checkCIF/PLATON report

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

Datablock: sw208II

Bond precision: C-C = 0.0175 A   Wavelength=1.54178

Cell: a=18.7735(11)   b=18.7735(11)   c=10.0369(8)
               alpha=90   beta=90   gamma=120
Temperature: 100 K

	Calculated	Reported
Volume	3063.5(4)	3063.5(4)
Space group	P 63/m	P 63/m
Hall group	-P 6c	-P 6c
Moiety formula	C12 Al F27 O3, 3(C7 H5 Mo O2 P3), C4, 0.97(F4), 0.33(O3), 0.	C16 AL F36 O4, 3(C7 H5 MO O2 P3), TL
Sum formula	C37 H15 Al F36 Mo3 O10 P9 Tl	C37 H15 Al F36 Mo3 O10 P9 Tl
Mr	2101.34	2101.34
Dx,g cm-3	2.278	2.278
Z	2	2
Mu (mm-1)	13.752	13.752
F000	1992.0	1992.0
F000'	1996.63	
h,k,lmax	22,22,11	22,21,11
Nref	1834	1813
Tmin,Tmax	0.116,0.352	0.197,0.352
Tmin'	0.022	

Correction method= MULTI-SCAN

Data completeness= 0.989   Theta(max)= 64.770

R(reflections)= 0.0455(1449)   wR2(reflections)= 0.1185(1813)

S = 1.063   Npar= 261

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   Al1
PLAT307_ALERT_2_A Isolated Metal Atom (Unusual !) Tl1
PLAT431_ALERT_2_A Short Inter HL..A Contact F9A   .. F7F   ..   1.74 Ang.

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PLAT431_ALERT_2_A Short Inter HL..A Contact F9A  .. O3   ..    1.94 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F9A  .. F7A  ..    1.95 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F9A  .. F7C  ..    2.24 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F9B  .. F7F  ..    2.33 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F9C  .. F7A  ..    2.41 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7A  .. F7B  ..    1.69 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7A  .. F7A  ..    1.89 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7A  .. F7C  ..    2.14 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7A  .. F7B  ..    2.22 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7D  .. F7E  ..    2.04 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7D  .. F7E  ..    2.04 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7D  .. F7E  ..    2.11 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7D  .. F7E  ..    2.11 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7D  .. F7F  ..    2.22 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7D  .. F7F  ..    2.22 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7E  .. F7F  ..    1.69 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact F7E  .. F7F  ..    2.15 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact F9A  .. C7   ..    2.29 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact F9A  .. C6   ..    2.53 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. O3   ..    1.36 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. O3   ..    1.36 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. O3   ..    1.36 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7B  ..    1.75 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7B  ..    1.75 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7B  ..    1.75 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7E  ..    2.15 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7E  ..    2.15 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7E  ..    2.15 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7C  ..    2.38 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7C  ..    2.38 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7C  ..    2.38 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7B  ..    2.38 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7B  ..    2.38 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7B  ..    2.38 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. C6   ..    2.38 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7A  ..    2.38 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7A  ..    2.38 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7A  ..    2.38 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. C7   ..    2.42 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. C7   ..    2.42 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. C7   ..    2.42 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7E  ..    2.42 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7E  ..    2.42 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7E  ..    2.42 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7F  ..    2.44 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7F  ..    2.44 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7F  ..    2.44 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7D  ..    2.46 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7D  ..    2.46 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C6   .. F7D  ..    2.46 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C7   .. F7F  ..    1.34 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C7   .. F7B  ..    1.34 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C7   .. F7A  ..    1.34 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C7   .. F7C  ..    1.36 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C7   .. F7E  ..    1.37 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C7   .. F7D  ..    1.38 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C7   .. O3   ..    2.40 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C9A  .. F7F  ..    2.55 Ang.
PLAT780_ALERT_1_A Coordinates do not Form a Properly Connected Set       ?
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● Alert level B

REFNR01_ALERT_3_B Ratio of reflections to parameters is < 8 for a
            centrosymmetric structure
                sine(theta)/lambda   0.5867
                Proportion of unique data used   1.0000
                Ratio reflections to parameters   6.9464
PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.95
PLAT213_ALERT_2_B Atom F10A   has ADP max/min Ratio .....   4.10 prola
PLAT241_ALERT_2_B Check High   Ueq as Compared to Neighbors for   C2
PLAT242_ALERT_2_B Check Low   Ueq as Compared to Neighbors for   C8
PLAT242_ALERT_2_B Check Low   Ueq as Compared to Neighbors for   C10
PLAT242_ALERT_2_B Check Low   Ueq as Compared to Neighbors for   C4
PLAT431_ALERT_2_B Short Inter HL..A Contact F7A   .. F7B   ..   2.56 Ang.
PLAT432_ALERT_2_B Short Inter X...Y Contact C9A   .. F7A   ..   2.77 Ang.

● Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
            Calculated sin(theta_max)/wavelength =   0.5867
PLAT213_ALERT_2_C Atom F9D   has ADP max/min Ratio .....   3.50 prola
PLAT213_ALERT_2_C Atom O1   has ADP max/min Ratio .....   4.00 prola
PLAT215_ALERT_3_C Disordered F9C   has ADP max/min Ratio 3.10
PLAT215_ALERT_3_C Disordered F9F   has ADP max/min Ratio 3.20
PLAT215_ALERT_3_C Disordered O4   has ADP max/min Ratio 3.50
PLAT242_ALERT_2_C Check Low   Ueq as Compared to Neighbors for   F9E
PLAT242_ALERT_2_C Check Low   Ueq as Compared to Neighbors for   C9B
PLAT242_ALERT_2_C Check Low   Ueq as Compared to Neighbors for   Mo1
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.60
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ..   18
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ   ?
PLAT234_ALERT_4_C Large Hirshfeld Difference C2   -- C3   ..   0.18 Ang.

● Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.   18.14
PLAT301_ALERT_3_G Note: Main Residue Disorder ....   34.00 Perc.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints   121
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ....   29.00 Perc.
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.   P1
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....   !

  62 **ALERT level A** = In general: serious problem
   9 **ALERT level B** = Potentially serious problem
  13 **ALERT level C** = Check and explain
   6 **ALERT level G** = General alerts; check

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

Datablock sw208II - ellipsoid plot