checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: sw238

Bond precision: C-C = 0.0166 A Wavelength=1.54178

Cell: **a=14.5298(6) b=16.4844(5) c=18.4998(5)**
alpha=75.820(3) beta=84.986(3) gamma=88.705(3)
Temperature: 100 K

	Calculated	Reported
Volume	4279.5(3)	4279.5(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C93.40 H117 Mo8 O15.40 P8 Tl2, 2(C16 Al F36 O4)	TL C48 H60 MO4 O8 P4, C16 AL F36 O4
Sum formula	C125.40 H117 Al2 F72 Mo8 O23.40 P8 Tl2	C64 H60 AL F36 MO4 O12 P4 TL
Mr	4844.40	2444.11
Dx,g cm-3	1.880	1.897
Z	1	2
Mu (mm-1)	10.221	10.231
F000	2348.6	2372.0
F000’	2351.16	
h,k,lmax	17,19,22	17,19,21
Nref	15243	14773
Tmin,Tmax	0.377,0.809	0.510,0.860
Tmin’	0.215	

Correction method= GAUSSIAN

Data completeness= 0.969 Theta(max)= 66.930

R(reflections)= 0.0656(12262) wR2(reflections)= 0.1964(14773)

S = 1.054 Npar= 1295

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A
PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C49B

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C50B

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C51B

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C52B

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C49A

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C50A

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C51A

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C52A

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT431_ALERT_2_A Short Inter HL..A Contact F32A .. F36A .. 1.82 Ang.

Author Response: Wrongly assigned intermolecular contact between atoms of disordered fragments with occupancy < 1.

PLAT432_ALERT_2_A Short Inter X...Y Contact F34B .. C9B .. 2.01 Ang.

Author Response: The involved atoms are part of different disordered fragments with sof < 1.

PLAT432_ALERT_2_A Short Inter X...Y Contact F35B .. C8B .. 1.95 Ang.

Author Response: The involved atoms are part of different disordered fragments with sof < 1.

PLAT234_ALERT_4_A Large Hirshfeld Difference F3B -- C53B .. 0.36 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_A Large Hirshfeld Difference F6B -- C54B .. 0.39 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_A Large Hirshfeld Difference F13B -- C57B .. 0.32 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_A Large Hirshfeld Difference F28B -- C62B .. 0.31 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_A Large Hirshfeld Difference C49B -- C54B .. 0.32 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_A Large Hirshfeld Difference C51B -- C59B .. 0.33 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT780_ALERT_1_A Coordinates do not Form a Properly Connected Set ?

Author Response: Due to wrongly assigned close contacts between disordered fragments no properly connected set is identified by the checkcif routine.

Alert level B

PLAT213_ALERT_2_B Atom F8B has ADP max/min Ratio ..... 4.60 prola
PLAT213_ALERT_2_B Atom F8A has ADP max/min Ratio ..... 4.60 prola
PLAT230_ALERT_2_B Hirshfeld Test Diff for C51B -- C61B .. 7.37 su
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for C24
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for Al1B

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C58B

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for Al1A

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C58A

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT432_ALERT_2_B Short Inter X...Y Contact F34B .. C4B .. 2.72 Ang.

Author Response: The involved atoms are part of different disordered fragments with sof < 1.

PLAT432_ALERT_2_B Short Inter X...Y Contact C64B .. C8B .. 2.91 Ang.

Author Response: The involved atoms are part of different disordered fragments with sof < 1.

PLAT432_ALERT_2_B Short Inter X...Y Contact F36A .. C63A .. 2.72 Ang.

Author Response: The involved atoms are part of different disordered fragments with sof < 1.

PLAT234_ALERT_4_B Large Hirshfeld Difference C50B -- C57B .. 0.28 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_B Large Hirshfeld Difference C51B -- C60B .. 0.27 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.97
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.20
PLAT213_ALERT_2_C Atom F1B has ADP max/min Ratio ..... 3.30 prola
PLAT213_ALERT_2_C Atom F7B has ADP max/min Ratio ..... 3.10 oblat
PLAT213_ALERT_2_C Atom F1A has ADP max/min Ratio ..... 3.30 prola
PLAT213_ALERT_2_C Atom F7A has ADP max/min Ratio ..... 3.10 oblat
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.33 Ratio
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.33 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for F33B -- C63B .. 5.45 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for O11B -- C51B .. 5.32 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for C52B -- C63B .. 6.28 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Al1B -- O9B .. 7.51 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Al1B -- O10B .. 8.29 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Al1B -- O11B .. 8.25 su
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Mo1A

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Mo2A

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Mo1B

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Mo1C

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Mo2B

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C55B

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

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PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C55A
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Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others. Within the dicationic coordination complex the organic ligands show a higher thermal mobility than the heavy Mo atoms.

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PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds (x 1000) Ang ..         17
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond  C13    -   C14    ...       1.39 Ang.
PLAT430_ALERT_2_C Short Inter D...A Contact  O8     ..  O2B     ..       2.85 Ang.
PLAT432_ALERT_2_C Short Inter X...Y Contact  F34B   ..  C8B     ..       2.93 Ang.
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Author Response: The involved atoms are part of different disordered fragments with sof < 1.

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PLAT432_ALERT_2_C Short Inter X...Y Contact  O3A    ..  C44     ..       2.97 Ang.
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Author Response: The involved atoms are part of different disordered fragments with sof < 1.

