1140210000 |
| C | -1.0714360000 | 3.3892310000 | 1.0677680000 |
| C | -0.5829990000 | 3.9995930000 | -0.0858030000 |
| C | -0.3932100000 | 3.2208860000 | -1.2268400000 |
| C | -0.6484040000 | 1.8510390000 | -1.2284360000 |
| C | -1.8656050000 | 1.3636880000 | 2.3627030000 |
| H | -1.2413410000 | 3.9872390000 | 1.9580320000 |
| C | -0.2248030000 | 5.4619500000 | -0.0888580000 |
| H | -0.0274220000 | 3.6876090000 | -2.1371940000 |
| C | -0.4484830000 | 1.0113850000 | -2.4608110000 |
| C | -3.5973440000 | -3.0420470000 | -0.7251220000 |
| C | -4.9655500000 | -2.6981160000 | -0.1209180000 |
| H | -3.3030920000 | -4.0462730000 | -0.4135710000 |
| H | -3.6786910000 | -3.0658920000 | -1.8184870000 |
| C | -5.6445910000 | -1.4697170000 | -0.7337970000 |
| H | -4.8548010000 | -2.5611280000 | 0.9601170000 |
| H | -5.6228620000 | -3.5597300000 | -0.2670860000 |
| H | -6.6693020000 | -1.4233890000 | -0.3543220000 |
| C | -3.6139700000 | 0.0762040000 | -1.1411100000 |
| H | -3.3386160000 | 1.1323740000 | -1.1114020000 |
| C | -4.9766770000 | -0.1185380000 | -0.4604530000 |
| H | -3.6994950000 | -0.1990510000 | -2.1994210000 |
| H | -5.6431000000 | 0.6699120000 | -0.8204470000 |
| H | -5.7240430000 | -1.6121970000 | -1.8188670000 |
| H | -4.8646610000 | 0.0295890000 | 0.6190570000 |
| H | 0.1791250000 | 0.1474790000 | -2.2329610000 |
| H | 0.0258820000 | 1.5948880000 | -3.2506170000 |
| H | -1.4049320000 | 0.6423690000 | -2.8434470000 |
| H | -1.1143330000 | 0.6997340000 | 2.8012220000 |
| H | -2.7469740000 | 0.7545280000 | 2.1426310000 |
| H | -2.1410840000 | 2.1155200000 | 3.1022840000 |
| H | -0.8158450000 | 6.0168440000 | 0.6410320000 |
| H | -0.3783010000 | 5.9064960000 | -1.0734650000 |
| H | 0.8308490000 | 5.5865730000 | 0.1711830000 |
| H | 0.9777320000 | 0.6440880000 | 1.6046380000 |

Thermochemie

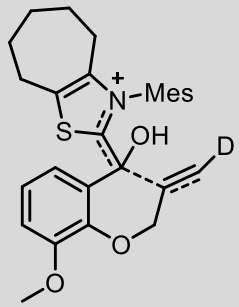
Zero-point correction= 0.527451 (Hartree/Particle)
Thermal correction to Energy= 0.559801
Thermal correction to Enthalpy= 0.560745
Thermal correction to Gibbs Free Energy= 0.462379
Sum of electronic and zero-point Energies= -1763.395710
Sum of electronic and thermal Energies= -1763.363360
Sum of electronic and thermal Enthalpies= -1763.362416
Sum of electronic and thermal Free Energies= -1763.460781

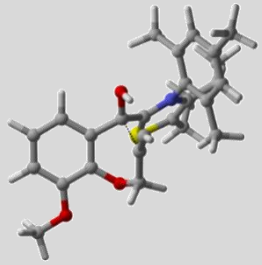
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 351.280 | 123.311 | 207.028 |

Imaginäre Frequenz

-127.2716

**TS-3e**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -5.0736770000 | -0.3315270000 | 1.3552910000 |
| C | -4.2228610000 | -0.8086340000 | 2.3560350000 |
| C | -2.8726550000 | -0.9915140000 | 2.1161110000 |
| C | -2.3483410000 | -0.6815090000 | 0.8578810000 |
| C | -3.1990970000 | -0.2476130000 | -0.1539390000 |
| C | -4.5688800000 | -0.0578140000 | 0.0874850000 |
| H | -6.1246390000 | -0.1941960000 | 1.5702270000 |
| H | -4.6353130000 | -1.0334690000 | 3.3324840000 |
| H | -2.2046950000 | -1.3728720000 | 2.8777310000 |
| C | -0.9066590000 | -0.8763060000 | 0.5417600000 |
| O | -5.3065180000 | 0.3713240000 | -0.9672600000 |
| C | -6.6902580000 | 0.5489310000 | -0.7598770000 |
| H | -7.1724290000 | -0.3905220000 | -0.4701710000 |
| H | -7.0959530000 | 0.8868220000 | -1.7111170000 |
| H | -6.8821580000 | 1.3066670000 | 0.0068890000 |
| O | -0.2408320000 | -1.8045100000 | 1.2783440000 |
| H | -0.1745270000 | -2.6066030000 | 0.6302980000 |
| N | 1.2100400000 | 0.3363980000 | 0.0669430000 |
| C | -0.1406960000 | 0.2804900000 | 0.2162830000 |
| S | -0.8133550000 | 1.8596390000 | -0.0112300000 |
| C | 0.7639410000 | 2.5578150000 | -0.2811770000 |
| C | 1.7237640000 | 1.6167420000 | -0.2041460000 |
| C | 2.0622460000 | -0.8294540000 | 0.0261330000 |
| C | 2.6775580000 | -1.2496870000 | 1.2099950000 |
| C | 3.5264770000 | -2.3450660000 | 1.1445710000 |
| C | 3.7689730000 | -3.0129200000 | -0.0597520000 |
| C | 3.1577140000 | -2.5449860000 | -1.2149870000 |
| C | 2.2980440000 | -1.4430420000 | -1.1987070000 |
| C | 2.3929160000 | -0.5406700000 | 2.5032750000 |
| H | 4.0064320000 | -2.6941270000 | 2.0538700000 |
| C | 4.6559490000 | -4.2303560000 | -0.0890310000 |
| H | 3.3433930000 | -3.0464440000 | -2.1604680000 |
| C | 1.6870530000 | -0.9512240000 | -2.4843410000 |
| C | 0.9164910000 | 4.0176690000 | -0.5965340000 |
| C | 1.9152380000 | 4.7467290000 | 0.3097460000 |
| H | -0.0611920000 | 4.4984900000 | -0.5125170000 |
| H | 1.2255940000 | 4.1320580000 | -1.6430480000 |
| C | 3.3805350000 | 4.3752980000 | 0.0708690000 |
| H | 1.6517520000 | 4.5584220000 | 1.3559820000 |
| H | 1.8003680000 | 5.8212660000 | 0.1403790000 |
| H | 4.0060460000 | 5.0762900000 | 0.6311580000 |
| C | 3.1968190000 | 1.8355390000 | -0.4005680000 |
| H | 3.7239880000 | 0.9036830000 | -0.1920650000 |
| C | 3.7826710000 | 2.9539400000 | 0.4715090000 |
| H | 3.3826390000 | 2.0659440000 | -1.4573930000 |
| H | 4.8722740000 | 2.8786950000 | 0.4131980000 |
| H | 3.6208790000 | 4.5289280000 | -0.9888960000 |
| H | 3.5108830000 | 2.7744090000 | 1.5173990000 |
| H | 1.1925840000 | -1.7768080000 | -2.9999160000 |
| H | 2.4624990000 | -0.5490740000 | -3.1429200000 |

| | | | |
|---|---|---|---|
| H | 0.9432710000 | -0.1721190000 | -2.3146660000 |
| H | 1.3476160000 | -0.7015670000 | 2.7787650000 |
| H | 2.5532890000 | 0.5375440000 | 2.4091920000 |
| H | 3.0340070000 | -0.9171370000 | 3.3003810000 |
| H | 4.0869270000 | -5.1215140000 | 0.1898910000 |
| H | 5.4827250000 | -4.1318210000 | 0.6165540000 |
| H | 5.0693710000 | -4.3954260000 | -1.0848970000 |
| C | -1.1798240000 | -1.9199480000 | -1.1528290000 |
| C | -2.0178750000 | -1.0628940000 | -2.0371150000 |
| H | -1.3995920000 | -0.5887810000 | -2.8034910000 |
| O | -2.6970390000 | 0.0229750000 | -1.3955000000 |
| H | -2.7617670000 | -1.6952960000 | -2.5322840000 |
| C | -0.6461670000 | -3.0392310000 | -0.9720450000 |
| H | -0.5421720000 | -4.0213100000 | -1.3955160000 |

Thermochemie

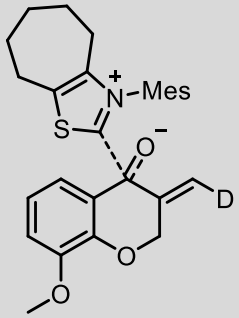
Zero-point correction= 0.527561 (Hartree/Particle)
Thermal correction to Energy= 0.559366
Thermal correction to Enthalpy= 0.560310
Thermal correction to Gibbs Free Energy= 0.464612
Sum of electronic and zero-point Energies= -1763.391821
Sum of electronic and thermal Energies= -1763.360016
Sum of electronic and thermal Enthalpies= -1763.359072
Sum of electronic and thermal Free Energies= -1763.454770

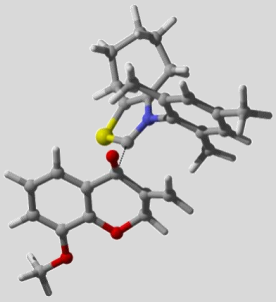
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 351.008 | 123.273 | 201.415 |

Imaginäre Frequenz

-584.3723

**TS-4e**



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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -4.9345980000 | 0.7568920000 | 1.1547750000 |
| C | -3.9435900000 | 0.9189440000 | 2.1306110000 |
| C | -2.7198760000 | 0.2953240000 | 1.9889550000 |
| C | -2.4502630000 | -0.4908330000 | 0.8636700000 |
| C | -3.4310010000 | -0.6541020000 | -0.1103640000 |
| C | -4.6893290000 | -0.0299020000 | 0.0385680000 |
| H | -5.8913300000 | 1.2457090000 | 1.2803420000 |
| H | -4.1520620000 | 1.5320050000 | 2.9990800000 |
| H | -1.9446420000 | 0.3898440000 | 2.7404540000 |
| C | -1.1133530000 | -1.2190140000 | 0.7650480000 |
| O | -5.5818380000 | -0.2622240000 | -0.9570940000 |
| C | -6.8525970000 | 0.3548470000 | -0.8472870000 |
| H | -7.3784040000 | 0.0155040000 | 0.0496970000 |
| H | -7.4102480000 | 0.0545990000 | -1.7310870000 |
| H | -6.7588860000 | 1.4444230000 | -0.8263300000 |
| O | -0.5426220000 | -1.5579160000 | 1.8239420000 |
| N | 1.2621590000 | 0.3630990000 | -0.1701260000 |

| | | | |
|---|---|---|---|
| C | -0.0611850000 | 0.3177260000 | -0.0196160000 |
| S | -0.6730610000 | 1.8951260000 | -0.2280880000 |
| C | 0.8940510000 | 2.5862580000 | -0.5328590000 |
| C | 1.8362820000 | 1.6178790000 | -0.4577910000 |
| C | 2.0665610000 | -0.8349320000 | -0.0407740000 |
| C | 2.5574310000 | -1.1706050000 | 1.2195260000 |
| C | 3.3214020000 | -2.3313560000 | 1.3194590000 |
| C | 3.5988200000 | -3.1251340000 | 0.2058610000 |
| C | 3.1106520000 | -2.7299080000 | -1.0392610000 |
| C | 2.3377400000 | -1.5797380000 | -1.1861540000 |
| C | 2.2712910000 | -0.2994530000 | 2.4103980000 |
| H | 3.7113700000 | -2.6204920000 | 2.2905250000 |
| C | 4.3971120000 | -4.3944730000 | 0.3520570000 |
| H | 3.3334560000 | -3.3299120000 | -1.9162960000 |
| C | 1.7995460000 | -1.1554550000 | -2.5249180000 |
| C | 1.0918870000 | 4.0441480000 | -0.8306870000 |
| C | 2.1222990000 | 4.7249650000 | 0.0783040000 |
| H | 0.1314630000 | 4.5553370000 | -0.7368530000 |
| H | 1.4012590000 | 4.1541280000 | -1.8769690000 |
| C | 3.5736920000 | 4.3147060000 | -0.1811770000 |
| H | 1.8631640000 | 4.5296050000 | 1.1244070000 |
| H | 2.0365950000 | 5.8041460000 | -0.0747110000 |
| H | 4.2238410000 | 4.9945980000 | 0.3765600000 |
| C | 3.3138950000 | 1.7846950000 | -0.6606860000 |
| H | 3.8088750000 | 0.8330720000 | -0.4581650000 |
| C | 3.9430100000 | 2.8815000000 | 0.2100180000 |
| H | 3.4986350000 | 2.0156880000 | -1.7170620000 |
| H | 5.0283990000 | 2.7744330000 | 0.1347650000 |
| H | 3.8053380000 | 4.4671710000 | -1.2426520000 |
| H | 3.6812660000 | 2.7068710000 | 1.2590610000 |
| H | 2.0959670000 | -0.1310390000 | -2.7678530000 |
| H | 0.7065680000 | -1.1868540000 | -2.5246190000 |
| H | 2.1624550000 | -1.8152600000 | -3.3124420000 |
| H | 1.1943460000 | -0.2790470000 | 2.5936510000 |
| H | 2.6119090000 | 0.7258140000 | 2.2373520000 |
| H | 2.7754250000 | -0.6837200000 | 3.2968780000 |
| H | 5.1579160000 | -4.2927580000 | 1.1275570000 |
| H | 4.8880600000 | -4.6618630000 | -0.5844930000 |
| H | 3.7443180000 | -5.2244550000 | 0.6360880000 |
| C | -1.0671540000 | -2.1106920000 | -0.4573270000 |
| C | -1.9124040000 | -1.6534650000 | -1.6084110000 |
| H | -1.5285340000 | -0.7120970000 | -2.0204090000 |
| O | -3.2714760000 | -1.4286330000 | -1.2182150000 |
| H | -1.9466240000 | -2.4001030000 | -2.4007070000 |
| C | -0.3426560000 | -3.2228260000 | -0.4678170000 |
| H | 0.2653370000 | -3.4759310000 | 0.3947460000 |
| H | -0.3198630000 | -3.8789160000 | -1.3319970000 |

Thermochemie

Zero-point correction= 0.529604 (Hartree/Particle)
Thermal correction to Energy= 0.560581
Thermal correction to Enthalpy= 0.561525
Thermal correction to Gibbs Free Energy= 0.467345
Sum of electronic and zero-point Energies= -1763.455618
Sum of electronic and thermal Energies= -1763.424641
Sum of electronic and thermal Enthalpies= -1763.423697
Sum of electronic and thermal Free Energies= -1763.517877

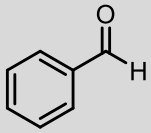
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 351.770 | 120.544 | 198.218 |

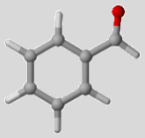
Imaginäre Frequenz
-173.6175

## Benzaldehyd

M06-2X/6-311+G**

**31**



14
XYZ-Matrix in Ångström

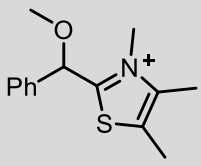
| | | | |
|---|---|---|---|
| C | 0.0445640000 | -1.0988030000 | 0.0000080000 |
| C | -1.3233500000 | -1.3249850000 | -0.0000030000 |
| C | -2.2084370000 | -0.2464760000 | -0.0000080000 |
| C | -1.7279290000 | 1.0588860000 | -0.0000020000 |
| C | -0.3561070000 | 1.2862370000 | 0.0000090000 |
| C | 0.5292400000 | 0.2105780000 | 0.0000150000 |
| H | 0.7558070000 | -1.9168810000 | 0.0000130000 |
| H | -1.7062950000 | -2.3383460000 | -0.0000070000 |
| H | -3.2770390000 | -0.4270380000 | -0.0000160000 |
| H | -2.4184570000 | 1.8932890000 | -0.0000050000 |
| H | 0.0322630000 | 2.3001810000 | 0.0000140000 |
| C | 1.9908570000 | 0.4665210000 | 0.0000320000 |
| O | 2.8304110000 | -0.3949950000 | -0.0000340000 |
| H | 2.2773980000 | 1.5370100000 | -0.0000360000 |

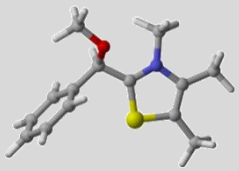
Thermochemie

| | |
|---|---|
| Zero-point correction= | 0.110578 (Hartree/Particle) |
| Thermal correction to Energy= | 0.116877 |
| Thermal correction to Enthalpy= | 0.117821 |
| Thermal correction to Gibbs Free Energy= | 0.080026 |
| Sum of electronic and zero-point Energies= | -345.405215 |
| Sum of electronic and thermal Energies= | -345.398916 |
| Sum of electronic and thermal Enthalpies= | -345.397971 |
| Sum of electronic and thermal Free Energies= | -345.435767 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 73.342 | 23.763 | 79.547 |

**35**



35
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -0.6246750000 | 0.2794960000 | 0.2069580000 |
| N | -1.8453820000 | 0.7949620000 | 0.2517320000 |
| C | -2.8715060000 | -0.1275670000 | 0.0559420000 |
| C | -2.3928060000 | -1.3876260000 | -0.1239500000 |
| S | -0.6664640000 | -1.3900280000 | -0.0634790000 |
| C | -4.3016430000 | 0.2999410000 | 0.0554950000 |
| H | -4.9297410000 | -0.5390320000 | -0.2394870000 |

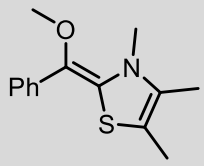
| | | | |
|---|---|---|---|
| H | -4.4712670000 | 1.1144660000 | -0.6518190000 |
| H | -4.6227670000 | 0.6287090000 | 1.0469430000 |
| C | -3.1739500000 | -2.6448820000 | -0.3585010000 |
| H | -2.5241590000 | -3.5194380000 | -0.3555850000 |
| H | -3.6809500000 | -2.6058430000 | -1.3247560000 |
| H | -3.9231860000 | -2.7815470000 | 0.4226770000 |
| C | -2.1162620000 | 2.2273160000 | 0.4554200000 |
| H | -3.0172000000 | 2.3250180000 | 1.0561650000 |
| H | -1.2773180000 | 2.6837580000 | 0.9716760000 |
| C | 0.6487440000 | 1.0830350000 | 0.3428920000 |
| H | -2.2449070000 | 2.7091840000 | -0.5130730000 |
| O | 0.5574690000 | 2.0801920000 | -0.6431230000 |
| C | 1.8683670000 | 0.1923000000 | 0.2152260000 |
| C | 2.3220420000 | -0.1734760000 | -1.0524360000 |
| C | 3.4142470000 | -1.0233420000 | -1.1757040000 |
| C | 4.0495090000 | -1.5122880000 | -0.0368590000 |
| C | 3.6000000000 | -1.1438900000 | 1.2265260000 |
| C | 2.5114750000 | -0.2864910000 | 1.3532640000 |
| H | 1.8269650000 | 0.2209190000 | -1.9338150000 |
| H | 3.7727490000 | -1.3019440000 | -2.1590180000 |
| H | 4.9012690000 | -2.1742640000 | -0.1349050000 |
| H | 4.1012770000 | -1.5141300000 | 2.1122370000 |
| H | 2.1682660000 | 0.0121570000 | 2.3390210000 |
| C | 1.5614340000 | 3.0838230000 | -0.5156540000 |
| H | 1.3811070000 | 3.8033910000 | -1.3105200000 |
| H | 2.5604740000 | 2.6549760000 | -0.6250890000 |
| H | 1.4819200000 | 3.5814610000 | 0.4575880000 |
| H | 0.6489530000 | 1.5382480000 | 1.3485700000 |

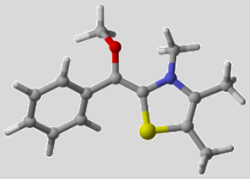
Thermochemie

Zero-point correction= 0.296276 (Hartree/Particle)
Thermal correction to Energy= 0.313559
Thermal correction to Enthalpy= 0.314504
Thermal correction to Gibbs Free Energy= 0.250851
Sum of electronic and zero-point Energies= -1071.846827
Sum of electronic and thermal Energies= -1071.829543
Sum of electronic and thermal Enthalpies= -1071.828599
Sum of electronic and thermal Free Energies= -1071.892252

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 196.762 | 64.640 | 133.969 |

