checkCIF/PLATON report

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

Datablock: sw218

Bond precision: C-C = 0.0134 A Wavelength=1.54178

Cell: **a=38.9470(7)** **b=14.3778(2)** **c=31.5972(5)**
alpha=90 **beta=113.475(2)** **gamma=90**
Temperature: **100 K**

	Calculated	Reported
Volume	16229.1(5)	16229.1(5)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C20 H30 Mo2 P4 S), C16 Al F36 O4, C H2 Cl2, Tl	2(C20 H30 Mo2 P4 S), C16 Al F36 O4, C H2 Cl2, Tl
Sum formula	C57 H62 Al Cl2 F36 Mo4 O4 P8 S2 Tl	C57 H62 Al Cl2 F36 Mo4 O4 P8 S2 Tl
Mr	2492.99	2492.99
Dx,g cm-3	2.041	2.041
Z	8	8
Mu (mm-1)	12.510	12.510
F000	9664.0	9664.0
F000’	9691.67	
h,k,lmax	46,17,37	46,16,37
Nref	14381	13971
Tmin,Tmax	0.460,0.808	0.545,0.810
Tmin’	0.057	

Correction method= MULTI-SCAN

Data completeness= 0.971 **Theta(max)= 66.700**

R(reflections)= 0.0548(9850) **wR2(reflections)= 0.1608(13971)**

S = 1.043 **Npar= 1045**

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
PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 5.06 Ratio

Author Response: Different parts of the anion are unequally affected by its strong thermal movement even at very low temperature.

```
PLAT242_ALERT_2_A Check Low       Ueq as Compared to Neighbors for        C43
```

Author Response: Different parts of the anion are unequally affected by its strong thermal movement even at very low temperature.

```
PLAT242_ALERT_2_A Check Low       Ueq as Compared to Neighbors for        C44
```

Author Response: Different parts of the anion are unequally affected by its strong thermal movement even at very low temperature.

```
PLAT307_ALERT_2_A Isolated Metal Atom (Unusual !) ...............        Tl1
```

Author Response: There are rather long coordinative bonds between the P1 and P5 atoms and Tl1, and the P3 and P7 atoms and Tl2 respectively.

```
PLAT307_ALERT_2_A Isolated Metal Atom (Unusual !) ...............        Tl2
```

Author Response: There are rather long coordinative bonds between the P1 and P5 atoms and Tl1, and the P3 and P7 atoms and Tl2 respectively.

Alert level B

```
PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       4.50 Ratio
```

Author Response: Different parts of the anion are unequally affected by its strong thermal movement even at very low temperature.

```
PLAT220_ALERT_2_B Large Non-Solvent    F     Ueq(max)/Ueq(min) ...       4.20 Ratio
```

Author Response: Different parts of the anion are unequally affected by its strong thermal movement even at very low temperature.

```
PLAT230_ALERT_2_B Hirshfeld Test Diff for    F6     --  C46     ..       8.42 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    F23    --  C52     ..       7.98 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    F27    --  C53     ..       9.46 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    F29    --  C54     ..      13.29 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    F30    --  C54     ..       7.31 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    F32    --  C55     ..       9.23 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    F33    --  C55     ..       8.59 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    F35    --  C56     ..       9.37 su
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for         O1
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        C54
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        C55
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        C56
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for        C41
```

Author Response: Different parts of the anion are unequally affected by its strong thermal movement even at very low temperature.

```
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for        C51
```

Author Response: Different parts of the anion are unequally affected by its strong thermal movement even at very low temperature.

```
PLAT413_ALERT_2_B Short Inter XH3 .. XHn     H36A   ..  H37C    ..       2.08 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference F34    --  C56     ..       0.26 Ang.
```

Alert level C

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......       0.97
PLAT213_ALERT_2_C Atom C26             has ADP max/min Ratio .....       3.20 prola
PLAT213_ALERT_2_C Atom F19             has ADP max/min Ratio .....       3.10 prola
PLAT213_ALERT_2_C Atom F26             has ADP max/min Ratio .....       3.20 prola
PLAT213_ALERT_2_C Atom F28             has ADP max/min Ratio .....       3.70 prola
PLAT213_ALERT_2_C Atom F32             has ADP max/min Ratio .....       3.80 prola
PLAT213_ALERT_2_C Atom F34             has ADP max/min Ratio .....       3.10 prola
PLAT213_ALERT_2_C Atom F35             has ADP max/min Ratio .....       3.80 prola
PLAT213_ALERT_2_C Atom C55             has ADP max/min Ratio .....       3.20 prola
PLAT222_ALERT_3_C Large Non-Solvent    H     Uiso(max)/Uso(min) ...       4.36 Rati
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F36    --  C56     ..       5.08 su
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         O3
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C46
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C53
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C22
```

Author Response: Different parts of the anion are unequally affected by its strong thermal movement even at very low temperature.

```
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Al1
```

Author Response: Different parts of the anion are unequally affected by its strong thermal movement even at very low temperature.

```
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C42
```

Author Response: Different parts of the anion are unequally affected by its strong thermal movement even at very low temperature.

```
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C47
```

Author Response: Different parts of the anion are unequally affected by its strong thermal movement even at very low temperature.

```
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.51
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds (x 1000) Ang ..         13
PLAT234_ALERT_4_C Large Hirshfeld Difference F4     --  C46     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F11    --  C48     ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F17    --  C50     ..       0.15 Ang.
```

```
PLAT234_ALERT_4_C Large Hirshfeld Difference F19    --  C51     ..       0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F22    --  C52     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F28    --  C54     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F31    --  C55     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C41    --  C45     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C42    --  C49     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C42    --  C50     ..       0.16 Ang.
```

Alert level G

```
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large.       0.10
PLAT301_ALERT_3_G Note: Main Residue  Disorder ..................       3.00 Perc.
PLAT431_ALERT_2_G Short Inter HL..A Contact  F19    ..  F24     ..      2.69 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F28    ..  C33     ..      2.94 Ang.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......       128
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.        P1
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.        P3
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.        P5
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.        P7
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety        C6
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C10
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C16
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C19
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C36
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C37
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C40
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         2
```

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  5 ALERT level A = In general: serious problem
 18 ALERT level B = Potentially serious problem
 30 ALERT level C = Check and explain
 17 ALERT level G = General alerts; check

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 42 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 ALERT type 3 Indicator that the structure quality may be low
 23 ALERT type 4 Improvement, methodology, query or suggestion
  0 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 29/06/2010; check.def file version of 26/06/2010

Datablock sw218 - ellipsoid plot