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
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Author Response: One of the [Cp2Mo2(CO)4P2] ligands was found disordered over three positions. Of the third orientation with 10 % site occupancy only the Mo2P2 core tetrahedron could be refined from electron density. Therefore, there is a discrepancy between the true number of carbon, hydrogen and oxygen atoms and all related parameters (which are given in the cif file) and the number found from the atom site data.

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PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ          ?
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Author Response: One of the [Cp2Mo2(CO)4P2] ligands was found disordered over three positions. Of the third orientation with 10 % site occupancy only the Mo2P2 core tetrahedron could be refined from electron density. Therefore, there is a discrepancy between the true number of carbon, hydrogen and oxygen atoms and all related parameters (which are given in the cif file) and the number found from the atom site data.

PLAT045_ALERT_1_C Calculated and Reported Z Differ by ..... 0.50 Ratio

Author Response: Z is not found correctly by the checkcif routine due to wrongly assigned close contacts between disordered fragments.

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?

Author Response: One of the [Cp2Mo2(CO)4P2] ligands was found disordered over three positions. Of the third orientation with 10 % site occupancy only the Mo2P2 core tetrahedron could be refined from electron density. Therefore, there is a discrepancy between the true number of carbon, hydrogen and oxygen atoms and all related parameters (which are given in the cif file) and the number found from the atom site data.

PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms .. ?

Author Response: One of the [Cp2Mo2(CO)4P2] ligands was found disordered over three positions. Of the third orientation with 10 % site occupancy only the Mo2P2 core tetrahedron could be refined from electron density. Therefore, there is a discrepancy between the true number of carbon, hydrogen and oxygen atoms and all related parameters (which are given in the cif file) and the number found from the atom site data.

PLAT234_ALERT_4_C Large Hirshfeld Difference O4 -- C24 .. 0.18 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_C Large Hirshfeld Difference F17B -- C58B .. 0.24 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_C Large Hirshfeld Difference F22B -- C60B .. 0.23 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_C Large Hirshfeld Difference F27B -- C61B .. 0.22 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_C Large Hirshfeld Difference F30B -- C62B .. 0.23 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_C Large Hirshfeld Difference F32B -- C63B .. 0.23 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_C Large Hirshfeld Difference F36B -- C64B .. 0.24 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

PLAT234_ALERT_4_C Large Hirshfeld Difference C52B -- C64B .. 0.24 Ang.

Author Response: The [Al{OC(CF3)3}4]- anion shows a positional disorder with two sites for the whole molecule. In consequence, the individual disorder of parts of the anion due to rotation around O-C and C-C bonds could not be refined, but is expressed by rather large displacement parameters. Displacement parameters of the atoms at the outer parts of the ion (especially the F atoms) are thereby more affected by the thermal motion than others.

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C64 H60 Al1 F36 Mo4 O12 P4 Tl1
           Atom count from the _atom_site data:  C62.7 H58.5 Al1 F36 Mo4 O11.7
```

Author Response: One of the [Cp2Mo2(CO)4P2] ligands was found disordered over three positions. Of the third orientation with 10 % site occupancy only the Mo2P2 core tetrahedron could be refined from electron density. Therefore, there is a discrepancy between the true number of carbon, hydrogen and oxygen atoms and all related parameters (which are given in the cif file) and the number found from the atom site data.

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CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
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Author Response: One of the [Cp2Mo2(CO)4P2] ligands was found disordered over three positions. Of the third orientation with 10 % site occupancy only the Mo2P2 core tetrahedron could be refined from electron density. Therefore, there is a discrepancy between the true number of carbon, hydrogen and oxygen atoms and all related parameters (which are given in the cif file) and the number found from the atom site data. Z is not found correctly by the checkcif routine due to wrongly assigned close contacts between disordered fragments.

```
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C64 H60 Al F36 Mo4 O12 P4 Tl
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        128.00    125.40    2.60
           H        120.00    117.00    3.00
           Al         2.00      2.00    0.00
           F         72.00     72.00    0.00
           Mo         8.00      8.00    0.00
           O         24.00     23.40    0.60
           P          8.00      8.00    0.00
           Tl         2.00      2.00    0.00
```

Author Response: One of the [Cp2Mo2(CO)4P2] ligands was found disordered over three positions. Of the third orientation with 10 % site occupancy only the Mo2P2 core tetrahedron could be refined from electron density. Therefore, there is a discrepancy between the true number of carbon, hydrogen and oxygen atoms and all related parameters (which are given in the cif file) and the number found from the atom site data. Z is not found correctly by the checkcif routine due to wrongly assigned close contacts between disordered fragments.

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PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large..       0.14
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.       8.98
PLAT301_ALERT_3_G Note: Main Residue  Disorder ..................      32.00 Perc.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......       971
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal  (x 10000)       300 Deg.
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      >P2A
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.       P4
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      <P1C
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      <P2B
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      <P2C
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C9A
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C34
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C44
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       12
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....        !
```

```
  18 ALERT level A = In general: serious problem
  13 ALERT level B = Potentially serious problem
  39 ALERT level C = Check and explain
  18 ALERT level G = General alerts; check

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  49 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  26 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/08/2009; check.def file version of 12/08/2009

Datablock sw238 - ellipsoid plot