**36**



34

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -0.5944240000 | 0.2027440000 | 0.0010720000 |
| N | -1.8108530000 | 0.8820210000 | -0.0214130000 |
| C | -2.9329650000 | 0.0377620000 | -0.1048140000 |
| C | -2.6427770000 | -1.2705490000 | -0.1150090000 |
| S | -0.8987070000 | -1.5452240000 | 0.0081440000 |
| C | -4.2948390000 | 0.6495820000 | -0.2131430000 |
| H | -5.0194060000 | -0.0978890000 | -0.5296190000 |
| H | -4.2948540000 | 1.4549500000 | -0.9515370000 |
| H | -4.6358560000 | 1.0629230000 | 0.7398970000 |
| C | -3.5373390000 | -2.4614060000 | -0.2262910000 |

| | | | |
|---|---|---|---|
| H | -3.3765260000 | -3.1436060000 | 0.6131260000 |
| H | -3.3442420000 | -3.0187190000 | -1.1469970000 |
| H | -4.5866430000 | -2.1676130000 | -0.2186450000 |
| C | -1.8999100000 | 2.2384350000 | 0.5047970000 |
| H | -1.3123940000 | 2.3093640000 | 1.4261470000 |
| H | -1.5215000000 | 2.9688270000 | -0.2077850000 |
| C | 0.6362400000 | 0.7689700000 | -0.0731460000 |
| H | -2.9372930000 | 2.4649570000 | 0.7394390000 |
| O | 0.7129370000 | 2.1036600000 | -0.4376710000 |
| C | 1.9048550000 | 0.0268420000 | -0.0298220000 |
| C | 2.9520930000 | 0.4121430000 | -0.8801980000 |
| C | 4.1614270000 | -0.2686640000 | -0.8708700000 |
| C | 4.3556050000 | -1.3476400000 | -0.0116260000 |
| C | 3.3297760000 | -1.7290580000 | 0.8463240000 |
| C | 2.1203680000 | -1.0438140000 | 0.8457010000 |
| H | 2.7960850000 | 1.2453970000 | -1.5559230000 |
| H | 4.9551960000 | 0.0393690000 | -1.5417700000 |
| H | 5.2990840000 | -1.8800420000 | -0.0064310000 |
| H | 3.4756800000 | -2.5541850000 | 1.5337910000 |
| H | 1.3451340000 | -1.3256170000 | 1.5487390000 |
| C | 1.4037920000 | 2.9327250000 | 0.4833380000 |
| H | 1.4533240000 | 3.9256900000 | 0.0368560000 |
| H | 2.4175220000 | 2.5651900000 | 0.6664580000 |
| H | 0.8670670000 | 2.9827350000 | 1.4373310000 |

Thermochemie

Zero-point correction= 0.282181 (Hartree/Particle)
Thermal correction to Energy= 0.299663
Thermal correction to Enthalpy= 0.300607
Thermal correction to Gibbs Free Energy= 0.236835
Sum of electronic and zero-point Energies= -1071.445420
Sum of electronic and thermal Energies= -1071.427938
Sum of electronic and thermal Enthalpies= -1071.426994
Sum of electronic and thermal Free Energies= -1071.490766

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 188.041 | 65.058 | 134.219 |

# Projekt B

## Wasserstoffatom, Methylradikal, Methan und Borylradikal

(u)M06-2X/6-311+G**

### Wasserstoffatom H•

1

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| H | 0.0000000000 | 0.0000000000 | 0.0000000000 |

Thermochemie

ero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.010654
Sum of electronic and zero-point Energies= -0.498134
Sum of electronic and thermal Energies= -0.496718
Sum of electronic and thermal Enthalpies= -0.495774
Sum of electronic and thermal Free Energies= -0.508788

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 0.889 | 2.981 | 27.392 |

### Methylradikal $CH_3$•

4

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 0.0000930000 | 0.0002070000 | -0.0000460000 |
| H | -0.8704400000 | 0.6376330000 | 0.0000910000 |
| H | 0.9881010000 | 0.4334120000 | 0.0000910000 |
| H | -0.1182200000 | -1.0722880000 | 0.0000910000 |

Thermochemie

Zero-point correction= 0.029714 (Hartree/Particle)
Thermal correction to Energy= 0.032826
Thermal correction to Enthalpy= 0.033770
Thermal correction to Gibbs Free Energy= 0.009893
Sum of electronic and zero-point Energies= -39.791163
Sum of electronic and thermal Energies= -39.788050
Sum of electronic and thermal Enthalpies= -39.787106
Sum of electronic and thermal Free Energies= -39.810983

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 20.599 | 7.531 | 50.253 |

### Methan $CH_4$

5

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 0.0002210000 | 0.0001500000 | -0.0002620000 |
| H | 0.6591930000 | -0.7358250000 | -0.4580440000 |
| H | -0.8524140000 | 0.1821660000 | -0.6529650000 |
| H | -0.3534070000 | -0.3771090000 | 0.9584300000 |
| H | 0.5453020000 | 0.9298680000 | 0.1541520000 |

Thermochemie

Zero-point correction= 0.044931 (Hartree/Particle)
Thermal correction to Energy= 0.047799
Thermal correction to Enthalpy= 0.048744
Thermal correction to Gibbs Free Energy= 0.025272
Sum of electronic and zero-point Energies= -40.451821
Sum of electronic and thermal Energies= -40.448953
Sum of electronic and thermal Enthalpies= -40.448009
Sum of electronic and thermal Free Energies= -40.471480

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 29.995 | 6.465 | 49.400 |

**Borylradikal $BH_2$•**

4
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 0.0000930000 | 0.0002070000 | -0.0000460000 |
| H | -0.8704400000 | 0.6376330000 | 0.0000910000 |
| H | 0.9881010000 | 0.4334120000 | 0.0000910000 |
| H | -0.1182200000 | -1.0722880000 | 0.0000910000 |

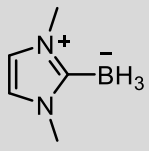
Thermochemie
Zero-point correction= 0.029714 (Hartree/Particle)
Thermal correction to Energy= 0.032826
Thermal correction to Enthalpy= 0.033770
Thermal correction to Gibbs Free Energy= 0.009893
Sum of electronic and zero-point Energies= -39.791163
Sum of electronic and thermal Energies= -39.788050
Sum of electronic and thermal Enthalpies= -39.787106
Sum of electronic and thermal Free Energies= -39.810983

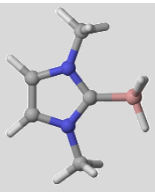
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 20.599 | 7.531 | 50.253 |

## Imd-$BH_3$

(u)M06-2X/6-311+G** SCRF=(PCM,Solvent=Acetonitrile)

**56**



19
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -0.0095860000 | 0.5819180000 | 0.0008720000 |
| N | 1.0836670000 | -0.2076130000 | 0.0039260000 |
| C | 0.7224530000 | -1.5414890000 | 0.0011330000 |
| C | -0.6308240000 | -1.5776890000 | -0.0042650000 |
| N | -1.0585370000 | -0.2657100000 | -0.0066760000 |
| C | -2.4490240000 | 0.1686930000 | 0.0071730000 |
| B | -0.0969170000 | 2.1831370000 | -0.0027800000 |
| H | 1.4517400000 | -2.3330440000 | 0.0002020000 |
| H | -1.3174570000 | -2.4064880000 | -0.0097810000 |
| H | -3.0798000000 | -0.6808390000 | -0.2447870000 |
| H | -2.5827770000 | 0.9602010000 | -0.7279940000 |

| | | | |
|---|---|---|---|
| H | -2.7134500000 | 0.5457650000 | 0.9949980000 |
| C | 2.4605490000 | 0.2762570000 | 0.0023390000 |
| H | 3.1222550000 | -0.5864570000 | -0.0238910000 |
| H | 2.6514310000 | 0.8579770000 | 0.9021700000 |
| H | 2.6341170000 | 0.8980240000 | -0.8738190000 |
| H | -0.8366180000 | 2.5181330000 | 0.9058690000 |
| H | -0.5930390000 | 2.5240040000 | -1.0645660000 |
| H | 1.0108700000 | 2.6541660000 | 0.1312420000 |

Thermochemie

Zero-point correction= 0.160305 (Hartree/Particle)
Thermal correction to Energy= 0.169307
Thermal correction to Enthalpy= 0.170252
Thermal correction to Gibbs Free Energy= 0.126818
Sum of electronic and zero-point Energies= -331.281300
Sum of electronic and thermal Energies= -331.272298
Sum of electronic and thermal Enthalpies= -331.271353
Sum of electronic and thermal Free Energies= -331.314787

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 106.242 | 32.543 | 91.414 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 6.0709 eV 204.23 nm f=0.0742 <S**2>=0.000
30 -> 31 0.66166
30 -> 34 0.12756
30 -> 36 -0.11533
30 -> 39 -0.10683
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -331.218504455
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 6.2635 eV 197.95 nm f=0.2994 <S**2>=0.000
30 -> 31 0.10572
30 -> 33 0.45279
30 -> 34 -0.37065
30 -> 37 -0.32708
30 -> 40 -0.10065

Excited State 3: Singlet-A 6.7318 eV 184.18 nm f=0.1173 <S**2>=0.000
28 -> 33 -0.10097
28 -> 37 0.10252
30 -> 34 0.10127
30 -> 35 0.63542
30 -> 43 -0.15799

Excited State 4: Singlet-A 6.7661 eV 183.24 nm f=0.0071 <S**2>=0.000
27 -> 31 -0.11196
30 -> 33 0.40353
30 -> 34 0.45972
30 -> 35 -0.10302
30 -> 36 0.24634

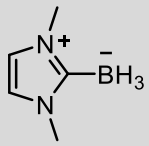
Excited State 5: Singlet-A 6.8719 eV 180.42 nm f=0.0004 <S**2>=0.000
30 -> 32 0.67741
30 -> 38 -0.11174

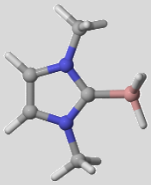
Excited State 6: Singlet-A 7.1143 eV 174.27 nm f=0.0233 <S**2>=0.000
30 -> 33 0.30041

| | |
|---|---|
| 30 -> 34 | -0.17910 |
| 30 -> 36 | -0.36057 |
| 30 -> 37 | 0.41645 |
| 30 -> 40 | 0.17997 |

(u)M06-2X/6-311+G**

**56**





19

XYZ-Matrix in Ångström

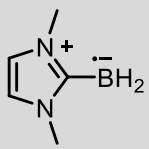
| | | | |
|---|---|---|---|
| C | -0.0102390000 | 0.5806730000 | 0.0022860000 |
| N | 1.0840070000 | -0.2105170000 | 0.0042630000 |
| C | 0.7263580000 | -1.5460100000 | 0.0001470000 |
| C | -0.6263760000 | -1.5848130000 | -0.0044710000 |
| N | -1.0563960000 | -0.2733330000 | -0.0058320000 |
| C | -2.4399620000 | 0.1759420000 | 0.0077510000 |
| B | -0.1046790000 | 2.1766400000 | -0.0039510000 |
| H | 1.4549380000 | -2.3378660000 | -0.0026740000 |
| H | -1.3088600000 | -2.4168080000 | -0.0106320000 |
| H | -3.0812100000 | -0.6567100000 | -0.2769250000 |
| H | -2.5481790000 | 0.9958140000 | -0.7006360000 |
| H | -2.7074590000 | 0.5338330000 | 1.0022720000 |
| C | 2.4515400000 | 0.2925860000 | 0.0034360000 |
| H | 3.1291250000 | -0.5586030000 | -0.0393460000 |
| H | 2.6346580000 | 0.8696770000 | 0.9082320000 |
| H | 2.6065330000 | 0.9356450000 | -0.8609320000 |
| H | -0.8622380000 | 2.4913570000 | 0.8933400000 |
| H | -0.5930410000 | 2.4879350000 | -1.0764070000 |
| H | 0.9979310000 | 2.6492070000 | 0.1395560000 |

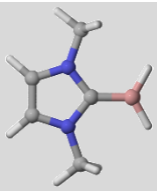
Thermochemie

| | |
|---|---|
| Zero-point correction= | 0.160287 (Hartree/Particle) |
| Thermal correction to Energy= | 0.169376 |
| Thermal correction to Enthalpy= | 0.170320 |
| Thermal correction to Gibbs Free Energy= | 0.126334 |
| Sum of electronic and zero-point Energies= | -331.266270 |
| Sum of electronic and thermal Energies= | -331.257181 |
| Sum of electronic and thermal Enthalpies= | -331.256236 |
| Sum of electronic and thermal Free Energies= | -331.300223 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 106.285 | 32.616 | 92.577 |

**81**





18

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 0.0000350000 | 0.6493510000 | -0.0003760000 |

| | | | |
|---|---|---|---|
| N | 1.0885760000 | -0.2001510000 | -0.0010710000 |
| C | 0.6772390000 | -1.5148650000 | -0.0001230000 |
| C | -0.6773250000 | -1.5148220000 | 0.0002870000 |
| N | -1.0885870000 | -0.2001050000 | 0.0000370000 |
| C | -2.4569920000 | 0.2668710000 | 0.0001500000 |
| B | 0.0000430000 | 2.1538560000 | -0.0000710000 |
| H | 1.3746920000 | -2.3347000000 | -0.0000860000 |
| H | -1.3747860000 | -2.3346550000 | 0.0006070000 |
| H | -3.1223060000 | -0.5952600000 | 0.0009390000 |
| H | -2.6451980000 | 0.8757350000 | -0.8864460000 |
| H | -2.6445820000 | 0.8768910000 | 0.8860830000 |
| C | 2.4570120000 | 0.2668130000 | 0.0006000000 |
| H | 3.1222990000 | -0.5953150000 | -0.0046590000 |
| H | 2.6457130000 | 0.8715030000 | 0.8899900000 |
| H | 2.6441250000 | 0.8809980000 | -0.8825060000 |
| H | -1.0412700000 | 2.7336140000 | 0.0006050000 |
| H | 1.0413660000 | 2.7335980000 | -0.0001560000 |

Thermochemie

Zero-point correction= 0.150171 (Hartree/Particle)
Thermal correction to Energy= 0.158763
Thermal correction to Enthalpy= 0.159707
Thermal correction to Gibbs Free Energy= 0.116917
Sum of electronic and zero-point Energies= -330.651283
Sum of electronic and thermal Energies= -330.642691
Sum of electronic and thermal Enthalpies= -330.641746
Sum of electronic and thermal Free Energies= -330.684537

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 99.625 | 31.922 | 90.060 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: 2.031-A 3.0598 eV 405.21 nm f=0.0321 <S**2>=0.781
30A -> 31A 0.95601
30A -> 33A -0.15083
30A -> 37A -0.10617
30A -> 38A -0.15587
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -330.689008470
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.174-A 3.1378 eV 395.13 nm f=0.0169 <S**2>=0.931
29A -> 34A -0.10831
30A -> 34A 0.88751
30A -> 42A 0.34974
30A -> 49A -0.16877
29B -> 34B 0.12107

Excited State 3: 2.030-A 3.4330 eV 361.15 nm f=0.0000 <S**2>=0.781
30A -> 32A 0.98979

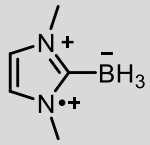
Excited State 4: 2.035-A 3.6659 eV 338.21 nm f=0.0154 <S**2>=0.785
30A -> 31A 0.19767
30A -> 33A 0.93217
30A -> 37A 0.22087
30A -> 56A -0.10887

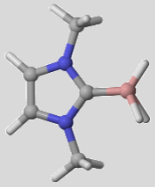
Excited State 5: 2.016-A 3.9830 eV 311.28 nm f=0.1160 <S**2>=0.766
30A -> 36A -0.28944

30A -> 39A 0.79645
30A -> 44A 0.19196
30A -> 48A 0.38946
30A -> 52A -0.10903
29B -> 30B 0.24667

Excited State 6: 2.024-A 4.0659 eV 304.93 nm f=0.0066 <S**2>=0.774
30A -> 31A 0.16721
30A -> 33A -0.24197
30A -> 37A 0.47124
30A -> 38A 0.80728
30A -> 53A -0.13849

**64**



19
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -0.0062480000 | 0.5744650000 | -0.0003530000 |
| N | 1.0991480000 | -0.2054120000 | 0.0000390000 |
| C | 0.7397800000 | -1.5233220000 | 0.0000820000 |
| C | -0.6236240000 | -1.5663820000 | -0.0000080000 |
| N | -1.0633770000 | -0.2724260000 | -0.0003290000 |
| C | -2.4651680000 | 0.1439700000 | 0.0002190000 |
| B | 0.0004730000 | 2.1088060000 | -0.0001780000 |
| H | 1.4654850000 | -2.3193380000 | 0.0001770000 |
| H | -1.2989680000 | -2.4054750000 | 0.0000200000 |
| H | -3.0889670000 | -0.7464340000 | -0.0036200000 |
| H | -2.6775920000 | 0.7298900000 | -0.8943520000 |
| H | -2.6789780000 | 0.7234300000 | 0.8986560000 |
| C | 2.4781530000 | 0.2945970000 | 0.0001120000 |
| H | 3.1475950000 | -0.5619340000 | 0.0018310000 |
| H | 2.6500970000 | 0.8944820000 | 0.8922220000 |
| H | 2.6511860000 | 0.8917540000 | -0.8936250000 |
| H | -1.0546230000 | 2.6275900000 | 0.5157040000 |
| H | -1.0550570000 | 2.6282220000 | -0.5143320000 |
| H | 0.9497090000 | 2.7986870000 | -0.0000750000 |

Thermochemie
Zero-point correction= 0.158442 (Hartree/Particle)
Thermal correction to Energy= 0.167438
Thermal correction to Enthalpy= 0.168383
Thermal correction to Gibbs Free Energy= 0.124357
Sum of electronic and zero-point Energies= -330.973234
Sum of electronic and thermal Energies= -330.964237
Sum of electronic and thermal Enthalpies= -330.963293
Sum of electronic and thermal Free Energies= -331.007318

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 105.069 | 33.373 | 92.659 |

Elektronisch angeregte Zustände
Excitation energies and oscillator strengths:

Excited State 1: 2.156-A 3.1319 eV 395.88 nm f=0.0597 <S**2>=0.912
30A -> 31A 0.26860
29B -> 30B 0.94608

29B -> 32B -0.12044
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -331.016580619
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.284-A 4.2955 eV 288.63 nm f=0.0133 <S**2>=1.054
28A -> 31A -0.18538
28B -> 30B 0.95327
28B -> 32B -0.18364

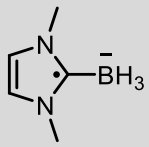
Excited State 3: 2.026-A 4.9114 eV 252.44 nm f=0.0010 <S**2>=0.776
25B -> 30B 0.15420
27B -> 30B 0.96625

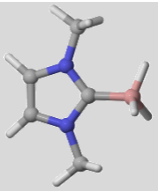
Excited State 4: 2.252-A 4.9939 eV 248.27 nm f=0.2417 <S**2>=1.018
30A -> 31A 0.92685
29B -> 30B -0.27996
29B -> 32B -0.11263

Excited State 5: 3.016-A 5.2973 eV 234.05 nm f=0.0227 <S**2>=2.024
29A -> 33A -0.34244
30A -> 31A 0.11865
30A -> 33A 0.74446
30A -> 41A 0.11238
29B -> 33B 0.47261
29B -> 47B 0.10036

Excited State 6: 2.081-A 6.0201 eV 205.95 nm f=0.0367 <S**2>=0.832
29A -> 34A -0.11587
30A -> 32A 0.86585
30A -> 34A -0.24854
30A -> 35A -0.15665
30A -> 38A -0.12267
30A -> 40A 0.13788
30A -> 43A -0.14308
30A -> 54A -0.13613

**65**



19
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -0.0103360000 | 0.5820150000 | 0.0014160000 |
| N | 1.0824470000 | -0.2077420000 | 0.0019660000 |
| C | 0.7250580000 | -1.5439100000 | -0.0021970000 |
| C | -0.6257920000 | -1.5827600000 | -0.0070560000 |
| N | -1.0554100000 | -0.2702490000 | -0.0088780000 |
| C | -2.4384110000 | 0.1689470000 | 0.0124540000 |
| B | -0.1048080000 | 2.1827640000 | -0.0073850000 |
| H | 1.4501980000 | -2.3383450000 | -0.0014600000 |
| H | -1.3042120000 | -2.4175640000 | -0.0123970000 |
| H | -3.0737310000 | -0.6711150000 | -0.2655270000 |
| H | -2.5585110000 | 0.9868660000 | -0.6979950000 |
| H | -2.7022950000 | 0.5188590000 | 1.0128360000 |
| C | 2.4502350000 | 0.2853920000 | 0.0080470000 |
| H | 3.1212960000 | -0.5717630000 | -0.0294830000 |
| H | 2.6315990000 | 0.8582040000 | 0.9180000000 |
| H | 2.6151910000 | 0.9237810000 | -0.8598740000 |

| | | | |
|---|---|---|---|
| H | -0.8657540000 | 2.5146650000 | 0.8852650000 |
| H | -0.5822470000 | 2.5091660000 | -1.0840560000 |
| H | 0.9987250000 | 2.6612560000 | 0.1440120000 |

Thermochemie

Zero-point correction= 0.159416 (Hartree/Particle)
Thermal correction to Energy= 0.168614
Thermal correction to Enthalpy= 0.169558
Thermal correction to Gibbs Free Energy= 0.124477
Sum of electronic and zero-point Energies= -331.236372
Sum of electronic and thermal Energies= -331.227174
Sum of electronic and thermal Enthalpies= -331.226230
Sum of electronic and thermal Free Energies= -331.271311

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 105.807 | 32.737 | 94.881 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: 2.001-A 0.4476 eV 2769.80 nm f=0.1464 <S**2>=0.751
31A -> 32A 0.97888
31A -> 38A -0.18746
31A -> 42A -0.17151
31A <- 42A -0.12620
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -331.379337360
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.001-A 0.7052 eV 1758.05 nm f=0.1358 <S**2>=0.751
31A -> 33A 0.49117
31A -> 34A 0.84132
31A -> 41A -0.16565
31A -> 46A 0.10333
31A -> 49A -0.11559

Excited State 3: 2.001-A 0.7793 eV 1590.92 nm f=0.1167 <S**2>=0.751
31A -> 33A 0.78272
31A -> 34A -0.43743
31A -> 35A 0.37228
31A -> 38A 0.20942

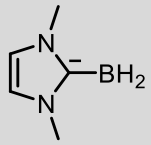
Excited State 4: 2.001-A 0.8923 eV 1389.52 nm f=0.0006 <S**2>=0.751
31A -> 36A 0.98136
31A -> 37A 0.11459
31A -> 51A 0.14921
31A <- 36A -0.10322

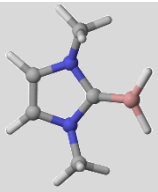
Excited State 5: 2.002-A 1.1338 eV 1093.55 nm f=0.0131 <S**2>=0.752
31A -> 32A 0.21532
31A -> 33A -0.14789
31A -> 35A -0.17039
31A -> 38A 0.90753
31A -> 42A 0.17460
31A -> 43A -0.17968
31A -> 48A -0.16192
31A <- 32A -0.12332

Excited State 6: 2.002-A 1.4663 eV 845.59 nm f=0.0079 <S**2>=0.752
31A -> 33A -0.33694
31A -> 34A 0.18814

| | |
|---|---|
| 31A -> 35A | 0.83679 |
| 31A -> 37A | -0.16763 |
| 31A -> 39A | -0.25265 |
| 31A -> 40A | 0.15696 |
| 31A -> 41A | -0.16909 |

**66**



18

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -0.0001250000 | 0.6827210000 | -0.2145040000 |
| N | 1.1267250000 | -0.2185910000 | -0.3035300000 |
| C | 0.6727620000 | -1.4897650000 | 0.0562240000 |
| C | -0.6723050000 | -1.4898010000 | 0.0564910000 |
| N | -1.1264940000 | -0.2188590000 | -0.3027280000 |
| C | -2.3890610000 | 0.2557850000 | 0.1934450000 |
| B | -0.0002610000 | 2.1233200000 | 0.0215660000 |
| H | 1.3553660000 | -2.3189420000 | 0.1680240000 |
| H | -1.3548560000 | -2.3188650000 | 0.1694740000 |
| H | -3.1313110000 | -0.5454380000 | 0.1296340000 |
| H | -2.7192700000 | 1.1039430000 | -0.4091800000 |
| H | -2.2966730000 | 0.6059610000 | 1.2364990000 |
| C | 2.3888790000 | 0.2561680000 | 0.1938890000 |
| H | 3.1313590000 | -0.5448520000 | 0.1301660000 |
| H | 2.2954820000 | 0.6059040000 | 1.2369690000 |
| H | 2.7193800000 | 1.1046880000 | -0.4080850000 |
| H | -1.0407020000 | 2.7310830000 | 0.0849950000 |
| H | 1.0400070000 | 2.7314080000 | 0.0842110000 |

Thermochemie

Zero-point correction= 0.147813 (Hartree/Particle)
Thermal correction to Energy= 0.156134
Thermal correction to Enthalpy= 0.157079
Thermal correction to Gibbs Free Energy= 0.115766
Sum of electronic and zero-point Energies= -330.655809
Sum of electronic and thermal Energies= -330.647488
Sum of electronic and thermal Enthalpies= -330.646544
Sum of electronic and thermal Free Energies= -330.687856

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 97.976 | 31.897 | 86.949 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.5740 eV 787.69 nm f=0.0247 <S**2>=0.000
30 -> 31 0.69633
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -330.745778363
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 1.8261 eV 678.97 nm f=0.0101 <S**2>=0.000
30 -> 32 0.70123

Excited State 3: Singlet-A 2.1302 eV 582.02 nm f=0.0096 <S**2>=0.000
30 -> 33 0.67942

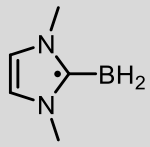
30 -> 35 0.15493

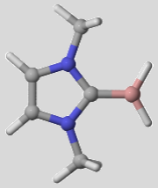
Excited State 4: Singlet-A 2.3372 eV 530.47 nm f=0.0091 <S**2>=0.000
30 -> 34 0.66306
30 -> 37 -0.16515
30 -> 42 0.13415

Excited State 5: Singlet-A 2.5540 eV 485.44 nm f=0.0054 <S**2>=0.000
30 -> 33 -0.14260
30 -> 35 0.38936
30 -> 36 0.55241

Excited State 6: Singlet-A 2.5797 eV 480.61 nm f=0.0302 <S**2>=0.000
30 -> 35 0.55141
30 -> 36 -0.41946

**67**



18

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 0.0000350000 | 0.6493510000 | -0.0003760000 |
| N | 1.0885760000 | -0.2001510000 | -0.0010710000 |
| C | 0.6772390000 | -1.5148650000 | -0.0001230000 |
| C | -0.6773250000 | -1.5148220000 | 0.0002870000 |
| N | -1.0885870000 | -0.2001050000 | 0.0000370000 |
| C | -2.4569920000 | 0.2668710000 | 0.0001500000 |
| B | 0.0000430000 | 2.1538560000 | -0.0000710000 |
| H | 1.3746920000 | -2.3347000000 | -0.0000860000 |
| H | -1.3747860000 | -2.3346550000 | 0.0006070000 |
| H | -3.1223060000 | -0.5952600000 | 0.0009390000 |
| H | -2.6451980000 | 0.8757350000 | -0.8864460000 |
| H | -2.6445820000 | 0.8768910000 | 0.8860830000 |
| C | 2.4570120000 | 0.2668130000 | 0.0006000000 |
| H | 3.1222990000 | -0.5953150000 | -0.0046590000 |
| H | 2.6457130000 | 0.8715030000 | 0.8899900000 |
| H | 2.6441250000 | 0.8809980000 | -0.8825060000 |
| H | -1.0412700000 | 2.7336140000 | 0.0006050000 |
| H | 1.0413660000 | 2.7335980000 | -0.0001560000 |

Thermochemie

Zero-point correction= 0.150171 (Hartree/Particle)
Thermal correction to Energy= 0.158763
Thermal correction to Enthalpy= 0.159707
Thermal correction to Gibbs Free Energy= 0.116917
Sum of electronic and zero-point Energies= -330.651283
Sum of electronic and thermal Energies= -330.642691
Sum of electronic and thermal Enthalpies= -330.641746
Sum of electronic and thermal Free Energies= -330.684537

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 99.625 | 31.922 | 90.060 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: 2.031-A 3.0598 eV 405.21 nm f=0.0321 <S**2>=0.781

30A -> 31A 0.95601
30A -> 33A -0.15083
30A -> 37A -0.10617
30A -> 38A -0.15587
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -330.689008470
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.174-A 3.1378 eV 395.13 nm f=0.0169 <S**2>=0.931
29A -> 34A -0.10831
30A -> 34A 0.88751
30A -> 42A 0.34974
30A -> 49A -0.16877
29B -> 34B 0.12107

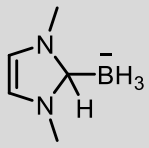
Excited State 3: 2.030-A 3.4330 eV 361.15 nm f=0.0000 <S**2>=0.781
30A -> 32A 0.98979

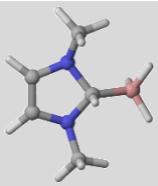
Excited State 4: 2.035-A 3.6659 eV 338.21 nm f=0.0154 <S**2>=0.785
30A -> 31A 0.19767
30A -> 33A 0.93217
30A -> 37A 0.22087
30A -> 56A -0.10887

Excited State 5: 2.016-A 3.9830 eV 311.28 nm f=0.1160 <S**2>=0.766
30A -> 36A -0.28944
30A -> 39A 0.79645
30A -> 44A 0.19196
30A -> 48A 0.38946
30A -> 52A -0.10903
29B -> 30B 0.24667

Excited State 6: 2.024-A 4.0659 eV 304.93 nm f=0.0066 <S**2>=0.774
30A -> 31A 0.16721
30A -> 33A -0.24197
30A -> 37A 0.47124
30A -> 38A 0.80728
30A -> 53A -0.13849

**68**



20
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 0.0000400000 | 0.6490620000 | 0.1414940000 |
| N | 1.1383480000 | -0.2070150000 | -0.2830900000 |
| C | 0.6718760000 | -1.5247150000 | -0.1612230000 |
| C | -0.6720890000 | -1.5246260000 | -0.1612440000 |
| N | -1.1383930000 | -0.2068340000 | -0.2832080000 |
| C | -2.3886800000 | 0.1173470000 | 0.3541170000 |
| B | 0.0001780000 | 2.2019510000 | -0.3579870000 |
| H | 1.3454880000 | -2.3687780000 | -0.2152920000 |
| H | -1.3458260000 | -2.3685840000 | -0.2153430000 |
| H | -3.1658960000 | -0.5794580000 | 0.0252800000 |
| H | -2.6752260000 | 1.1325230000 | 0.0797200000 |
| H | -2.3098070000 | 0.0666020000 | 1.4571880000 |
| C | 2.3886940000 | 0.1171510000 | 0.3540780000 |
| H | 3.1658810000 | -0.5796680000 | 0.0252010000 |

| | | | |
|---|---|---|---|
| H | 2.3099480000 | 0.0664850000 | 1.4571690000 |
| H | 2.6752130000 | 1.1323170000 | 0.0796060000 |
| H | -0.9943750000 | 2.7620720000 | 0.1027650000 |
| H | 0.0006900000 | 2.2592730000 | -1.5814170000 |
| H | 0.9943190000 | 2.7620960000 | 0.1036560000 |
| H | -0.0000270000 | 0.5969880000 | 1.2721610000 |

Thermochemie

Zero-point correction= 0.168228 (Hartree/Particle)
Thermal correction to Energy= 0.176927
Thermal correction to Enthalpy= 0.177871
Thermal correction to Gibbs Free Energy= 0.135798
Sum of electronic and zero-point Energies= -331.852155
Sum of electronic and thermal Energies= -331.843456
Sum of electronic and thermal Enthalpies= -331.842512
Sum of electronic and thermal Free Energies= -331.884584

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 111.023 | 33.506 | 88.550 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: 3.000-A 3.0486 eV 406.69 nm f=0.0000 <S**2>=2.000
31A -> 35A 0.21313
31A -> 38A -0.33716
31A -> 40A 0.17195
31A -> 43A -0.43604
31A -> 46A 0.15665
31A -> 50A -0.21222
31A -> 53A 0.13764
31B -> 35B -0.21313
31B -> 38B 0.33716
31B -> 40B -0.17195
31B -> 43B 0.43604
31B -> 46B -0.15665
31B -> 50B 0.21222
31B -> 53B -0.13764
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -331.908348437
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 1.000-A 3.1149 eV 398.03 nm f=0.0221 <S**2>=0.000
31A -> 32A 0.68820
31A -> 34A 0.11619
31B -> 32B 0.68820
31B -> 34B 0.11619

Excited State 3: 3.000-A 3.1993 eV 387.54 nm f=0.0000 <S**2>=2.000
31A -> 32A 0.69120
31B -> 32B -0.69120

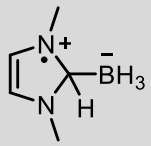
Excited State 4: 1.000-A 3.4424 eV 360.16 nm f=0.0078 <S**2>=0.000
31A -> 33A 0.69171
31A -> 35A 0.10941
31B -> 33B 0.69171
31B -> 35B 0.10941

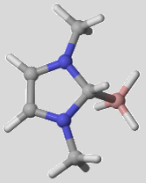
Excited State 5: 3.000-A 3.4816 eV 356.12 nm f=0.0000 <S**2>=2.000
31A -> 33A 0.68771
31A -> 35A 0.12375

31B -> 33B -0.68771
31B -> 35B -0.12375

Excited State 6: 1.000-A 3.8537 eV 321.72 nm f=0.0062 <S**2>=0.000
31A -> 32A -0.11144
31A -> 34A 0.67993
31B -> 32B -0.11144
31B -> 34B 0.67993

**69**



20
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -0.0000450000 | 0.6296660000 | 0.4402010000 |
| N | 1.1191890000 | -0.2715540000 | 0.2317540000 |
| C | 0.6867050000 | -1.4422600000 | -0.2824740000 |
| C | -0.6866380000 | -1.4423590000 | -0.2823010000 |
| N | -1.1191910000 | -0.2717330000 | 0.2321000000 |
| C | -2.4808740000 | 0.2140290000 | 0.1702120000 |
| B | -0.0001050000 | 1.9203170000 | -0.6385590000 |
| H | 1.3637460000 | -2.2114740000 | -0.6177710000 |
| H | -1.3636580000 | -2.2116760000 | -0.6174020000 |
| H | -3.1614660000 | -0.6367630000 | 0.2017690000 |
| H | -2.6323740000 | 0.7921580000 | -0.7442580000 |
| H | -2.6700600000 | 0.8636760000 | 1.0249690000 |
| C | 2.4809260000 | 0.2140440000 | 0.1703380000 |
| H | 3.1614580000 | -0.6367530000 | 0.2031740000 |
| H | 2.6695170000 | 0.8645070000 | 1.0245930000 |
| H | 2.6331890000 | 0.7913020000 | -0.7445590000 |
| H | -1.0037210000 | 2.5587070000 | -0.4015460000 |
| H | -0.0004050000 | 1.4166640000 | -1.7482830000 |
| H | 1.0037600000 | 2.5584480000 | -0.4019260000 |
| H | 0.0001090000 | 1.0139090000 | 1.4712070000 |

Thermochemie
Zero-point correction= 0.170099 (Hartree/Particle)
Thermal correction to Energy= 0.179247
Thermal correction to Enthalpy= 0.180192
Thermal correction to Gibbs Free Energy= 0.136268
Sum of electronic and zero-point Energies= -331.797958
Sum of electronic and thermal Energies= -331.788810
Sum of electronic and thermal Enthalpies= -331.787865
Sum of electronic and thermal Free Energies= -331.831789

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 112.479 | 34.042 | 92.444 |

Elektronisch angeregte Zustände
Excitation energies and oscillator strengths:

Excited State 1: 2.028-A 3.3704 eV 367.86 nm f=0.0195 <S**2>=0.779
31A -> 35A 0.86563
31A -> 40A -0.28035
31A -> 47A 0.17507
27B -> 31B -0.29962
This state for optimization and/or second-order correction.

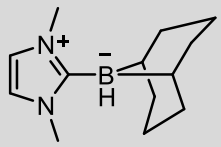
Total Energy, E(TD-HF/TD-KS) = -331.844197486
Copying the excited state density for this state as the 1-particle RhoCI density.

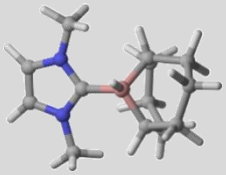
| | | | | | |
|---|---|---|---|---|---|
| Excited State | 2: | 2.022-A | 3.9191 eV | 316.36 nm | f=0.0131 <S**2>=0.772 |
| 31A -> 32A | | 0.95983 | | | |
| 31A -> 34A | | -0.10836 | | | |
| 31A -> 36A | | 0.15561 | | | |
| 31A -> 39A | | -0.11858 | | | |
| Excited State | 3: | 2.025-A | 4.0674 eV | 304.82 nm | f=0.0028 <S**2>=0.775 |
| 30B -> 31B | | 0.98997 | | | |
| Excited State | 4: | 2.033-A | 4.1970 eV | 295.41 nm | f=0.0127 <S**2>=0.783 |
| 31A -> 35A | | -0.15228 | | | |
| 27B -> 31B | | -0.26685 | | | |
| 29B -> 31B | | 0.93786 | | | |
| Excited State | 5: | 2.015-A | 4.2442 eV | 292.12 nm | f=0.1179 <S**2>=0.765 |
| 28B -> 31B | | 0.97846 | | | |
| Excited State | 6: | 2.023-A | 4.4136 eV | 280.92 nm | f=0.0002 <S**2>=0.773 |
| 31A -> 33A | | 0.96375 | | | |
| 31A -> 37A | | -0.10253 | | | |
| 27B -> 31B | | -0.14374 | | | |

## Imd-9BBN

(u)M06-2X/6-311+G** SCRF=(PCM,Solvent=Acetonitrile)

**57**



39
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2079490000 | 0.0813090000 | -0.3627830000 |
| N | 1.9907450000 | -1.0211210000 | -0.2740640000 |
| C | 3.3154040000 | -0.6732920000 | -0.0879210000 |
| C | 3.3640490000 | 0.6763770000 | -0.0624280000 |
| N | 2.0692750000 | 1.1186020000 | -0.2362800000 |
| C | 1.7095380000 | 2.5296040000 | -0.3116720000 |
| H | 4.0917050000 | -1.4127520000 | 0.0073380000 |
| H | 4.1902180000 | 1.3553550000 | 0.0597190000 |
| H | 2.5919400000 | 3.0898750000 | -0.6147990000 |
| H | 1.3644700000 | 2.8874810000 | 0.6578370000 |
| H | 0.9207580000 | 2.6543040000 | -1.0503750000 |
| C | 1.5682550000 | -2.4115350000 | -0.4200620000 |
| H | 1.2888670000 | -2.6138200000 | -1.4527790000 |
| H | 0.7285920000 | -2.6241930000 | 0.2358950000 |
| H | 2.4094150000 | -3.0438050000 | -0.1436450000 |
| C | -1.3149040000 | -1.0939760000 | -0.6429810000 |
| C | -2.6388310000 | -0.7359980000 | -1.3639640000 |
| C | -3.0842310000 | 0.7223530000 | -1.1380980000 |
| C | -2.6610900000 | 1.2488390000 | 0.2348860000 |
| H | -0.8866480000 | -1.9306510000 | -1.2013650000 |
| H | -2.5206240000 | -0.9022880000 | -2.4404760000 |

| | | | |
|---|---|---|---|
| H | -3.4345570000 | -1.4173900000 | -1.0335120000 |
| H | -2.6353040000 | 1.3610600000 | -1.9044370000 |
| H | -4.1693950000 | 0.8078740000 | -1.2592060000 |
| H | -3.0316740000 | 2.2730140000 | 0.3566860000 |
| H | -3.1708250000 | 0.6624430000 | 1.0080510000 |
| C | -1.1191190000 | 1.2112760000 | 0.4747630000 |
| C | -1.5921290000 | -1.5783740000 | 0.8179040000 |
| C | -0.8129070000 | 0.6476210000 | 1.8785390000 |
| C | -0.7401810000 | -0.8960960000 | 1.9016900000 |
| H | -0.7744430000 | 2.2486990000 | 0.4528040000 |
| H | -1.5705700000 | 0.9946650000 | 2.5936260000 |
| H | 0.1451950000 | 1.0433950000 | 2.2390490000 |
| H | 0.3036720000 | -1.2006800000 | 1.7768680000 |
| H | -1.0367320000 | -1.2700610000 | 2.8869930000 |
| H | -1.4412060000 | -2.6627200000 | 0.8923980000 |
| H | -2.6488330000 | -1.4233260000 | 1.0608210000 |
| B | -0.3905310000 | 0.2583560000 | -0.6581710000 |
| H | -0.3923250000 | 0.7807230000 | -1.7714700000 |

Thermochemie

Zero-point correction= 0.352214 (Hartree/Particle)
Thermal correction to Energy= 0.366963
Thermal correction to Enthalpy= 0.367907
Thermal correction to Gibbs Free Energy= 0.312130
Sum of electronic and zero-point Energies= -643.110245
Sum of electronic and thermal Energies= -643.095496
Sum of electronic and thermal Enthalpies= -643.094552
Sum of electronic and thermal Free Energies= -643.150329

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 230.273 | 61.143 | 117.393 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 5.6520 eV 219.36 nm f=0.0440 <S**2>=0.000
60 -> 61 0.49522
60 -> 62 0.22524
60 -> 63 -0.20254
60 -> 66 0.18115
60 -> 67 -0.15043
60 -> 68 0.16315
60 -> 70 0.13547
60 -> 71 0.12352
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -643.254750927
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 5.7213 eV 216.71 nm f=0.0789 <S**2>=0.000
60 -> 61 0.43026
60 -> 62 -0.19906
60 -> 63 0.10188
60 -> 64 -0.26933
60 -> 67 0.22059
60 -> 68 -0.20029
60 -> 70 -0.18593
60 -> 71 -0.12503

Excited State 3: Singlet-A 5.9826 eV 207.24 nm f=0.0336 <S**2>=0.000
59 -> 61 0.51051
59 -> 64 -0.12000

60 -> 62 0.16558
60 -> 63 0.36657
60 -> 64 0.10129

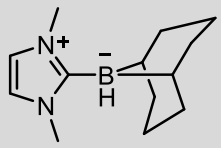
Excited State 4: Singlet-A 6.0896 eV 203.60 nm f=0.0163 <S**2>=0.000
60 -> 62 0.52296
60 -> 63 -0.14286
60 -> 64 -0.28899
60 -> 67 0.12631
60 -> 69 0.18989

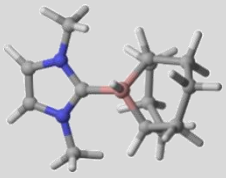
Excited State 5: Singlet-A 6.1049 eV 203.09 nm f=0.1719 <S**2>=0.000
59 -> 62 0.27678
59 -> 63 -0.21281
59 -> 64 0.21185
59 -> 66 0.18798
59 -> 67 -0.27437
59 -> 68 0.27549
59 -> 69 -0.12155
59 -> 70 0.21770
59 -> 71 0.14997
59 -> 72 -0.11727

Excited State 6: Singlet-A 6.1681 eV 201.01 nm f=0.0122 <S**2>=0.000
59 -> 61 -0.14098
60 -> 62 0.15008
60 -> 64 0.53842
60 -> 66 -0.13603
60 -> 67 0.19090
60 -> 68 -0.17849
60 -> 69 0.10803
60 -> 70 -0.12011

(u)M06-2X/6-311+G**

**57**



39
XYZ-Matrix in Ångström

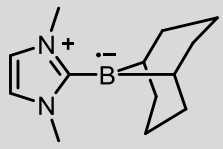
| | | | |
|---|---|---|---|
| C | -1.2057960000 | -0.0870010000 | -0.3504050000 |
| N | -1.9934000000 | 1.0140470000 | -0.2744400000 |
| C | -3.3187800000 | 0.6651790000 | -0.0953130000 |
| C | -3.3644270000 | -0.6837960000 | -0.0586000000 |
| N | -2.0678450000 | -1.1244910000 | -0.2197310000 |
| C | -1.6942500000 | -2.5304230000 | -0.2935570000 |
| H | -4.0981820000 | 1.4021630000 | -0.0092190000 |
| H | -4.1905060000 | -1.3619490000 | 0.0672170000 |
| H | -2.5680130000 | -3.0997850000 | -0.6081830000 |
| H | -1.3512490000 | -2.8859320000 | 0.6777480000 |
| H | -0.8946200000 | -2.6408060000 | -1.0237520000 |
| C | -1.5639120000 | 2.3989000000 | -0.4353490000 |
| H | -1.3093470000 | 2.5951410000 | -1.4760660000 |
| H | -0.7012830000 | 2.6025220000 | 0.1930300000 |
| H | -2.3908350000 | 3.0409560000 | -0.1353650000 |
| C | 1.3094740000 | 1.0808190000 | -0.6695220000 |

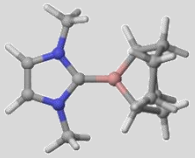
| | | | |
|---|---|---|---|
| C | 2.6258250000 | 0.6977250000 | -1.3926270000 |
| C | 3.0630930000 | -0.7571970000 | -1.1347540000 |
| C | 2.6547010000 | -1.2437240000 | 0.2562740000 |
| H | 0.8826510000 | 1.9036490000 | -1.2500240000 |
| H | 2.4965020000 | 0.8374230000 | -2.4707420000 |
| H | 3.4262610000 | 1.3834700000 | -1.0855130000 |
| H | 2.5995330000 | -1.4116390000 | -1.8783960000 |
| H | 4.1455370000 | -0.8529170000 | -1.2667630000 |
| H | 3.0227990000 | -2.2645440000 | 0.4045470000 |
| H | 3.1718230000 | -0.6377000000 | 1.0087030000 |
| C | 1.1153060000 | -1.1964870000 | 0.5087990000 |
| C | 1.5978170000 | 1.5998390000 | 0.7774570000 |
| C | 0.8222880000 | -0.5984100000 | 1.9004520000 |
| C | 0.7546600000 | 0.9459450000 | 1.8862660000 |
| H | 0.7721830000 | -2.2350340000 | 0.5161860000 |
| H | 1.5839590000 | -0.9306660000 | 2.6169820000 |
| H | -0.1338770000 | -0.9809750000 | 2.2817220000 |
| H | -0.2917490000 | 1.2487930000 | 1.7697210000 |
| H | 1.0625220000 | 1.3423370000 | 2.8589160000 |
| H | 1.4551550000 | 2.6871880000 | 0.8281300000 |
| H | 2.6552680000 | 1.4484470000 | 1.0158080000 |
| B | 0.3878930000 | -0.2697720000 | -0.6454620000 |
| H | 0.3687290000 | -0.8163910000 | -1.7428970000 |

Zero-point correction= 0.352708 (Hartree/Particle)
Thermal correction to Energy= 0.367489
Thermal correction to Enthalpy= 0.368433
Thermal correction to Gibbs Free Energy= 0.312519
Sum of electronic and zero-point Energies= -643.099451
Sum of electronic and thermal Energies= -643.084670
Sum of electronic and thermal Enthalpies= -643.083726
Sum of electronic and thermal Free Energies= -643.139640

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 230.603 | 61.088 | 117.680 |

**82**



38
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2627850000 | 0.0000370000 | -0.0003570000 |
| N | 2.1274420000 | -1.0809260000 | -0.1579420000 |
| C | 3.4419200000 | -0.6680930000 | -0.0957580000 |
| C | 3.4419220000 | 0.6679730000 | 0.0962320000 |
| N | 2.1274300000 | 1.0809390000 | 0.1574850000 |
| C | 1.7257650000 | 2.4688470000 | 0.2111620000 |
| H | 4.2613870000 | -1.3600530000 | -0.1876420000 |
| H | 4.2613910000 | 1.3599030000 | 0.1882920000 |
| H | 2.5936360000 | 3.0885210000 | -0.0138700000 |
| H | 1.3412890000 | 2.7359100000 | 1.1976580000 |
| H | 0.9491370000 | 2.6538660000 | -0.5336220000 |
| C | 1.7255670000 | -2.4687460000 | -0.2120700000 |
| H | 1.3404110000 | -2.7351550000 | -1.1984760000 |
| H | 0.9493570000 | -2.6540910000 | 0.5330860000 |
| H | 2.5935140000 | -3.0886460000 | 0.0120110000 |
| C | -1.2049390000 | -1.1277100000 | -0.6211000000 |

| | | | |
|---|---|---|---|
| C | -1.8287190000 | -0.5108090000 | -1.9072430000 |
| C | -1.9836190000 | 1.0205890000 | -1.8323670000 |
| C | -2.3118160000 | 1.5051080000 | -0.4170860000 |
| H | -0.7068220000 | -2.0484190000 | -0.9239120000 |
| H | -1.2040740000 | -0.7581670000 | -2.7712120000 |
| H | -2.8073210000 | -0.9722510000 | -2.0884540000 |
| H | -1.0433790000 | 1.4898820000 | -2.1466610000 |
| H | -2.7478090000 | 1.3555400000 | -2.5401960000 |
| H | -2.4541740000 | 2.5904690000 | -0.4280530000 |
| H | -3.2744350000 | 1.0837630000 | -0.1093170000 |
| C | -1.2045820000 | 1.1276810000 | 0.6211020000 |
| C | -2.3116720000 | -1.5050150000 | 0.4177120000 |
| C | -1.8277360000 | 0.5107270000 | 1.9076180000 |
| C | -1.9825220000 | -1.0206470000 | 1.8327940000 |
| H | -0.7062660000 | 2.0483570000 | 0.9236930000 |
| H | -2.8062890000 | 0.9721300000 | 2.0891360000 |
| H | -1.2027330000 | 0.7581910000 | 2.7712840000 |
| H | -1.0420490000 | -1.4899170000 | 2.1464240000 |
| H | -2.7462120000 | -1.3557020000 | 2.5411230000 |
| H | -2.4542600000 | -2.5903350000 | 0.4285750000 |
| H | -3.2742960000 | -1.0833090000 | 0.1104940000 |
| B | -0.2516440000 | -0.0000450000 | -0.0001990000 |

Thermochemie

Zero-point correction= 0.341743 (Hartree/Particle)
Thermal correction to Energy= 0.356868
Thermal correction to Enthalpy= 0.357813
Thermal correction to Gibbs Free Energy= 0.299670
Sum of electronic and zero-point Energies= -642.485879
Sum of electronic and thermal Energies= -642.470753
Sum of electronic and thermal Enthalpies= -642.469809
Sum of electronic and thermal Free Energies= -642.527952

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 223.938 | 60.853 | 122.372 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: 2.027-A 2.7386 eV 452.72 nm f=0.0229 <S**2>=0.777
60A -> 61A 0.95419
60A -> 65A 0.17172
60A -> 68A -0.13206
60A -> 73A -0.11486
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -642.726978428
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.143-A 2.8793 eV 430.60 nm f=0.0143 <S**2>=0.898
60A -> 67A 0.78983
60A -> 70A -0.42959
60A -> 76A 0.19686
60A -> 78A 0.21684
60A -> 85A 0.15475

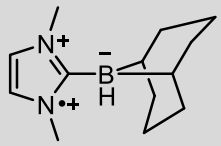
Excited State 3: 2.026-A 3.0081 eV 412.16 nm f=0.0002 <S**2>=0.776
60A -> 62A 0.98814

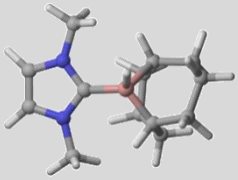
Excited State 4: 2.032-A 3.2268 eV 384.23 nm f=0.0014 <S**2>=0.782
60A -> 63A 0.94252
60A -> 65A 0.27657

| | | | | | |
|---|---|---|---|---|---|
| Excited State | 5: | 2.027-A | 3.5279 eV | 351.44 nm | f=0.0058 <S**2>=0.777 |
| 60A -> 61A | | 0.25598 | | | |
| 60A -> 63A | | 0.18877 | | | |
| 60A -> 65A | | -0.57291 | | | |
| 60A -> 68A | | 0.68268 | | | |
| 60A -> 72A | | 0.13373 | | | |
| 60A -> 73A | | 0.19278 | | | |
| 60A -> 90A | | -0.11132 | | | |

| | | | | | |
|---|---|---|---|---|---|
| Excited State | 6: | 2.022-A | 3.5344 eV | 350.80 nm | f=0.0018 <S**2>=0.772 |
| 60A -> 64A | | 0.96344 | | | |
| 60A -> 66A | | 0.13115 | | | |
| 60A -> 69A | | -0.16183 | | | |

**70**



39

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2383050000 | 0.1061560000 | -0.3917650000 |
| N | 2.0128650000 | -0.9974040000 | -0.2925400000 |
| C | 3.3209940000 | -0.6424630000 | -0.0463980000 |
| C | 3.3598660000 | 0.7087800000 | 0.0123220000 |
| N | 2.0774380000 | 1.1502430000 | -0.2154180000 |
| C | 1.7094370000 | 2.5641290000 | -0.2665290000 |
| H | 4.1025260000 | -1.3757200000 | 0.0572680000 |
| H | 4.1777190000 | 1.3862320000 | 0.1898390000 |
| H | 2.5958970000 | 3.1378530000 | -0.5285540000 |
| H | 1.3385280000 | 2.8965290000 | 0.7037520000 |
| H | 0.9516690000 | 2.7098830000 | -1.0344970000 |
| C | 1.6100460000 | -2.3858760000 | -0.5302730000 |
| H | 1.3841500000 | -2.5326340000 | -1.5858980000 |
| H | 0.7482830000 | -2.6450140000 | 0.0792700000 |
| H | 2.4450010000 | -3.0250700000 | -0.2521700000 |
| C | -1.3531360000 | -1.0089110000 | -0.6709240000 |
| C | -2.6544900000 | -0.6344830000 | -1.3951210000 |
| C | -3.1088400000 | 0.8067610000 | -1.0883460000 |
| C | -2.7218590000 | 1.1929050000 | 0.3418340000 |
| H | -0.8064290000 | -1.7281980000 | -1.3044890000 |
| H | -2.5238060000 | -0.7417680000 | -2.4741490000 |
| H | -3.4405930000 | -1.3349380000 | -1.0969710000 |
| H | -2.6420300000 | 1.5020850000 | -1.7894190000 |
| H | -4.1874320000 | 0.9051830000 | -1.2182170000 |
| H | -3.0533630000 | 2.2210690000 | 0.5333400000 |
| H | -3.2534580000 | 0.5593090000 | 1.0558160000 |
| C | -1.2335710000 | 1.1349570000 | 0.6096950000 |
| C | -1.5846230000 | -1.6306710000 | 0.7236960000 |
| C | -0.8006560000 | 0.5025020000 | 1.9091080000 |
| C | -0.7138880000 | -1.0437840000 | 1.8420340000 |
| H | -0.7359300000 | 2.0768100000 | 0.3591340000 |
| H | -1.5400800000 | 0.7845180000 | 2.6684950000 |
| H | 0.1622250000 | 0.9070550000 | 2.2326010000 |
| H | 0.3330890000 | -1.3224260000 | 1.7000530000 |
| H | -1.0084570000 | -1.4762380000 | 2.7994770000 |
| H | -1.4265890000 | -2.7137820000 | 0.6851670000 |
| H | -2.6362630000 | -1.5117880000 | 0.9947520000 |
| B | -0.3206440000 | 0.2562450000 | -0.7574220000 |

H -0.4190620000 0.9499390000 -1.7277790000

Thermochemie

Zero-point correction= 0.351018 (Hartree/Particle)
Thermal correction to Energy= 0.366434
Thermal correction to Enthalpy= 0.367378
Thermal correction to Gibbs Free Energy= 0.309571
Sum of electronic and zero-point Energies= -642.844995
Sum of electronic and thermal Energies= -642.829580
Sum of electronic and thermal Enthalpies= -642.828635
Sum of electronic and thermal Free Energies= -642.886443

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 229.941 | 63.113 | 121.666 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: 2.017-A 2.3579 eV 525.83 nm f=0.0141 <S**2>=0.767
51B -> 60B -0.13285
54B -> 60B 0.10627
57B -> 60B -0.32338
58B -> 60B -0.38420
59B -> 60B 0.83020
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -643.109363367
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.010-A 2.9986 eV 413.47 nm f=0.0036 <S**2>=0.760
55B -> 60B -0.13175
57B -> 60B 0.68876
58B -> 60B -0.67711

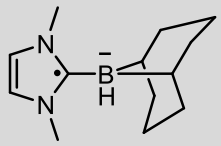
Excited State 3: 2.099-A 3.5554 eV 348.72 nm f=0.0220 <S**2>=0.852
57B -> 60B 0.60114
58B -> 60B 0.57260
59B -> 60B 0.48471
59B -> 61B 0.10893

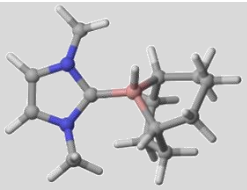
Excited State 4: 2.013-A 3.8688 eV 320.47 nm f=0.0257 <S**2>=0.763
52B -> 60B 0.53165
53B -> 60B -0.15512
54B -> 60B 0.14424
56B -> 60B 0.78730

Excited State 5: 2.025-A 4.0432 eV 306.65 nm f=0.0040 <S**2>=0.775
48B -> 60B -0.13546
52B -> 60B 0.79376
54B -> 60B -0.18210
56B -> 60B -0.50616

Excited State 6: 2.030-A 4.1543 eV 298.45 nm f=0.0047 <S**2>=0.780
51B -> 60B -0.32572
53B -> 60B -0.16772
54B -> 60B 0.64034
55B -> 60B -0.58628
56B -> 60B -0.13247
57B -> 60B -0.11659
58B -> 60B 0.15189
59B -> 60B -0.14806

**71**





39

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2185150000 | 0.1423180000 | -0.1780750000 |
| N | 2.0140400000 | -1.0346990000 | -0.0343930000 |
| C | 3.3552620000 | -0.6743410000 | -0.0044570000 |
| C | 3.4542530000 | 0.6583660000 | -0.1647910000 |
| N | 2.1832660000 | 1.1741040000 | -0.4060730000 |
| C | 1.8654250000 | 2.5240050000 | -0.0168760000 |
| H | 4.1335910000 | -1.4127580000 | 0.1130820000 |
| H | 4.3300730000 | 1.2881840000 | -0.1533880000 |
| H | 2.6608900000 | 3.1977930000 | -0.3464820000 |
| H | 1.7491510000 | 2.6005330000 | 1.0817040000 |
| H | 0.9262240000 | 2.8160580000 | -0.4851570000 |
| C | 1.6273680000 | -2.3229100000 | -0.5627090000 |
| H | 1.5298230000 | -2.3063680000 | -1.6595250000 |
| H | 0.6719300000 | -2.6350970000 | -0.1430160000 |
| H | 2.3870440000 | -3.0582900000 | -0.2834070000 |
| C | -1.2963500000 | -0.9548990000 | -0.8216270000 |
| C | -2.5527610000 | -0.4566380000 | -1.5775910000 |
| C | -3.0206640000 | 0.9483180000 | -1.1434470000 |
| C | -2.7188400000 | 1.2355360000 | 0.3310060000 |
| H | -0.8154070000 | -1.6844750000 | -1.4818270000 |
| H | -2.3342830000 | -0.4278730000 | -2.6514260000 |
| H | -3.3794250000 | -1.1729970000 | -1.4481500000 |
| H | -2.5036830000 | 1.6970050000 | -1.7489710000 |
| H | -4.0941690000 | 1.0645470000 | -1.3411180000 |
| H | -3.0946810000 | 2.2359840000 | 0.5834960000 |
| H | -3.3082400000 | 0.5431710000 | 0.9461380000 |
| C | -1.2067400000 | 1.1132400000 | 0.6991940000 |
| C | -1.7031790000 | -1.6875340000 | 0.4981990000 |
| C | -1.0478720000 | 0.3011010000 | 2.0026000000 |
| C | -0.9368780000 | -1.2173790000 | 1.7452950000 |
| H | -0.8302140000 | 2.1247010000 | 0.8957980000 |
| H | -1.8899220000 | 0.5032310000 | 2.6831750000 |
| H | -0.1390460000 | 0.6210600000 | 2.5233040000 |
| H | 0.1219140000 | -1.4601950000 | 1.6198770000 |
| H | -1.2821160000 | -1.7764300000 | 2.6245350000 |
| H | -1.5661200000 | -2.7733630000 | 0.3920810000 |
| H | -2.7777000000 | -1.5551070000 | 0.6785630000 |
| B | -0.3510940000 | 0.3690000000 | -0.5258190000 |
| H | -0.3465420000 | 1.0947530000 | -1.5272560000 |

Thermochemie

Zero-point correction= 0.346545 (Hartree/Particle)
Thermal correction to Energy= 0.362082
Thermal correction to Enthalpy= 0.363026
Thermal correction to Gibbs Free Energy= 0.304141
Sum of electronic and zero-point Energies= -643.070097
Sum of electronic and thermal Energies= -643.054559
Sum of electronic and thermal Enthalpies= -643.053615
Sum of electronic and thermal Free Energies= -643.112500

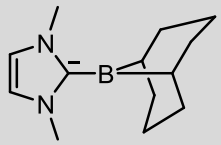
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 227.210 | 63.092 | 123.934 |

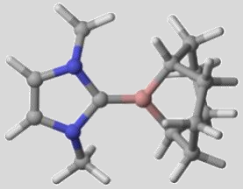
Elektronisch angeregte Zustände
Excitation energies and oscillator strengths:

```
Excited State   1:  2.026-A     0.7501 eV 1652.86 nm  f=0.0152  <S**2>=0.777
   61A -> 62A       0.87980
   61A -> 63A       0.37015
   61A -> 73A      -0.10066
   61A -> 74A       0.16474
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) =  -643.389012769
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State   2:  2.035-A     1.1170 eV 1110.00 nm  f=0.0042  <S**2>=0.785
   61A -> 62A      -0.24895
   61A -> 63A       0.76430
   61A -> 64A      -0.18452
   61A -> 65A      -0.29489
   61A -> 67A      -0.27557
   61A -> 68A       0.10979
   61A -> 73A       0.23679
   61A -> 74A      -0.16566
   61A -> 80A       0.10760

Excited State   3:  2.036-A     1.1809 eV 1049.95 nm  f=0.0262  <S**2>=0.787
   61A -> 62A       0.33333
   61A -> 63A      -0.26981
   61A -> 64A       0.42846
   61A -> 65A      -0.10205
   61A -> 66A       0.22941
   61A -> 67A      -0.21820
   61A -> 68A       0.28306
   61A -> 73A       0.48657
   61A -> 74A      -0.30319
   61A -> 76A       0.15997
   61A -> 80A       0.15803

Excited State   4:  2.030-A     1.3497 eV  918.58 nm  f=0.0011  <S**2>=0.781
   61A -> 62A      -0.15653
   61A -> 63A       0.39576
   61A -> 64A       0.73606
   61A -> 65A       0.38886
   61A -> 66A       0.21621
   61A -> 67A       0.10217
   61A -> 73A      -0.17411
   61A -> 74A       0.10481

Excited State   5:  2.033-A     1.3959 eV  888.17 nm  f=0.0034  <S**2>=0.784
   61A -> 64A      -0.29545
   61A -> 65A       0.78489
   61A -> 67A      -0.10127
   61A -> 69A       0.15862
   61A -> 70A      -0.19061
   61A -> 71A       0.13810
   61A -> 72A       0.10234
   61A -> 73A       0.22501
   61A -> 74A      -0.10432
   61A -> 75A      -0.21377
   61A -> 80A       0.17267

Excited State   6:  2.032-A     1.5757 eV  786.85 nm  f=0.0031  <S**2>=0.782
   61A -> 64A      -0.30326
```

| | |
|---|---|
| 61A -> 65A | 0.12241 |
| 61A -> 66A | 0.85061 |
| 61A -> 67A | -0.16451 |
| 61A -> 68A | -0.14178 |
| 61A -> 69A | -0.17853 |
| 61A -> 71A | -0.17738 |
| 61A -> 73A | -0.10062 |
| 61A -> 75A | 0.14496 |

**72**



38

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -1.2141250000 | -0.0537530000 | 0.1622730000 |
| N | -2.0739790000 | 1.0596710000 | 0.5953620000 |
| C | -3.4068440000 | 0.6266280000 | 0.4354140000 |
| C | -3.4363960000 | -0.6551600000 | 0.0472030000 |
| N | -2.1455400000 | -1.1579350000 | -0.0292550000 |
| C | -1.8429160000 | -2.1936190000 | -0.9778030000 |
| H | -4.2329770000 | 1.2764420000 | 0.6829430000 |
| H | -4.2908520000 | -1.3018910000 | -0.0934930000 |
| H | -2.7280680000 | -2.8209490000 | -1.1181010000 |
| H | -1.0287100000 | -2.8227190000 | -0.6109360000 |
| H | -1.5358320000 | -1.7683910000 | -1.9495090000 |
| C | -1.8251470000 | 2.3399900000 | -0.0529000000 |
| H | -1.8333630000 | 2.2259380000 | -1.1504460000 |
| H | -0.8594820000 | 2.7439940000 | 0.2397030000 |
| H | -2.6041720000 | 3.0495330000 | 0.2478630000 |
| C | 1.2025710000 | 1.1613140000 | 0.5438740000 |
| C | 1.8577850000 | 1.8554840000 | -0.6739060000 |
| C | 2.0217520000 | 0.8831020000 | -1.8594030000 |
| C | 2.3565480000 | -0.5446710000 | -1.4096160000 |
| H | 0.6713950000 | 1.9075600000 | 1.1404660000 |
| H | 1.2374020000 | 2.6977690000 | -1.0032150000 |
| H | 2.8380720000 | 2.2758560000 | -0.3992890000 |
| H | 1.0727260000 | 0.8437950000 | -2.4037560000 |
| H | 2.7830220000 | 1.2549790000 | -2.5568010000 |
| H | 2.5137210000 | -1.1667650000 | -2.2998000000 |
| H | 3.3192640000 | -0.5367150000 | -0.8836300000 |
| C | 1.2487830000 | -1.1890820000 | -0.5043380000 |
| C | 2.3012220000 | 0.5482290000 | 1.4804700000 |
| C | 1.8800490000 | -1.8546240000 | 0.7454130000 |
| C | 1.9722730000 | -0.8782310000 | 1.9339840000 |
| H | 0.7770640000 | -1.9713090000 | -1.1007720000 |
| H | 2.8823500000 | -2.2463140000 | 0.5091880000 |
| H | 1.2716130000 | -2.7148560000 | 1.0493340000 |
| H | 1.0009350000 | -0.8523720000 | 2.4382770000 |
| H | 2.7114350000 | -1.2333260000 | 2.6631280000 |
| H | 2.4335260000 | 1.1858160000 | 2.3634780000 |
| H | 3.2735110000 | 0.5435060000 | 0.9727140000 |
| B | 0.2341460000 | -0.0310740000 | 0.0151810000 |

Thermochemie

Zero-point correction= 0.338024 (Hartree/Particle)
Thermal correction to Energy= 0.353243
Thermal correction to Enthalpy= 0.354187
Thermal correction to Gibbs Free Energy= 0.296426

Sum of electronic and zero-point Energies= -642.494334
Sum of electronic and thermal Energies= -642.479115
Sum of electronic and thermal Enthalpies= -642.478171
Sum of electronic and thermal Free Energies= -642.535932

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 221.663 | 61.510 | 121.568 |

Elektronisch angeregte Zustände
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.5529 eV 798.39 nm f=0.0250 <S**2>=0.000
60 -> 61 0.55459
60 -> 62 0.31684
60 -> 63 0.26056
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -642.775182097
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 1.7520 eV 707.67 nm f=0.0178 <S**2>=0.000
60 -> 61 -0.23691
60 -> 62 0.61382
60 -> 63 -0.20781

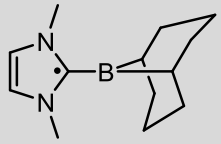
Excited State 3: Singlet-A 1.8082 eV 685.70 nm f=0.0050 <S**2>=0.000
60 -> 61 -0.32758
60 -> 63 0.60001
60 -> 66 -0.10733

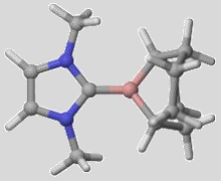
Excited State 4: Singlet-A 2.0644 eV 600.57 nm f=0.0229 <S**2>=0.000
60 -> 64 0.63721
60 -> 68 0.10739
60 -> 69 0.20584

Excited State 5: Singlet-A 2.2372 eV 554.20 nm f=0.0173 <S**2>=0.000
60 -> 61 0.12167
60 -> 65 0.59551
60 -> 66 -0.20802
60 -> 67 0.16749
60 -> 68 -0.12670
60 -> 74 -0.12774

Excited State 6: Singlet-A 2.3006 eV 538.92 nm f=0.0007 <S**2>=0.000
60 -> 65 0.23463
60 -> 66 0.63886
60 -> 70 0.10572

**73**



38
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2627850000 | 0.0000370000 | -0.0003570000 |
| N | 2.1274420000 | -1.0809260000 | -0.1579420000 |
| C | 3.4419200000 | -0.6680930000 | -0.0957580000 |
| C | 3.4419220000 | 0.6679730000 | 0.0962320000 |
| N | 2.1274300000 | 1.0809390000 | 0.1574850000 |

| | | | |
|---|---|---|---|
| C | 1.7257650000 | 2.4688470000 | 0.2111620000 |
| H | 4.2613870000 | -1.3600530000 | -0.1876420000 |
| H | 4.2613910000 | 1.3599030000 | 0.1882920000 |
| H | 2.5936360000 | 3.0885210000 | -0.0138700000 |
| H | 1.3412890000 | 2.7359100000 | 1.1976580000 |
| H | 0.9491370000 | 2.6538660000 | -0.5336220000 |
| C | 1.7255670000 | -2.4687460000 | -0.2120700000 |
| H | 1.3404110000 | -2.7351550000 | -1.1984760000 |
| H | 0.9493570000 | -2.6540910000 | 0.5330860000 |
| H | 2.5935140000 | -3.0886460000 | 0.0120110000 |
| C | -1.2049390000 | -1.1277100000 | -0.6211000000 |
| C | -1.8287190000 | -0.5108090000 | -1.9072430000 |
| C | -1.9836190000 | 1.0205890000 | -1.8323670000 |
| C | -2.3118160000 | 1.5051080000 | -0.4170860000 |
| H | -0.7068220000 | -2.0484190000 | -0.9239120000 |
| H | -1.2040740000 | -0.7581670000 | -2.7712120000 |
| H | -2.8073210000 | -0.9722510000 | -2.0884540000 |
| H | -1.0433790000 | 1.4898820000 | -2.1466610000 |
| H | -2.7478090000 | 1.3555400000 | -2.5401960000 |
| H | -2.4541740000 | 2.5904690000 | -0.4280530000 |
| H | -3.2744350000 | 1.0837630000 | -0.1093170000 |
| C | -1.2045820000 | 1.1276810000 | 0.6211020000 |
| C | -2.3116720000 | -1.5050150000 | 0.4177120000 |
| C | -1.8277360000 | 0.5107270000 | 1.9076180000 |
| C | -1.9825220000 | -1.0206470000 | 1.8327940000 |
| H | -0.7062660000 | 2.0483570000 | 0.9236930000 |
| H | -2.8062890000 | 0.9721300000 | 2.0891360000 |
| H | -1.2027330000 | 0.7581910000 | 2.7712840000 |
| H | -1.0420490000 | -1.4899170000 | 2.1464240000 |
| H | -2.7462120000 | -1.3557020000 | 2.5411230000 |
| H | -2.4542600000 | -2.5903350000 | 0.4285750000 |
| H | -3.2742960000 | -1.0833090000 | 0.1104940000 |
| B | -0.2516440000 | -0.0000450000 | -0.0001990000 |

Thermochemie

Zero-point correction= 0.341743 (Hartree/Particle)
Thermal correction to Energy= 0.356869
Thermal correction to Enthalpy= 0.357813
Thermal correction to Gibbs Free Energy= 0.299671
Sum of electronic and zero-point Energies= -642.485878
Sum of electronic and thermal Energies= -642.470753
Sum of electronic and thermal Enthalpies= -642.469809
Sum of electronic and thermal Free Energies= -642.527951

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 223.938 | 60.853 | 122.370 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: 2.027-A 2.7386 eV 452.72 nm f=0.0229 <S**2>=0.777
60A -> 61A 0.95419
60A -> 65A 0.17172
60A -> 68A -0.13206
60A -> 73A -0.11486
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -642.726978428
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.143-A 2.8793 eV 430.60 nm f=0.0143 <S**2>=0.898
60A -> 67A 0.78983

60A -> 70A -0.42959
60A -> 76A 0.19686
60A -> 78A 0.21684
60A -> 85A 0.15475

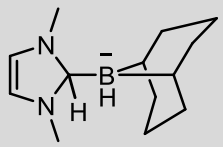
Excited State 3: 2.026-A 3.0081 eV 412.16 nm f=0.0002 <S**2>=0.776
60A -> 62A 0.98814

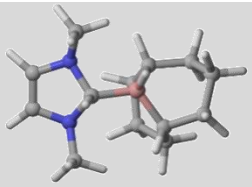
Excited State 4: 2.032-A 3.2268 eV 384.23 nm f=0.0014 <S**2>=0.782
60A -> 63A 0.94252
60A -> 65A 0.27657

Excited State 5: 2.027-A 3.5279 eV 351.44 nm f=0.0058 <S**2>=0.777
60A -> 61A 0.25598
60A -> 63A 0.18877
60A -> 65A -0.57291
60A -> 68A 0.68268
60A -> 72A 0.13373
60A -> 73A 0.19278
60A -> 90A -0.11132

Excited State 6: 2.022-A 3.5344 eV 350.80 nm f=0.0018 <S**2>=0.772
60A -> 64A 0.96344
60A -> 66A 0.13115
60A -> 69A -0.16183

**74**



40
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2123760000 | 0.2007810000 | -0.5927250000 |
| N | 1.8498480000 | -1.0476170000 | -0.0896470000 |
| C | 3.1793100000 | -0.6881330000 | 0.1995050000 |
| C | 3.2654010000 | 0.6436120000 | 0.3390190000 |
| N | 1.9999640000 | 1.2170000000 | 0.1525810000 |
| C | 1.9419670000 | 2.5470250000 | -0.4015700000 |
| H | 3.9293880000 | -1.4385650000 | 0.4057820000 |
| H | 4.1034220000 | 1.2322080000 | 0.6854310000 |
| H | 2.6114210000 | 3.2064100000 | 0.1588510000 |
| H | 0.9222090000 | 2.9252130000 | -0.3298350000 |
| H | 2.2382690000 | 2.5582590000 | -1.4668460000 |
| C | 1.6714060000 | -2.1823700000 | -0.9638260000 |
| H | 2.0072150000 | -1.9582210000 | -1.9929980000 |
| H | 0.6171510000 | -2.4601590000 | -1.0003050000 |
| H | 2.2434560000 | -3.0344410000 | -0.5845040000 |
| C | -1.4461520000 | -0.7214790000 | -1.0248180000 |
| C | -2.7503000000 | -0.0088670000 | -1.4577590000 |
| C | -3.0910310000 | 1.2218850000 | -0.5835570000 |
| C | -2.5447460000 | 1.1268380000 | 0.8483690000 |
| H | -1.0867410000 | -1.2818730000 | -1.8985470000 |
| H | -2.6459710000 | 0.3291980000 | -2.4952020000 |
| H | -3.5943970000 | -0.7160440000 | -1.4433100000 |
| H | -2.6564690000 | 2.1116720000 | -1.0468180000 |
| H | -4.1774080000 | 1.3775140000 | -0.5621360000 |
| H | -2.8235540000 | 2.0405290000 | 1.3905330000 |
| H | -3.0633920000 | 0.3129970000 | 1.3714790000 |
| C | -1.0030870000 | 0.8966560000 | 0.9230110000 |

| | | | |
|---|---|---|---|
| C | -1.7632380000 | -1.7394840000 | 0.1179710000 |
| C | -0.6884410000 | -0.2127520000 | 1.9425930000 |
| C | -0.8762620000 | -1.6423270000 | 1.3735400000 |
| H | -0.5338120000 | 1.8187670000 | 1.2910580000 |
| H | -1.3076160000 | -0.0849820000 | 2.8447470000 |
| H | 0.3558970000 | -0.1110400000 | 2.2572620000 |
| H | 0.1133870000 | -2.0308190000 | 1.1289350000 |
| H | -1.2853880000 | -2.3056230000 | 2.1463860000 |
| H | -1.6951810000 | -2.7692950000 | -0.2613770000 |
| H | -2.8114920000 | -1.6219010000 | 0.4193880000 |
| B | -0.4141680000 | 0.4759270000 | -0.5520290000 |
| H | -0.5371280000 | 1.4093560000 | -1.3508720000 |
| H | 1.5556800000 | 0.2772150000 | -1.6660020000 |

Thermochemie

Zero-point correction= 0.359216 (Hartree/Particle)
Thermal correction to Energy= 0.374262
Thermal correction to Enthalpy= 0.375206
Thermal correction to Gibbs Free Energy= 0.318856
Sum of electronic and zero-point Energies= -643.697807
Sum of electronic and thermal Energies= -643.682761
Sum of electronic and thermal Enthalpies= -643.681817
Sum of electronic and thermal Free Energies= -643.738166

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 234.853 | 62.480 | 118.597 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.2254 eV 384.40 nm f=0.0185 <S**2>=0.000
61 -> 62 0.58005
61 -> 63 -0.33352
61 -> 64 0.14837
61 -> 67 0.11077
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -643.938492526
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.5146 eV 352.77 nm f=0.0092 <S**2>=0.000
61 -> 62 0.24112
61 -> 63 0.54142
61 -> 64 0.30626
61 -> 66 0.18421

Excited State 3: Singlet-A 3.8495 eV 322.08 nm f=0.0067 <S**2>=0.000
61 -> 62 -0.27855
61 -> 63 -0.13131
61 -> 64 0.42873
61 -> 66 -0.15392
61 -> 67 0.41120

Excited State 4: Singlet-A 4.0167 eV 308.67 nm f=0.0585 <S**2>=0.000
61 -> 64 -0.10825
61 -> 65 0.59960
61 -> 66 -0.22703
61 -> 70 0.21140

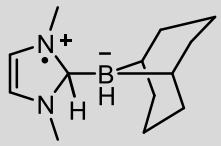
Excited State 5: Singlet-A 4.0343 eV 307.32 nm f=0.0329 <S**2>=0.000
61 -> 63 -0.19545
61 -> 65 0.20730

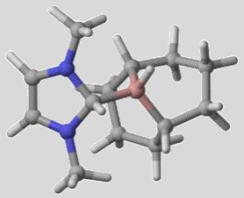
| | |
|---|---|
| 61 -> 66 | 0.49736 |
| 61 -> 68 | 0.24944 |
| 61 -> 69 | -0.10615 |
| 61 -> 71 | 0.17099 |
| 61 -> 72 | 0.12977 |
| 61 -> 73 | 0.10793 |

Excited State 6: Singlet-A 4.2073 eV 294.69 nm f=0.0350 <S**2>=0.000

| | |
|---|---|
| 61 -> 63 | 0.16300 |
| 61 -> 64 | -0.29481 |
| 61 -> 65 | -0.11069 |
| 61 -> 66 | -0.18860 |
| 61 -> 67 | 0.26602 |
| 61 -> 68 | 0.34083 |
| 61 -> 69 | -0.12918 |
| 61 -> 73 | 0.26735 |
| 61 -> 74 | -0.15336 |
| 61 -> 80 | 0.10808 |

**75**



40

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2383720000 | 0.2261350000 | -0.8796740000 |
| N | 1.8723010000 | -0.9775460000 | -0.3891610000 |
| C | 2.8333660000 | -0.6844890000 | 0.5151820000 |
| C | 2.9250130000 | 0.6822520000 | 0.6214780000 |
| N | 2.0492130000 | 1.2423830000 | -0.2387140000 |
| C | 1.8172600000 | 2.6564720000 | -0.4306070000 |
| H | 3.3841550000 | -1.4466520000 | 1.0428330000 |
| H | 3.5521280000 | 1.2719580000 | 1.2708670000 |
| H | 2.5837320000 | 3.2131590000 | 0.1078010000 |
| H | 0.8248010000 | 2.9263200000 | -0.0675830000 |
| H | 1.8741350000 | 2.8956700000 | -1.4947410000 |
| C | 1.6580140000 | -2.2588880000 | -1.0225810000 |
| H | 2.1804280000 | -2.2983640000 | -1.9843690000 |
| H | 0.5912010000 | -2.4067000000 | -1.1863720000 |
| H | 2.0346120000 | -3.0495600000 | -0.3738330000 |
| C | -1.4445240000 | -0.6831280000 | -1.0397770000 |
| C | -2.7847630000 | 0.0385590000 | -1.3363600000 |
| C | -3.0566040000 | 1.2248810000 | -0.3804400000 |
| C | -2.3881580000 | 1.0721630000 | 0.9936210000 |
| H | -1.1510630000 | -1.1962230000 | -1.9649740000 |
| H | -2.7687900000 | 0.4192100000 | -2.3623500000 |
| H | -3.6121670000 | -0.6806990000 | -1.2838390000 |
| H | -2.6841090000 | 2.1443860000 | -0.8394140000 |
| H | -4.1351710000 | 1.3602140000 | -0.2513330000 |
| H | -2.6184290000 | 1.9574500000 | 1.5962860000 |
| H | -2.8553710000 | 0.2335500000 | 1.5224120000 |
| C | -0.8398990000 | 0.8475900000 | 0.9422440000 |
| C | -1.6644210000 | -1.7547920000 | 0.0771390000 |
| C | -0.4614530000 | -0.3048240000 | 1.8915470000 |
| C | -0.7174500000 | -1.7115070000 | 1.2938150000 |
| H | -0.3599320000 | 1.7552910000 | 1.3316610000 |
| H | -1.0139410000 | -0.1979180000 | 2.8334810000 |
| H | 0.5986000000 | -0.2282130000 | 2.1596650000 |
| H | 0.2415150000 | -2.1552880000 | 1.0181600000 |

| | | | |
|---|---|---|---|
| H | -1.1213550000 | -2.3745830000 | 2.0652720000 |
| H | -1.6130900000 | -2.7638410000 | -0.3516760000 |
| H | -2.6904400000 | -1.6663310000 | 0.4475660000 |
| B | -0.4325660000 | 0.5151590000 | -0.5998300000 |
| H | -0.5611270000 | 1.4817190000 | -1.3383980000 |
| H | 1.3433910000 | 0.2732450000 | -1.9763680000 |

Thermochemie

Zero-point correction= 0.361549 (Hartree/Particle)
Thermal correction to Energy= 0.377020
Thermal correction to Enthalpy= 0.377964
Thermal correction to Gibbs Free Energy= 0.319990
Sum of electronic and zero-point Energies= -643.629603
Sum of electronic and thermal Energies= -643.614132
Sum of electronic and thermal Enthalpies= -643.613188
Sum of electronic and thermal Free Energies= -643.671161

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 236.584 | 63.050 | 122.016 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: 2.026-A 2.9854 eV 415.30 nm f=0.0009 <S**2>=0.776
60B -> 61B 0.98473
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -643.881439385
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.035-A 3.3280 eV 372.55 nm f=0.0188 <S**2>=0.785
61A -> 63A -0.13368
61A -> 64A 0.30127
61A -> 65A 0.73672
61A -> 66A 0.24637
61A -> 71A -0.28562
61A -> 77A 0.16072
61A -> 78A 0.14147
55B -> 61B -0.22027
56B -> 61B -0.12373

Excited State 3: 2.027-A 3.5357 eV 350.66 nm f=0.0089 <S**2>=0.777
57B -> 61B 0.21858
58B -> 61B -0.19754
59B -> 61B 0.93853

Excited State 4: 2.018-A 3.7128 eV 333.94 nm f=0.0984 <S**2>=0.768
53B -> 61B 0.12396
54B -> 61B 0.14421
57B -> 61B -0.23429
58B -> 61B 0.89913
59B -> 61B 0.24689

Excited State 5: 2.023-A 3.9598 eV 313.10 nm f=0.0225 <S**2>=0.774
61A -> 62A 0.95865
61A -> 66A -0.10417

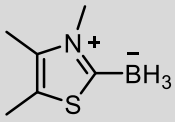
Excited State 6: 2.030-A 4.3831 eV 282.87 nm f=0.0064 <S**2>=0.780
61A -> 63A 0.82544
61A -> 64A 0.30217
61A -> 65A 0.14605
61A -> 67A -0.12167

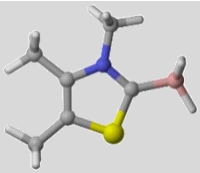
55B -> 61B 0.29661
56B -> 61B 0.18469

## Thz-$BH_3$

(u)M06-2X/6-311+G** SCRF=(PCM,Solvent=Acetonitrile)

**58**



21
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2353980000 | -0.5292880000 | -0.0078310000 |
| S | -0.0386770000 | -1.6657320000 | -0.0008000000 |
| C | -1.2707000000 | -0.4344680000 | 0.0028990000 |
| C | -0.6853750000 | 0.7855010000 | -0.0015290000 |
| N | 0.7154040000 | 0.6948590000 | -0.0112130000 |
| C | 1.5597110000 | 1.8918010000 | 0.0113200000 |
| B | 2.7891360000 | -0.9449670000 | 0.0010650000 |
| C | -2.7219570000 | -0.7947820000 | 0.0066220000 |
| C | -1.3344370000 | 2.1304540000 | -0.0065580000 |
| H | 1.2318230000 | 2.5824070000 | -0.7638150000 |
| H | 2.5845540000 | 1.5865140000 | -0.1746120000 |
| H | 1.4869140000 | 2.3721500000 | 0.9874990000 |
| H | 3.3015680000 | -0.4580580000 | 0.9929350000 |
| H | 3.3105260000 | -0.4780200000 | -0.9959520000 |
| H | 2.8607580000 | -2.1555240000 | 0.0121960000 |
| H | -0.9589250000 | 2.7492900000 | 0.8109020000 |
| H | -2.4106700000 | 2.0293570000 | 0.1122700000 |
| H | -1.1432550000 | 2.6551310000 | -0.9457190000 |
| H | -2.9745210000 | -1.3845640000 | 0.8897380000 |
| H | -2.9786570000 | -1.3827600000 | -0.8765180000 |
| H | -3.3406270000 | 0.1013050000 | 0.0074990000 |

Thermochemie
Zero-point correction= 0.172115 (Hartree/Particle)
Thermal correction to Energy= 0.183013
Thermal correction to Enthalpy= 0.183957
Thermal correction to Gibbs Free Energy= 0.135933
Sum of electronic and zero-point Energies= -713.406506
Sum of electronic and thermal Energies= -713.395609
Sum of electronic and thermal Enthalpies= -713.394665
Sum of electronic and thermal Free Energies= -713.442689

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 114.842 | 39.615 | 101.076 |

Elektronisch angeregte Zustände
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 5.3292 eV 232.65 nm f=0.2888 <S**2>=0.000
38 -> 39 0.69404
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -713.382776118

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 6.0304 eV 205.60 nm f=0.0006 <S**2>=0.000
38 -> 40 0.54160
38 -> 41 0.24635
38 -> 45 -0.20466
38 -> 48 -0.21530

Excited State 3: Singlet-A 6.1263 eV 202.38 nm f=0.0058 <S**2>=0.000
37 -> 39 -0.17324
38 -> 40 0.37143
38 -> 41 -0.24725
38 -> 44 -0.32624
38 -> 45 0.13990
38 -> 46 -0.14368
38 -> 47 -0.12967
38 -> 48 0.13444
38 -> 52 0.10007
38 -> 54 0.14949

Excited State 4: Singlet-A 6.2420 eV 198.63 nm f=0.0049 <S**2>=0.000
34 -> 39 -0.21608
37 -> 39 0.62182
38 -> 44 -0.12859

Excited State 5: Singlet-A 6.4233 eV 193.02 nm f=0.0078 <S**2>=0.000
36 -> 39 0.58685
38 -> 43 0.17313
38 -> 46 0.16163
38 -> 47 -0.23380

Excited State 6: Singlet-A 6.6156 eV 187.41 nm f=0.0017 <S**2>=0.000
34 -> 39 0.63063
37 -> 39 0.24504

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(u)M06-2X/6-311+G**

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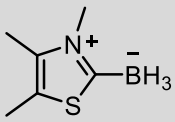
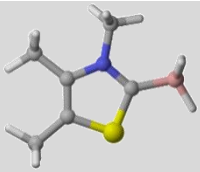
**58**



21
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -1.2334970000 | -0.5418150000 | 0.0112450000 |
| S | 0.0527600000 | -1.6680360000 | 0.0013640000 |
| C | 1.2751830000 | -0.4241020000 | -0.0029430000 |
| C | 0.6816540000 | 0.7903500000 | 0.0025650000 |
| N | -0.7176190000 | 0.6889550000 | 0.0180360000 |
| C | -1.5884670000 | 1.8635740000 | -0.0085970000 |
| B | -2.7809470000 | -0.9504420000 | -0.0072190000 |
| C | 2.7303170000 | -0.7708900000 | -0.0068590000 |
| C | 1.3209030000 | 2.1409170000 | 0.0018990000 |
| H | -1.2098290000 | 2.6152620000 | 0.6825130000 |
| H | -2.5832500000 | 1.5458720000 | 0.2917820000 |
| H | -1.6282520000 | 2.2737090000 | -1.0192760000 |
| H | -3.2621570000 | -0.4312670000 | -0.9974970000 |
| H | -3.2832950000 | -0.4678230000 | 0.9917020000 |

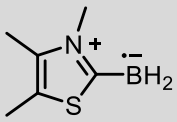
| | | | |
|---|---|---|---|
| H | -2.8632680000 | -2.1539640000 | -0.0265480000 |
| H | 0.9255560000 | 2.7622350000 | -0.8049090000 |
| H | 2.3958420000 | 2.0503580000 | -0.1394100000 |
| H | 1.1470490000 | 2.6632070000 | 0.9463620000 |
| H | 2.9883200000 | -1.3662090000 | -0.8852160000 |
| H | 2.9952570000 | -1.3498850000 | 0.8803860000 |
| H | 3.3453680000 | 0.1283990000 | -0.0157270000 |

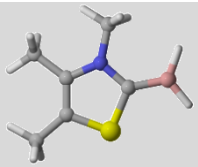
Thermochemie

Zero-point correction= 0.172592 (Hartree/Particle)
Thermal correction to Energy= 0.183249
Thermal correction to Enthalpy= 0.184193
Thermal correction to Gibbs Free Energy= 0.137423
Sum of electronic and zero-point Energies= -713.390649
Sum of electronic and thermal Energies= -713.379991
Sum of electronic and thermal Enthalpies= -713.379047
Sum of electronic and thermal Free Energies= -713.425817

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 114.991 | 39.524 | 98.436 |

**83**



20

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2526490000 | -0.6502630000 | -0.0013420000 |
| S | -0.1462910000 | -1.6935450000 | -0.0011440000 |
| C | -1.2506700000 | -0.3392120000 | 0.0002770000 |
| C | -0.5679170000 | 0.8304260000 | -0.0006540000 |
| N | 0.8109460000 | 0.6554060000 | -0.0039870000 |
| C | 1.7820990000 | 1.7370640000 | -0.0001290000 |
| B | 2.6651560000 | -1.1490100000 | 0.0034490000 |
| C | -2.7253220000 | -0.5862730000 | 0.0014600000 |
| C | -1.1487280000 | 2.2090550000 | 0.0013410000 |
| H | 1.2718970000 | 2.6956290000 | -0.0329890000 |
| H | 2.4376670000 | 1.6444850000 | -0.8678750000 |
| H | 2.3955450000 | 1.6811930000 | 0.9014510000 |
| H | 3.5759690000 | -0.3799770000 | 0.0063830000 |
| H | 2.8501450000 | -2.3252700000 | 0.0052220000 |
| H | -0.8319050000 | 2.7713150000 | 0.8833190000 |
| H | -2.2350120000 | 2.1597850000 | 0.0094480000 |
| H | -0.8451630000 | 2.7689680000 | -0.8868000000 |
| H | -3.0233890000 | -1.1591720000 | 0.8831290000 |
| H | -3.0252490000 | -1.1560580000 | -0.8816130000 |
| H | -3.2849170000 | 0.3482420000 | 0.0035870000 |

Thermochemie

Zero-point correction= 0.162632 (Hartree/Particle)
Thermal correction to Energy= 0.173213
Thermal correction to Enthalpy= 0.174157
Thermal correction to Gibbs Free Energy= 0.126241
Sum of electronic and zero-point Energies= -712.786938
Sum of electronic and thermal Energies= -712.776358
Sum of electronic and thermal Enthalpies= -712.775414
Sum of electronic and thermal Free Energies= -712.823329

| | E (Thermal) | CV | S |
|---|---|---|---|

| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 108.693 | 38.735 | 100.847 |

Elektronisch angeregte Zustände
Excitation energies and oscillator strengths:

Excited State 1: 2.174-A 3.2880 eV 377.08 nm f=0.0438 <S**2>=0.931
38A -> 42A 0.74824
38A -> 44A 0.42504
38A -> 49A -0.25189
38A -> 53A -0.21990
36B -> 38B -0.10899
37B -> 38B 0.22716
37B -> 50B 0.10181
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -712.828739312
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.056-A 3.2931 eV 376.50 nm f=0.0018 <S**2>=0.807
38A -> 39A 0.73366
38A -> 40A -0.18950
38A -> 41A -0.22675
38A -> 45A -0.39857
38A -> 48A -0.32394
38A -> 54A 0.23385

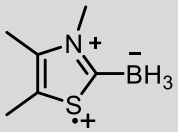
Excited State 3: 2.050-A 3.4266 eV 361.83 nm f=0.0047 <S**2>=0.801
38A -> 39A 0.53790
38A -> 40A 0.24354
38A -> 41A -0.17106
38A -> 43A 0.36580
38A -> 45A 0.39565
38A -> 48A 0.43018
38A -> 54A -0.29034
38A -> 58A 0.11579

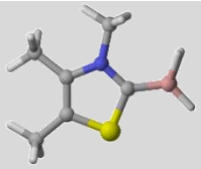
Excited State 4: 2.041-A 3.9994 eV 310.01 nm f=0.0789 <S**2>=0.791
38A -> 42A -0.20289
38A -> 49A 0.16983
38A -> 57A -0.10734
37B -> 38B 0.91823

Excited State 5: 2.151-A 4.0215 eV 308.30 nm f=0.1166 <S**2>=0.906
37A -> 42A 0.12465
38A -> 42A 0.39128
38A -> 44A -0.11761
38A -> 47A 0.48253
38A -> 49A 0.59993
38A -> 57A -0.25530
38A -> 60A 0.17728
36B -> 38B 0.13692
37B -> 38B -0.11703
37B -> 42B -0.12065

Excited State 6: 2.036-A 4.0418 eV 306.76 nm f=0.0011 <S**2>=0.787
38A -> 39A 0.18484
38A -> 40A 0.80452
38A -> 41A 0.31719
38A -> 43A -0.40043

**76**



21

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.1924410000 | -0.5880790000 | 0.0000750000 |
| S | -0.1252370000 | -1.6697000000 | -0.0000660000 |
| C | -1.2763880000 | -0.3883870000 | -0.0001270000 |
| C | -0.6384870000 | 0.8216710000 | -0.0000280000 |
| N | 0.7428240000 | 0.6782120000 | 0.0000260000 |
| C | 1.6776080000 | 1.8094070000 | -0.0002330000 |
| B | 2.6251360000 | -1.1164070000 | 0.0002130000 |
| C | -2.7411650000 | -0.6908070000 | 0.0000060000 |
| C | -1.2669610000 | 2.1766060000 | 0.0001810000 |
| H | 1.1236160000 | 2.7418680000 | 0.0000660000 |
| H | 2.2975680000 | 1.7686660000 | -0.8969410000 |
| H | 2.2982650000 | 1.7684260000 | 0.8959610000 |
| H | 3.4994890000 | -0.2956000000 | 0.4900030000 |
| H | 3.4995290000 | -0.2956990000 | -0.4896360000 |
| H | 2.9516500000 | -2.2428470000 | 0.0001890000 |
| H | -0.9818080000 | 2.7451170000 | 0.8882060000 |
| H | -2.3498030000 | 2.0844870000 | 0.0006650000 |
| H | -0.9824380000 | 2.7452170000 | -0.8879760000 |
| H | -3.0170070000 | -1.2651550000 | 0.8863260000 |
| H | -3.0156150000 | -1.2727320000 | -0.8817700000 |
| H | -3.3273740000 | 0.2255420000 | -0.0045290000 |

Thermochemie

Zero-point correction= 0.170823 (Hartree/Particle)
Thermal correction to Energy= 0.181600
Thermal correction to Enthalpy= 0.182544
Thermal correction to Gibbs Free Energy= 0.134725
Sum of electronic and zero-point Energies= -713.096327
Sum of electronic and thermal Energies= -713.085550
Sum of electronic and thermal Enthalpies= -713.084606
Sum of electronic and thermal Free Energies= -713.132425

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 113.956 | 40.314 | 100.643 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: 2.238-A 2.8330 eV 437.64 nm f=0.0373 <S**2>=1.002
38A -> 39A -0.38506
31B -> 38B -0.10883
37B -> 38B 0.89997
37B -> 39B -0.13427
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -713.163038258
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.406-A 3.7965 eV 326.57 nm f=0.0105 <S**2>=1.198
36A -> 39A 0.24038
38A -> 39A -0.12800
36B -> 38B 0.92481
36B -> 39B -0.20751

| | | | | | |
|---|---|---|---|---|---|
| Excited State | 3: | 2.125-A | 4.1620 eV | 297.90 nm | f=0.2991 <S**2>=0.878 |
| 38A -> 39A | | 0.89516 | | | |
| 36B -> 38B | | 0.12862 | | | |
| 37B -> 38B | | 0.38161 | | | |
| Excited State | 4: | 3.043-A | 4.9359 eV | 251.19 nm | f=0.0155 <S**2>=2.065 |
| 37A -> 39A | | -0.38568 | | | |
| 37A -> 42A | | 0.24947 | | | |
| 38A -> 39A | | 0.10346 | | | |
| 38A -> 42A | | 0.63200 | | | |
| 37B -> 39B | | -0.45307 | | | |
| 37B -> 42B | | 0.34799 | | | |
| Excited State | 5: | 2.032-A | 5.0287 eV | 246.55 nm | f=0.0017 <S**2>=0.782 |
| 30B -> 38B | | -0.12601 | | | |
| 32B -> 38B | | -0.16595 | | | |
| 34B -> 38B | | 0.91149 | | | |
| 34B -> 39B | | 0.13644 | | | |
| 35B -> 38B | | -0.22217 | | | |
| Excited State | 6: | 3.193-A | 5.4543 eV | 227.32 nm | f=0.0067 <S**2>=2.300 |
| 31A -> 39A | | 0.11375 | | | |
| 36A -> 39A | | -0.14867 | | | |
| 37A -> 39A | | 0.52200 | | | |
| 37A -> 42A | | 0.23236 | | | |
| 38A -> 42A | | 0.43895 | | | |
| 31B -> 39B | | -0.10981 | | | |
| 37B -> 38B | | 0.12380 | | | |
| 37B -> 39B | | 0.53265 | | | |
| 37B -> 42B | | 0.31281 | | | |

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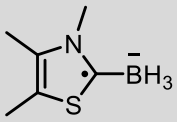
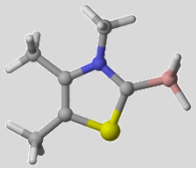


21

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2798430000 | -0.5197920000 | 0.1703540000 |
| S | -0.0321680000 | -1.7053030000 | -0.0054270000 |
| C | -1.2665980000 | -0.4325750000 | 0.0556740000 |
| C | -0.6847470000 | 0.7826070000 | -0.0339820000 |
| N | 0.6992040000 | 0.7403670000 | -0.1329290000 |
| C | 1.5202290000 | 1.9018820000 | 0.1260260000 |
| B | 2.8273930000 | -0.8851340000 | -0.0937760000 |
| C | -2.7128020000 | -0.8024400000 | 0.0349600000 |
| C | -1.3800240000 | 2.1091580000 | -0.0812940000 |
| H | 1.0987310000 | 2.7867380000 | -0.3540050000 |
| H | 2.5121670000 | 1.7076640000 | -0.2797440000 |
| H | 1.6267530000 | 2.0870380000 | 1.2073850000 |
| H | 3.5621520000 | -0.2160600000 | 0.6317470000 |
| H | 3.1145020000 | -0.6382460000 | -1.2742400000 |
| H | 2.9987200000 | -2.0740720000 | 0.1323690000 |
| H | -1.0782760000 | 2.7473500000 | 0.7551910000 |
| H | -2.4607440000 | 1.9807600000 | -0.0372330000 |
| H | -1.1375920000 | 2.6415500000 | -1.0069300000 |
| H | -2.9825360000 | -1.3996300000 | 0.9122130000 |
| H | -2.9483000000 | -1.4071170000 | -0.8502180000 |
| H | -3.3576870000 | 0.0789280000 | 0.0192490000 |

Thermochemie

Zero-point correction= 0.168218 (Hartree/Particle)
Thermal correction to Energy= 0.179430
Thermal correction to Enthalpy= 0.180374
Thermal correction to Gibbs Free Energy= 0.131578
Sum of electronic and zero-point Energies= -713.383161
Sum of electronic and thermal Energies= -713.371949
Sum of electronic and thermal Enthalpies= -713.371005
Sum of electronic and thermal Free Energies= -713.419801

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 112.594 | 40.841 | 102.700 |

Elektronisch angeregte Zustände
Excitation energies and oscillator strengths:

Excited State 1: 2.051-A 1.0790 eV 1149.07 nm f=0.0027 <S**2>=0.802
39A -> 40A 0.97894
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -713.511726514
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.049-A 1.4137 eV 876.99 nm f=0.0065 <S**2>=0.799
39A -> 41A 0.95982
39A -> 42A -0.11810
39A -> 44A 0.15572

Excited State 3: 2.057-A 1.7495 eV 708.68 nm f=0.0030 <S**2>=0.808
39A -> 40A -0.14270
39A -> 42A 0.78553
39A -> 43A 0.12273
39A -> 44A 0.26642
39A -> 45A 0.27418
39A -> 48A -0.12104
39A -> 49A -0.12052
39A -> 50A 0.14137
39A -> 55A -0.27483
39A -> 56A 0.15205
39A -> 58A 0.11783

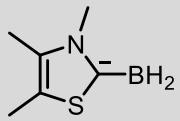
Excited State 4: 2.057-A 1.9056 eV 650.63 nm f=0.0006 <S**2>=0.808
39A -> 41A -0.23830
39A -> 42A -0.49046
39A -> 44A 0.50408
39A -> 46A 0.13853
39A -> 48A -0.27496
39A -> 50A 0.18790
39A -> 51A 0.19695
39A -> 55A -0.26107
39A -> 56A 0.23778
39A -> 58A 0.29806

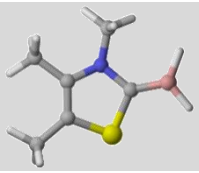
Excited State 5: 2.082-A 2.0225 eV 613.02 nm f=0.0191 <S**2>=0.834
39A -> 42A -0.29118
39A -> 44A -0.12383
39A -> 45A 0.58559
39A -> 46A 0.29806
39A -> 48A 0.24115
39A -> 49A -0.28769
39A -> 51A -0.14218
39A -> 52A 0.25257
39A -> 54A -0.12812

39A -> 55A -0.28117
39A -> 57A -0.17788
39A -> 58A -0.24316

Excited State 6: 2.053-A 2.1455 eV 577.87 nm f=0.0092 <S**2>=0.803
39A -> 43A 0.96897
39A -> 47A 0.12980

**78**



20
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2822720000 | -0.6762110000 | -0.0271930000 |
| S | -0.1790950000 | -1.7154880000 | -0.2114610000 |
| C | -1.2373470000 | -0.3156690000 | 0.0810500000 |
| C | -0.5385740000 | 0.8285850000 | -0.0322520000 |
| N | 0.8194810000 | 0.6604830000 | -0.3399900000 |
| C | 1.7611560000 | 1.7014060000 | -0.0095390000 |
| B | 2.5953810000 | -1.1398040000 | 0.3797650000 |
| C | -2.7081490000 | -0.5272460000 | 0.2242360000 |
| C | -1.0948220000 | 2.2180090000 | 0.0382030000 |
| H | 1.3746750000 | 2.6798230000 | -0.3004700000 |
| H | 2.6878000000 | 1.5104790000 | -0.5524360000 |
| H | 2.0088200000 | 1.6963280000 | 1.0664360000 |
| H | 3.5437590000 | -0.3942640000 | 0.4388620000 |
| H | 2.7550910000 | -2.3072510000 | 0.6367920000 |
| H | -0.6525040000 | 2.7873720000 | 0.8616730000 |
| H | -2.1745200000 | 2.1983390000 | 0.1812050000 |
| H | -0.8818520000 | 2.7615130000 | -0.8892620000 |
| H | -2.9380220000 | -1.1212150000 | 1.1150720000 |
| H | -3.1046240000 | -1.0770390000 | -0.6390860000 |
| H | -3.2535990000 | 0.4161170000 | 0.2986620000 |

Thermochemie
Zero-point correction= 0.160790 (Hartree/Particle)
Thermal correction to Energy= 0.171036
Thermal correction to Enthalpy= 0.171980
Thermal correction to Gibbs Free Energy= 0.126082
Sum of electronic and zero-point Energies= -712.811274
Sum of electronic and thermal Energies= -712.801027
Sum of electronic and thermal Enthalpies= -712.800083
Sum of electronic and thermal Free Energies= -712.845981

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 107.327 | 38.710 | 96.601 |

Elektronisch angeregte Zustände
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.8402 eV 673.74 nm f=0.0029 <S**2>=0.000
38 -> 39 0.68442
38 -> 41 -0.11600
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -712.904436000
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.1923 eV 565.55 nm f=0.0064 <S**2>=0.000

38 -> 40 0.67622
38 -> 41 0.13498

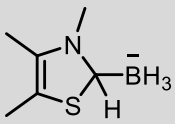
Excited State 3: Singlet-A 2.4361 eV 508.95 nm f=0.0080 <S**2>=0.000
38 -> 39 0.12934
38 -> 40 -0.10620
38 -> 41 0.63979
38 -> 43 -0.20213

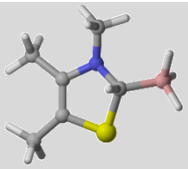
Excited State 4: Singlet-A 2.6925 eV 460.48 nm f=0.0399 <S**2>=0.000
38 -> 42 0.64905
38 -> 43 -0.12534
38 -> 46 0.10199
38 -> 47 -0.16411

Excited State 5: Singlet-A 2.7321 eV 453.80 nm f=0.0104 <S**2>=0.000
38 -> 41 0.15982
38 -> 42 0.16639
38 -> 43 0.53856
38 -> 44 -0.19045
38 -> 48 0.24406
38 -> 50 -0.10638
38 -> 55 0.10635

Excited State 6: Singlet-A 2.8648 eV 432.79 nm f=0.0037 <S**2>=0.000
38 -> 40 -0.12257
38 -> 43 0.29884
38 -> 44 0.44518
38 -> 45 0.15820
38 -> 46 0.10319
38 -> 47 -0.20576
38 -> 48 -0.18093
38 -> 55 -0.16402
38 -> 58 0.13150

**79**



22
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.2895010000 | -0.4511120000 | 0.3192270000 |
| S | 0.0098970000 | -1.7096150000 | -0.0743580000 |
| C | -1.2535640000 | -0.4600790000 | 0.0563310000 |
| C | -0.7124140000 | 0.7680370000 | -0.0490470000 |
| N | 0.6810070000 | 0.7810640000 | -0.2345440000 |
| C | 1.4205250000 | 1.9652100000 | 0.1377670000 |
| B | 2.8030370000 | -0.8364100000 | -0.1739620000 |
| C | -2.6910980000 | -0.8656760000 | 0.0885740000 |
| C | -1.4587700000 | 2.0656880000 | -0.1241830000 |
| H | 0.9948120000 | 2.8545730000 | -0.3323020000 |
| H | 2.4484430000 | 1.8411620000 | -0.2004430000 |
| H | 1.4399420000 | 2.1171230000 | 1.2341170000 |
| H | 3.5963820000 | -0.0528700000 | 0.3475330000 |
| H | 2.8769390000 | -0.7717090000 | -1.3938590000 |
| H | 3.0566250000 | -1.9691670000 | 0.2204610000 |
| H | -1.1640250000 | 2.7484500000 | 0.6787730000 |
| H | -2.5342530000 | 1.9060250000 | -0.0568980000 |
| H | -1.2456380000 | 2.5672830000 | -1.0747560000 |

| | | | |
|---|---|---|---|
| H | -2.9105120000 | -1.4701910000 | 0.9746170000 |
| H | -2.9410740000 | -1.4775750000 | -0.7867080000 |
| H | -3.3607340000 | -0.0028230000 | 0.0951640000 |
| H | 1.2374270000 | -0.3542470000 | 1.4236260000 |

Thermochemie

Zero-point correction= 0.181122 (Hartree/Particle)
Thermal correction to Energy= 0.191989
Thermal correction to Enthalpy= 0.192933
Thermal correction to Gibbs Free Energy= 0.145752
Sum of electronic and zero-point Energies= -714.010852
Sum of electronic and thermal Energies= -713.999985
Sum of electronic and thermal Enthalpies= -713.999041
Sum of electronic and thermal Free Energies= -714.046222

| | E (Thermal) | CV | S |
|---|---|---|---|
| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 120.475 | 40.734 | 99.301 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.1536 eV 393.15 nm f=0.0014 <S**2>=0.000
39 -> 40 0.68523
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -714.076081434
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.5657 eV 347.72 nm f=0.0054 <S**2>=0.000
39 -> 41 0.67960
39 -> 44 0.11388

Excited State 3: Singlet-A 3.9354 eV 315.05 nm f=0.0194 <S**2>=0.000
39 -> 42 0.60346
39 -> 44 -0.26273

Excited State 4: Singlet-A 3.9929 eV 310.51 nm f=0.0211 <S**2>=0.000
39 -> 43 0.64631
39 -> 44 -0.14610

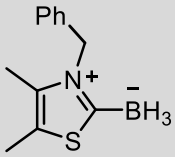
Excited State 5: Singlet-A 4.1405 eV 299.44 nm f=0.0018 <S**2>=0.000
39 -> 42 -0.19849
39 -> 43 -0.21990
39 -> 44 -0.18610
39 -> 45 0.37584
39 -> 49 0.25173
39 -> 50 -0.13361
39 -> 51 -0.10799
39 -> 55 -0.12468
39 -> 56 -0.13743
39 -> 59 -0.20565

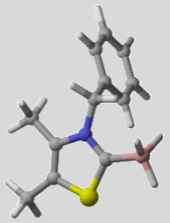
Excited State 6: Singlet-A 4.2364 eV 292.67 nm f=0.0193 <S**2>=0.000
39 -> 42 0.28728
39 -> 44 0.35469
39 -> 45 0.46492
39 -> 48 0.10538

## BnThz-$BH_3$

(u)M06-2X/6-311+G**

**59**



31

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -1.4710620000 | 1.3600530000 | -0.2413460000 |
| S | -2.8435410000 | 0.7284250000 | 0.5574150000 |
| C | -2.3732740000 | -0.9273470000 | 0.2710800000 |
| C | -1.2052170000 | -0.9546920000 | -0.4088170000 |
| N | -0.7320170000 | 0.3395300000 | -0.6822990000 |
| C | 0.5455110000 | 0.5789520000 | -1.3622570000 |
| B | -1.1684930000 | 2.9265670000 | -0.3926920000 |
| C | -3.2230120000 | -2.0605480000 | 0.7521620000 |
| C | -0.4302660000 | -2.1426710000 | -0.8798110000 |
| H | 0.5731690000 | -0.0260070000 | -2.2705600000 |
| H | 0.5423100000 | 1.6311410000 | -1.6488970000 |
| H | -1.1453110000 | 3.1607660000 | -1.5873690000 |
| H | -0.0661410000 | 3.1228980000 | 0.0840180000 |
| H | -2.0360620000 | 3.5425350000 | 0.1763790000 |
| H | -0.3497040000 | -2.1520040000 | -1.9700290000 |
| H | -0.9283430000 | -3.0606600000 | -0.5750680000 |
| H | 0.5799520000 | -2.1423000000 | -0.4643530000 |
| H | -4.1924590000 | -2.0633400000 | 0.2490970000 |
| H | -3.4024430000 | -1.9827470000 | 1.8263750000 |
| H | -2.7406680000 | -3.0185790000 | 0.5620030000 |
| C | 1.7316500000 | 0.2641410000 | -0.4782640000 |
| C | 2.8676780000 | -0.3264400000 | -1.0273350000 |
| C | 3.9773110000 | -0.5950790000 | -0.2323330000 |
| C | 3.9536970000 | -0.2806480000 | 1.1220130000 |
| C | 2.8201880000 | 0.3082270000 | 1.6745060000 |
| C | 1.7131940000 | 0.5819580000 | 0.8789900000 |
| H | 2.8844650000 | -0.5800460000 | -2.0829420000 |
| H | 4.8557080000 | -1.0544570000 | -0.6698250000 |
| H | 4.8146910000 | -0.4938480000 | 1.7442380000 |
| H | 2.7988910000 | 0.5611560000 | 2.7279530000 |
| H | 0.8367970000 | 1.0557210000 | 1.3083760000 |

Thermochemie

Zero-point correction= 0.254304 (Hartree/Particle)
Thermal correction to Energy= 0.269369
Thermal correction to Enthalpy= 0.270313
Thermal correction to Gibbs Free Energy= 0.211390
Sum of electronic and zero-point Energies= -944.324298
Sum of electronic and thermal Energies= -944.309234
Sum of electronic and thermal Enthalpies= -944.308289
Sum of electronic and thermal Free Energies= -944.367212

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 169.031 | 57.482 | 124.013 |

Elektronisch angeregte Zustände
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 5.2228 eV 237.39 nm f=0.2194 <S**2>=0.000
58 -> 59 0.66295
58 -> 61 -0.10605
58 -> 63 -0.14022
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -944.386667374
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 5.4739 eV 226.50 nm f=0.0012 <S**2>=0.000
55 -> 61 -0.13129
55 -> 62 -0.19874
56 -> 59 -0.21062
56 -> 60 -0.11857
56 -> 62 0.22318
56 -> 63 -0.23576
57 -> 59 0.10000
57 -> 61 0.38375
57 -> 62 0.18413
58 -> 61 -0.14169

Excited State 3: Singlet-A 5.6195 eV 220.63 nm f=0.0065 <S**2>=0.000
55 -> 59 0.46675
55 -> 63 -0.11934
56 -> 59 0.28716
57 -> 59 0.35032

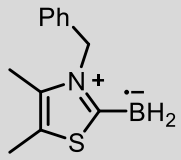
Excited State 4: Singlet-A 5.7999 eV 213.77 nm f=0.0012 <S**2>=0.000
54 -> 60 0.10686
58 -> 60 0.57673
58 -> 61 -0.16530
58 -> 62 0.11951
58 -> 65 0.14037
58 -> 68 -0.14861

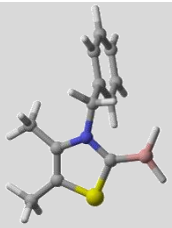
Excited State 5: Singlet-A 6.0649 eV 204.43 nm f=0.0234 <S**2>=0.000
55 -> 59 -0.10073
56 -> 61 0.12449
57 -> 59 0.11126
57 -> 62 -0.10048
58 -> 60 -0.21762
58 -> 62 0.31316
58 -> 66 -0.23209
58 -> 67 0.11883
58 -> 68 -0.17281
58 -> 70 0.24889
58 -> 73 -0.11075
58 -> 76 -0.11971

Excited State 6: Singlet-A 6.1220 eV 202.52 nm f=0.0283 <S**2>=0.000
52 -> 59 0.12808
55 -> 61 -0.10360
56 -> 61 0.22816
56 -> 62 0.14372
57 -> 59 0.24151
57 -> 60 0.14760
57 -> 62 -0.22495
57 -> 63 0.14952
58 -> 62 0.18454
58 -> 63 -0.19597

58 -> 66 0.19537
58 -> 70 -0.17553

**84**



30

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -1.3712690000 | 1.4290780000 | -0.3255170000 |
| S | -2.7961470000 | 0.9052700000 | 0.5396710000 |
| C | -2.4283850000 | -0.7866310000 | 0.2833360000 |
| C | -1.2879260000 | -0.9190630000 | -0.4320900000 |
| N | -0.7196610000 | 0.3012220000 | -0.7858330000 |
| C | 0.5759370000 | 0.3915680000 | -1.4391560000 |
| B | -0.9841070000 | 2.8704790000 | -0.4514520000 |
| C | -3.3436510000 | -1.8377310000 | 0.8230140000 |
| C | -0.6280440000 | -2.1875580000 | -0.8719860000 |
| H | 0.6147570000 | -0.3390310000 | -2.2501530000 |
| H | 0.6402240000 | 1.3821110000 | -1.8897300000 |
| H | 0.0120230000 | 3.1967330000 | -1.0183220000 |
| H | -1.7010950000 | 3.6842360000 | 0.0403310000 |
| H | -0.6562700000 | -2.2874330000 | -1.9605940000 |
| H | -1.1356290000 | -3.0486050000 | -0.4431210000 |
| H | 0.4175490000 | -2.2139360000 | -0.5541960000 |
| H | -4.3368630000 | -1.7594820000 | 0.3734810000 |
| H | -3.4594750000 | -1.7347960000 | 1.9048130000 |
| H | -2.9598250000 | -2.8367600000 | 0.6191970000 |
| C | 1.7394110000 | 0.1688710000 | -0.4924040000 |
| C | 2.9635430000 | -0.2585510000 | -1.0058740000 |
| C | 4.0540010000 | -0.4514980000 | -0.1656000000 |
| C | 3.9275070000 | -0.2234560000 | 1.2012230000 |
| C | 2.7076370000 | 0.1984510000 | 1.7184170000 |
| C | 1.6166740000 | 0.3947750000 | 0.8770390000 |
| H | 3.0630500000 | -0.4440570000 | -2.0711130000 |
| H | 4.9994750000 | -0.7860140000 | -0.5762810000 |
| H | 4.7742060000 | -0.3766560000 | 1.8595210000 |
| H | 2.6025160000 | 0.3787350000 | 2.7817690000 |
| H | 0.6692600000 | 0.7301540000 | 1.2853490000 |

Thermochemie

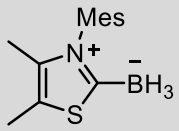
Zero-point correction= 0.244414 (Hartree/Particle)
Thermal correction to Energy= 0.259286
Thermal correction to Enthalpy= 0.260230
Thermal correction to Gibbs Free Energy= 0.198985
Sum of electronic and zero-point Energies= -943.720232
Sum of electronic and thermal Energies= -943.705360
Sum of electronic and thermal Enthalpies= -943.704416
Sum of electronic and thermal Free Energies= -943.765661

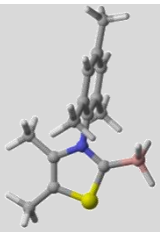
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 162.704 | 56.680 | 128.901 |

## MesThz-$BH_3$

(u)M06-2X/6-311+G**

**60**



37

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -1.3246010000 | 1.3485970000 | -0.0058600000 |
| S | -3.0156840000 | 1.0877840000 | -0.0052680000 |
| C | -2.8532580000 | -0.6515400000 | 0.0027670000 |
| C | -1.5430650000 | -0.9819900000 | 0.0047450000 |
| N | -0.7203640000 | 0.1571430000 | -0.0002340000 |
| B | -0.6306830000 | 2.7893840000 | -0.0115930000 |
| C | -4.0582980000 | -1.5380930000 | 0.0045700000 |
| C | -0.9054470000 | -2.3333310000 | 0.0099880000 |
| H | 0.0741030000 | 2.8332990000 | -1.0020210000 |
| H | 0.0708110000 | 2.8424890000 | 0.9807420000 |
| H | -1.4958880000 | 3.6324620000 | -0.0168620000 |
| H | -0.2813030000 | -2.4719360000 | -0.8765660000 |
| H | -1.6647200000 | -3.1127070000 | 0.0268260000 |
| H | -0.2598940000 | -2.4545720000 | 0.8834910000 |
| H | -4.6675880000 | -1.3696250000 | -0.8860280000 |
| H | -4.6828020000 | -1.3454970000 | 0.8795060000 |
| H | -3.7679860000 | -2.5881240000 | 0.0212870000 |
| C | 0.7187000000 | 0.0504080000 | 0.0007780000 |
| C | 1.3800270000 | -0.0100720000 | -1.2239410000 |
| C | 2.7660120000 | -0.1368000000 | -1.1982540000 |
| C | 3.4724760000 | -0.1923450000 | 0.0028130000 |
| C | 2.7660210000 | -0.1254510000 | 1.2019600000 |
| C | 1.3787760000 | 0.0013230000 | 1.2253970000 |
| C | 0.6109310000 | 0.0874830000 | -2.5129760000 |
| H | 3.3074270000 | -0.1837430000 | -2.1381800000 |
| C | 4.9761860000 | -0.2858780000 | -0.0014020000 |
| H | 3.3062030000 | -0.1638080000 | 2.1427540000 |
| C | 0.6091490000 | 0.1096380000 | 2.5132330000 |
| H | 1.2746470000 | 0.0043740000 | 3.3697030000 |
| H | -0.1677120000 | -0.6577050000 | 2.5841380000 |
| H | 0.1148670000 | 1.0833620000 | 2.5709080000 |
| H | 0.1221240000 | 1.0632410000 | -2.5819300000 |
| H | -0.1702920000 | -0.6761270000 | -2.5750260000 |
| H | 1.2759100000 | -0.0314720000 | -3.3680560000 |
| H | 5.3497470000 | -0.7017460000 | 0.9352300000 |
| H | 5.4180900000 | 0.7064610000 | -0.1263950000 |
| H | 5.3295170000 | -0.9117970000 | -0.8225350000 |

Thermochemie

| | |
|---|---|
| Zero-point correction= | 0.307167 (Hartree/Particle) |
| Thermal correction to Energy= | 0.326542 |
| Thermal correction to Enthalpy= | 0.327486 |
| Thermal correction to Gibbs Free Energy= | 0.259377 |
| Sum of electronic and zero-point Energies= | -1022.889437 |
| Sum of electronic and thermal Energies= | -1022.870062 |
| Sum of electronic and thermal Enthalpies= | -1022.869118 |

Sum of electronic and thermal Free Energies= -1022.937227

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 204.908 | 71.231 | 143.348 |

Elektronisch angeregte Zustände
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 5.1894 eV 238.92 nm f=0.2052 <S**2>=0.000
66 -> 67 0.68329
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1023.00589915
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 5.3233 eV 232.91 nm f=0.0029 <S**2>=0.000
64 -> 69 0.42101
64 -> 71 0.20926
64 -> 73 0.10834
65 -> 67 -0.12674
65 -> 70 0.37655
65 -> 72 0.19347
66 -> 69 -0.10208

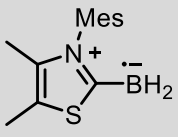
Excited State 3: Singlet-A 5.5257 eV 224.38 nm f=0.0024 <S**2>=0.000
63 -> 67 0.58653
65 -> 67 -0.32044

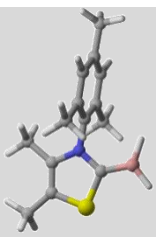
Excited State 4: Singlet-A 5.6596 eV 219.07 nm f=0.0000 <S**2>=0.000
66 -> 68 0.45460
66 -> 69 -0.38022
66 -> 71 -0.10448
66 -> 76 -0.20569
66 -> 85 0.11711

Excited State 5: Singlet-A 5.9510 eV 208.34 nm f=0.0076 <S**2>=0.000
63 -> 67 0.31369
65 -> 67 0.56392
65 -> 69 0.11998

Excited State 6: Singlet-A 5.9637 eV 207.90 nm f=0.0319 <S**2>=0.000
64 -> 67 0.16946
64 -> 70 -0.29937
64 -> 72 -0.13651
65 -> 67 -0.13242
65 -> 69 0.45086
65 -> 71 0.18474
66 -> 68 -0.11104
66 -> 70 0.10619

**85**



36
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -1.3405590000 | 1.3991310000 | -0.0016920000 |
| S | -3.0622700000 | 1.1083360000 | -0.0026210000 |

| | | | |
|---|---|---|---|
| C | -2.8530210000 | -0.6318060000 | 0.0003740000 |
| C | -1.5382320000 | -0.9487310000 | 0.0018260000 |
| N | -0.7099280000 | 0.1701920000 | 0.0007320000 |
| B | -0.7113220000 | 2.7585610000 | -0.0031660000 |
| C | -4.0499870000 | -1.5271380000 | 0.0001200000 |
| C | -0.9089870000 | -2.3052900000 | 0.0040330000 |
| H | 0.4764760000 | 2.8575500000 | -0.0023500000 |
| H | -1.4247470000 | 3.7122240000 | -0.0051180000 |
| H | -0.2759860000 | -2.4406190000 | -0.8770350000 |
| H | -1.6702170000 | -3.0825570000 | 0.0083970000 |
| H | -0.2712110000 | -2.4353590000 | 0.8823920000 |
| H | -4.6668480000 | -1.3538970000 | -0.8853040000 |
| H | -4.6730430000 | -1.3460600000 | 0.8795810000 |
| H | -3.7552940000 | -2.5761630000 | 0.0057640000 |
| C | 0.7203540000 | 0.0641880000 | 0.0012700000 |
| C | 1.3907450000 | 0.0148820000 | -1.2212930000 |
| C | 2.7776110000 | -0.1050380000 | -1.1983840000 |
| C | 3.4855800000 | -0.1631470000 | 0.0017430000 |
| C | 2.7782770000 | -0.1017210000 | 1.2006060000 |
| C | 1.3900290000 | 0.0182820000 | 1.2228920000 |
| C | 0.6215930000 | 0.1144730000 | -2.5106400000 |
| H | 3.3188170000 | -0.1471560000 | -2.1389200000 |
| C | 4.9895870000 | -0.2558480000 | -0.0033810000 |
| H | 3.3186830000 | -0.1415120000 | 2.1414610000 |
| C | 0.6214620000 | 0.1211450000 | 2.5123350000 |
| H | 1.2899300000 | 0.0387470000 | 3.3691970000 |
| H | -0.1395310000 | -0.6608400000 | 2.5889100000 |
| H | 0.0995870000 | 1.0806720000 | 2.5653190000 |
| H | 0.1005080000 | 1.0742790000 | -2.5662350000 |
| H | -0.1400750000 | -0.6671120000 | -2.5844350000 |
| H | 1.2896650000 | 0.0289230000 | -3.3675010000 |
| H | 5.3638240000 | -0.6673550000 | 0.9349620000 |
| H | 5.4330960000 | 0.7350980000 | -0.1341110000 |
| H | 5.3420830000 | -0.8866890000 | -0.8211880000 |

Thermochemie

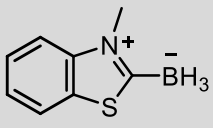
Zero-point correction= 0.297414 (Hartree/Particle)
Thermal correction to Energy= 0.316595
Thermal correction to Enthalpy= 0.317539
Thermal correction to Gibbs Free Energy= 0.248594
Sum of electronic and zero-point Energies= -1022.287472
Sum of electronic and thermal Energies= -1022.268291
Sum of electronic and thermal Enthalpies= -1022.267347
Sum of electronic and thermal Free Energies= -1022.336292

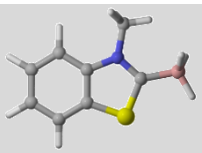
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 198.666 | 70.431 | 145.109 |

## BenzoThz-$BH_3$

(u)M06-2X/6-311+G**

**61**



21
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.7756530000 | -0.2237900000 | 0.0000940000 |
| S | 0.8677030000 | -1.6885330000 | 0.0000330000 |
| C | -0.6565650000 | -0.8336640000 | 0.0000290000 |
| C | -0.4159370000 | 0.5414800000 | 0.0000710000 |
| N | 0.9525930000 | 0.8254190000 | 0.0001720000 |
| C | 1.4432700000 | 2.2003850000 | -0.0001110000 |
| B | 3.3709450000 | -0.2053530000 | -0.0000720000 |
| H | 1.0823320000 | 2.7125000000 | -0.8933640000 |
| H | 2.5288610000 | 2.1705980000 | -0.0008300000 |
| H | 1.0835850000 | 2.7125420000 | 0.8936300000 |
| H | 3.7052390000 | 0.4121080000 | 0.9932170000 |
| H | 3.7046830000 | 0.4115040000 | -0.9939720000 |
| H | 3.7728850000 | -1.3416500000 | 0.0001420000 |
| C | -1.4644400000 | 1.4587030000 | 0.0000640000 |
| C | -2.7590600000 | 0.9619500000 | 0.0000160000 |
| C | -3.0049050000 | -0.4157130000 | -0.0000610000 |
| C | -1.9586200000 | -1.3261020000 | -0.0001120000 |
| H | -1.2749940000 | 2.5247920000 | 0.0001020000 |
| H | -3.5929180000 | 1.6526500000 | -0.0000050000 |
| H | -4.0257500000 | -0.7766880000 | -0.0001470000 |
| H | -2.1464210000 | -2.3925000000 | -0.0000890000 |

Thermochemie

Zero-point correction= 0.163264 (Hartree/Particle)
Thermal correction to Energy= 0.173486
Thermal correction to Enthalpy= 0.174430
Thermal correction to Gibbs Free Energy= 0.127517
Sum of electronic and zero-point Energies= -788.408643
Sum of electronic and thermal Energies= -788.398421
Sum of electronic and thermal Enthalpies= -788.397476
Sum of electronic and thermal Free Energies= -788.444389

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 108.864 | 39.544 | 98.736 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 4.9718 eV 249.38 nm f=0.2211 <S**2>=0.000
40 -> 44 0.10141
42 -> 45 0.23466
43 -> 44 0.63244
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -788.389197913
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 5.4015 eV 229.54 nm f=0.0826 <S**2>=0.000
42 -> 44 0.54967
42 -> 45 0.10627
43 -> 44 -0.11474
43 -> 45 -0.37574

Excited State 3: Singlet-A 5.4059 eV 229.35 nm f=0.0038 <S**2>=0.000
41 -> 44 0.62085
41 -> 45 0.19259
41 -> 49 0.25410

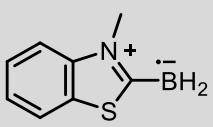
Excited State 4: Singlet-A 5.7218 eV 216.69 nm f=0.2400 <S**2>=0.000
40 -> 44 0.27268

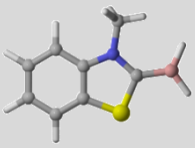
42 -> 44 -0.27510
42 -> 45 0.37029
42 -> 49 -0.10833
43 -> 44 -0.16422
43 -> 45 -0.17805
43 -> 49 -0.34234

Excited State 5: Singlet-A 5.9626 eV 207.94 nm f=0.0029 <S**2>=0.000
39 -> 44 0.41853
39 -> 45 0.13733
39 -> 49 0.19660
42 -> 46 0.11219
42 -> 47 0.14408
42 -> 50 0.13592
42 -> 54 -0.12176
43 -> 46 0.16565
43 -> 47 0.20421
43 -> 50 0.17907
43 -> 54 -0.16041

Excited State 6: Singlet-A 6.0210 eV 205.92 nm f=0.0019 <S**2>=0.000
39 -> 44 0.42306
39 -> 45 0.13583
39 -> 49 0.19938
42 -> 46 -0.12126
42 -> 47 -0.15146
42 -> 50 -0.13259
42 -> 54 0.11525
43 -> 46 -0.20490
43 -> 47 -0.19447
43 -> 50 -0.16427
43 -> 54 0.15928

**86**



20
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 1.8519540000 | -0.2071920000 | -0.0000010000 |
| S | 0.9244350000 | -1.6983010000 | 0.0000010000 |
| C | -0.5942530000 | -0.8342040000 | 0.0000000000 |
| C | -0.3629090000 | 0.5487360000 | -0.0000040000 |
| N | 0.9832730000 | 0.8633940000 | -0.0000060000 |
| C | 1.4231520000 | 2.2467510000 | 0.0000090000 |
| B | 3.3519760000 | -0.2252560000 | -0.0000020000 |
| H | 1.0494620000 | 2.7561980000 | -0.8913710000 |
| H | 2.5077610000 | 2.2701230000 | 0.0000180000 |
| H | 1.0494480000 | 2.7561820000 | 0.8913930000 |
| H | 3.9882070000 | 0.7806330000 | -0.0000120000 |
| H | 3.8901640000 | -1.2865620000 | -0.0000010000 |
| C | -1.4321140000 | 1.4455660000 | -0.0000050000 |
| C | -2.7234360000 | 0.9316530000 | -0.0000020000 |
| C | -2.9528030000 | -0.4448970000 | 0.0000020000 |
| C | -1.8873680000 | -1.3396270000 | 0.0000030000 |
| H | -1.2612680000 | 2.5146290000 | -0.0000080000 |
| H | -3.5641330000 | 1.6143720000 | -0.0000030000 |
| H | -3.9675970000 | -0.8220810000 | 0.0000040000 |
| H | -2.0591310000 | -2.4088820000 | 0.0000060000 |

Thermochemie

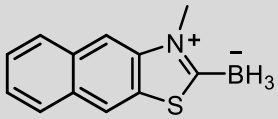
| | |
|---|---|
| Zero-point correction= | 0.154038 (Hartree/Particle) |
| Thermal correction to Energy= | 0.163887 |
| Thermal correction to Enthalpy= | 0.164831 |
| Thermal correction to Gibbs Free Energy= | 0.118262 |
| Sum of electronic and zero-point Energies= | -787.807586 |
| Sum of electronic and thermal Energies= | -787.797737 |
| Sum of electronic and thermal Enthalpies= | -787.796793 |
| Sum of electronic and thermal Free Energies= | -787.843362 |

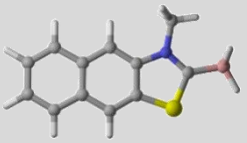
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 102.841 | 38.552 | 98.013 |

## NaphthoThz-$BH_3$

(u)M06-2X/6-311+G**

**62**



27

XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 2.9204700000 | -0.1067700000 | -0.0000310000 |
| S | 2.1525690000 | -1.6530470000 | -0.0000210000 |
| C | 0.5497470000 | -0.9414090000 | -0.0000050000 |
| C | 0.6675330000 | 0.4698650000 | -0.0000090000 |
| N | 2.0110850000 | 0.8666290000 | -0.0000240000 |
| C | 2.3787280000 | 2.2785280000 | -0.0000290000 |
| B | 4.5055300000 | 0.0499800000 | -0.0000450000 |
| H | 1.9732010000 | 2.7565630000 | -0.8931850000 |
| H | 3.4624280000 | 2.3460410000 | -0.0000420000 |
| H | 1.9732230000 | 2.7565630000 | 0.8931380000 |
| H | 4.7827530000 | 0.6964190000 | 0.9926260000 |
| H | 4.7827390000 | 0.6964240000 | -0.9927160000 |
| H | 5.0071500000 | -1.0455280000 | -0.0000510000 |
| C | -0.4367380000 | 1.2827780000 | 0.0000020000 |
| C | -1.7189890000 | 0.6857360000 | 0.0000170000 |
| C | -1.8424750000 | -0.7363530000 | 0.0000200000 |
| C | -0.6804690000 | -1.5437500000 | 0.0000090000 |
| H | -0.3452360000 | 2.3625940000 | -0.0000010000 |
| C | -2.9014120000 | 1.4757170000 | 0.0000280000 |
| C | -3.1424060000 | -1.3129480000 | 0.0000360000 |
| H | -0.7770350000 | -2.6233280000 | 0.0000130000 |
| C | -4.1355590000 | 0.8887650000 | 0.0000430000 |
| C | -4.2582260000 | -0.5239600000 | 0.0000460000 |
| H | -2.8047990000 | 2.5558950000 | 0.0000250000 |
| H | -5.0282070000 | 1.5024320000 | 0.0000510000 |
| H | -5.2430000000 | -0.9750310000 | 0.0000580000 |
| H | -3.2307900000 | -2.3937900000 | 0.0000380000 |

Thermochemie

| | |
|---|---|
| Zero-point correction= | 0.210265 (Hartree/Particle) |
| Thermal correction to Energy= | 0.223067 |
| Thermal correction to Enthalpy= | 0.224011 |
| Thermal correction to Gibbs Free Energy= | 0.171475 |

Sum of electronic and zero-point Energies= -941.976416
Sum of electronic and thermal Energies= -941.963615
Sum of electronic and thermal Enthalpies= -941.962671
Sum of electronic and thermal Free Energies= -942.015207

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 139.977 | 51.368 | 110.572 |

Elektronisch angeregte Zustände
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 4.2762 eV 289.94 nm f=0.0806 <S**2>=0.000
55 -> 58 -0.12059
56 -> 57 0.67796
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -942.029446364
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.4005 eV 281.75 nm f=0.1006 <S**2>=0.000
53 -> 57 0.16119
55 -> 57 0.54190
56 -> 57 -0.12518
56 -> 58 0.36827
56 -> 61 0.10475

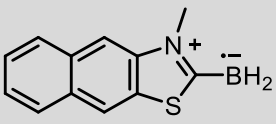
Excited State 3: Singlet-A 5.2042 eV 238.24 nm f=1.1219 <S**2>=0.000
53 -> 57 0.22506
55 -> 57 -0.38073
55 -> 58 -0.20991
55 -> 61 0.19141
56 -> 58 0.43930

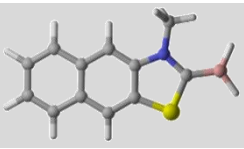
Excited State 4: Singlet-A 5.2292 eV 237.10 nm f=0.0035 <S**2>=0.000
54 -> 57 0.58496
54 -> 58 0.23631
54 -> 61 -0.26813
54 -> 63 -0.13523

Excited State 5: Singlet-A 5.5763 eV 222.34 nm f=0.0145 <S**2>=0.000
52 -> 57 -0.33251
53 -> 57 0.11604
55 -> 58 -0.11087
56 -> 58 -0.22620
56 -> 61 0.52201

Excited State 6: Singlet-A 5.6567 eV 219.18 nm f=0.0004 <S**2>=0.000
52 -> 64 0.10556
55 -> 60 0.11892
55 -> 64 0.12486
56 -> 59 -0.34944
56 -> 60 0.39078
56 -> 62 -0.10696
56 -> 64 0.23289
56 -> 68 0.17965





26
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | -2.9935230000 | -0.0890800000 | 0.0000950000 |
| S | -2.1985990000 | -1.6552560000 | -0.0001160000 |
| C | -0.6074790000 | -0.9290620000 | -0.0002090000 |
| C | -0.7224640000 | 0.4893010000 | -0.0002370000 |
| N | -2.0424620000 | 0.9047190000 | -0.0004560000 |
| C | -2.3648880000 | 2.3199020000 | -0.0003310000 |
| B | -4.4912990000 | 0.0177420000 | 0.0009060000 |
| H | -1.9496050000 | 2.7935200000 | 0.8927030000 |
| H | -3.4433310000 | 2.4366120000 | -0.0040430000 |
| H | -1.9434200000 | 2.7947450000 | -0.8897730000 |
| H | -5.0415360000 | 1.0729550000 | 0.0012770000 |
| H | -5.1154190000 | -0.9948720000 | 0.0012290000 |
| C | 0.3965730000 | 1.2880160000 | -0.0000040000 |
| C | 1.6769470000 | 0.6812320000 | 0.0000390000 |
| C | 1.7910750000 | -0.7396830000 | -0.0000650000 |
| C | 0.6173650000 | -1.5370490000 | -0.0001530000 |
| H | 0.3173190000 | 2.3685590000 | 0.0002680000 |
| C | 2.8642620000 | 1.4600340000 | 0.0002000000 |
| C | 3.0830200000 | -1.3259260000 | -0.0000050000 |
| H | 0.7049000000 | -2.6175420000 | -0.0001220000 |
| C | 4.0968910000 | 0.8638320000 | 0.0002390000 |
| C | 4.2089930000 | -0.5466150000 | 0.0001390000 |
| H | 2.7765250000 | 2.5412010000 | 0.0002730000 |
| H | 4.9933740000 | 1.4724100000 | 0.0003400000 |
| H | 5.1895360000 | -1.0069290000 | 0.0001800000 |
| H | 3.1623390000 | -2.4077290000 | -0.0000740000 |

Thermochemie

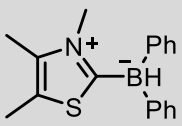
| | |
|---|---|
| Zero-point correction= | 0.200429 (Hartree/Particle) |
| Thermal correction to Energy= | 0.213009 |
| Thermal correction to Enthalpy= | 0.213953 |
| Thermal correction to Gibbs Free Energy= | 0.161074 |
| Sum of electronic and zero-point Energies= | -941.377622 |
| Sum of electronic and thermal Energies= | -941.365042 |
| Sum of electronic and thermal Enthalpies= | -941.364098 |
| Sum of electronic and thermal Free Energies= | -941.416978 |

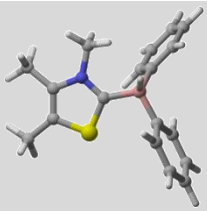
| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 133.665 | 50.518 | 111.295 |

## Thz-BHPh$_2$

(u)M06-2X/6-311+G**

**63**



41
XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 0.8254870000 | -0.1923800000 | -0.4675860000 |
| S | 1.3229580000 | -1.5769990000 | 0.3980720000 |

| | | | |
|---|---|---|---|
| C | 2.9753600000 | -1.0367970000 | 0.4826930000 |
| C | 3.0992490000 | 0.1593250000 | -0.1383840000 |
| N | 1.8782520000 | 0.5998440000 | -0.6655350000 |
| C | 1.7429450000 | 1.8863610000 | -1.3552740000 |
| C | 4.0232660000 | -1.8708910000 | 1.1502060000 |
| C | 4.3278890000 | 0.9923670000 | -0.3104020000 |
| H | 2.6287420000 | 2.0640180000 | -1.9621550000 |
| H | 1.6143600000 | 2.6845820000 | -0.6221010000 |
| H | 0.8591240000 | 1.8424460000 | -1.9859190000 |
| B | -0.7118750000 | 0.0973800000 | -0.9109110000 |
| H | -0.6725680000 | 0.1995450000 | -2.1265800000 |
| C | -1.6106160000 | -1.1785610000 | -0.4794110000 |
| C | -2.3807220000 | -1.2047670000 | 0.6901490000 |
| C | -3.0995160000 | -2.3368350000 | 1.0701080000 |
| C | -3.0670830000 | -3.4825330000 | 0.2821950000 |
| C | -2.3151530000 | -3.4831200000 | -0.8897150000 |
| C | -1.6032830000 | -2.3455990000 | -1.2579150000 |
| H | -2.4273500000 | -0.3158890000 | 1.3128110000 |
| H | -3.6904840000 | -2.3229150000 | 1.9797120000 |
| H | -3.6288480000 | -4.3633020000 | 0.5724680000 |
| H | -2.2920080000 | -4.3670720000 | -1.5182490000 |
| H | -1.0285100000 | -2.3562080000 | -2.1806770000 |
| C | -1.1681210000 | 1.5051310000 | -0.2480980000 |
| C | -2.0293960000 | 2.3647520000 | -0.9426880000 |
| C | -2.4565950000 | 3.5744250000 | -0.4031000000 |
| C | -2.0267860000 | 3.9660020000 | 0.8619920000 |
| C | -1.1746180000 | 3.1320040000 | 1.5785150000 |
| C | -0.7567070000 | 1.9225780000 | 1.0258130000 |
| H | -2.3720190000 | 2.0726810000 | -1.9309820000 |
| H | -3.1243610000 | 4.2143550000 | -0.9699040000 |
| H | -2.3553690000 | 4.9083960000 | 1.2851930000 |
| H | -0.8388540000 | 3.4222560000 | 2.5684020000 |
| H | -0.0959050000 | 1.2841040000 | 1.6105240000 |
| H | 4.1650460000 | 2.0122430000 | 0.0451740000 |
| H | 4.6314990000 | 1.0424730000 | -1.3593000000 |
| H | 5.1531830000 | 0.5638730000 | 0.2545250000 |
| H | 4.2790180000 | -2.7401080000 | 0.5399440000 |
| H | 3.6729680000 | -2.2327920000 | 2.1183350000 |
| H | 4.9330270000 | -1.2952800000 | 1.3183230000 |

Thermochemie

Zero-point correction= 0.338514 (Hartree/Particle)
Thermal correction to Energy= 0.358617
Thermal correction to Enthalpy= 0.359561
Thermal correction to Gibbs Free Energy= 0.286900
Sum of electronic and zero-point Energies= -1175.275967
Sum of electronic and thermal Energies= -1175.255864
Sum of electronic and thermal Enthalpies= -1175.254919
Sum of electronic and thermal Free Energies= -1175.327581

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 225.036 | 76.413 | 152.929 |

Elektronisch angeregte Zustände

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 4.7240 eV 262.46 nm f=0.0294 <S**2>=0.000
77 -> 79 -0.12140
78 -> 79 0.66159
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1175.44087770

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.9777 eV 249.08 nm f=0.0518 <S**2>=0.000
71 -> 79 -0.11022
76 -> 79 0.19757
77 -> 79 0.62630
78 -> 79 0.11186

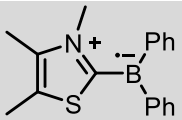
Excited State 3: Singlet-A 5.3002 eV 233.92 nm f=0.0612 <S**2>=0.000
74 -> 79 0.36885
76 -> 79 0.51674
77 -> 79 -0.17518
78 -> 79 -0.11046

Excited State 4: Singlet-A 5.3586 eV 231.38 nm f=0.0095 <S**2>=0.000
75 -> 79 0.11178
75 -> 86 0.11148
75 -> 88 -0.14625
75 -> 90 0.14631
75 -> 92 0.10469
76 -> 79 -0.12609
76 -> 93 -0.12397
77 -> 84 -0.12569
77 -> 89 0.24570
77 -> 94 -0.12410
78 -> 84 -0.18518
78 -> 85 -0.20622
78 -> 89 0.25263

Excited State 5: Singlet-A 5.3908 eV 229.99 nm f=0.0072 <S**2>=0.000
74 -> 79 0.18336
76 -> 89 0.17217
76 -> 93 0.21864
77 -> 84 -0.10683
77 -> 85 -0.14328
77 -> 89 0.12923
77 -> 93 -0.10555
78 -> 80 -0.10143
78 -> 85 0.17078
78 -> 94 -0.23434
78 -> 96 0.21472

Excited State 6: Singlet-A 5.5212 eV 224.56 nm f=0.0973 <S**2>=0.000
74 -> 79 0.47267
76 -> 79 -0.37744
78 -> 80 -0.15404

**88**

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XYZ-Matrix in Ångström

| | | | |
|---|---|---|---|
| C | 0.9132330000 | -0.1542690000 | -0.1079210000 |
| S | 1.7385590000 | -1.5854300000 | 0.4724120000 |
| C | 3.3093910000 | -0.8324030000 | 0.3234250000 |
| C | 3.1888070000 | 0.4221950000 | -0.1634550000 |
| N | 1.8701090000 | 0.7894780000 | -0.4240330000 |
| C | 1.5565340000 | 2.0002470000 | -1.1756340000 |
| C | 4.5365850000 | -1.5899300000 | 0.7170880000 |
| C | 4.2921340000 | 1.3958230000 | -0.4376230000 |

| | | | |
|---|---|---|---|
| H | 2.3224530000 | 2.1618170000 | -1.9340620000 |
| H | 1.4953820000 | 2.8752910000 | -0.5249140000 |
| H | 0.5938720000 | 1.8688970000 | -1.6633630000 |
| B | -0.5972440000 | -0.0293130000 | -0.1058250000 |
| C | -1.4853550000 | -1.3280270000 | -0.0928640000 |
| C | -2.6795300000 | -1.3674140000 | 0.6467260000 |
| C | -3.4826460000 | -2.5017990000 | 0.6770190000 |
| C | -3.1218270000 | -3.6314250000 | -0.0523410000 |
| C | -1.9534790000 | -3.6152040000 | -0.8081870000 |
| C | -1.1490740000 | -2.4808000000 | -0.8220620000 |
| H | -2.9781210000 | -0.4909610000 | 1.2134900000 |
| H | -4.3921580000 | -2.5054030000 | 1.2673760000 |
| H | -3.7490090000 | -4.5155640000 | -0.0364450000 |
| H | -1.6716690000 | -4.4860260000 | -1.3897220000 |
| H | -0.2474540000 | -2.4831400000 | -1.4267490000 |
| C | -1.2955190000 | 1.3780620000 | 0.0155740000 |
| C | -2.4835130000 | 1.6723050000 | -0.6724630000 |
| C | -3.1170310000 | 2.9033020000 | -0.5381180000 |
| C | -2.5899400000 | 3.8705710000 | 0.3135550000 |
| C | -1.4260950000 | 3.5964470000 | 1.0266760000 |
| C | -0.7905960000 | 2.3690940000 | 0.8726750000 |
| H | -2.9148510000 | 0.9185410000 | -1.3243000000 |
| H | -4.0272040000 | 3.1075700000 | -1.0908690000 |
| H | -3.0872180000 | 4.8268980000 | 0.4283320000 |
| H | -1.0205510000 | 4.3368580000 | 1.7075310000 |
| H | 0.1121190000 | 2.1612540000 | 1.4416460000 |
| H | 4.0587550000 | 2.3768870000 | -0.0179310000 |
| H | 4.4633910000 | 1.5211370000 | -1.5100740000 |
| H | 5.2207930000 | 1.0501080000 | 0.0114870000 |
| H | 4.5994160000 | -2.5337130000 | 0.1698850000 |
| H | 4.5291180000 | -1.8249580000 | 1.7843970000 |
| H | 5.4389800000 | -1.0190420000 | 0.5006180000 |

Thermochemie

Zero-point correction= 0.329147 (Hartree/Particle)
Thermal correction to Energy= 0.348898
Thermal correction to Enthalpy= 0.349842
Thermal correction to Gibbs Free Energy= 0.279386
Sum of electronic and zero-point Energies= -1174.672641
Sum of electronic and thermal Energies= -1174.652890
Sum of electronic and thermal Enthalpies= -1174.651946
Sum of electronic and thermal Free Energies= -1174.722402

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 218.937 | 75.657 | 148.287 |