checkCIF/PLATON report

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

Datablock: sw139

Bond precision: C-C = 0.0101 A   Wavelength=1.54178

Cell: a=9.6229(1)   b=23.3032(2)   c=36.1442(2)
               alpha=90   beta=91.045(1)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	8103.79(12)	8103.79(12)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C16 Al F36 O4, C24 H21 N2 P Tl, C24 H21 N2 P, 2(C7 H8)	C16 Al F36 O4, 2(C24 H21 N2 P), TL, 2(C7 H8)
Sum formula	C78 H58 Al F36 N4 O4 P2 Tl	C78 H58 Al F36 N4 O4 P2 Tl
Mr	2092.58	2092.58
Dx,g cm-3	1.715	1.715
Z	4	4
Mu (mm-1)	5.541	5.541
F000	4136.0	4136.0
F000'	4139.52	
h,k,lmax	11,26,41	11,26,41
Nref	12863	12511
Tmin,Tmax	0.255,0.355	0.286,0.355
Tmin'	0.161	

Correction method= MULTI-SCAN

Data completeness= 0.973   Theta(max)= 62.380

R(reflections)= 0.0516(11802)   wR2(reflections)= 0.1270(12511)

S = 1.048   Npar= 1566

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

PLAT083_ALERT_2_A SHELXL Second Parameter in WGHT unusually Large.   58.00

Author Response: Possibly a result of the weak diffraction at high theta angles and/or a strong disorder of the counterion.

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PLAT308_ALERT_2_A Single Bonded Metal Atom (Unusual !) ...........        Tl1
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Author Response: There are rather long coordinative bonds between P1, P2, N1, N3 and the Tl(I) cation. Additionally, the thallium cation is pi-coordinated by one of the toluene solvent molecules.

🟠 Alert level B
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REFNR01_ALERT_3_B  Ratio of reflections to parameters is < 8 for a
           centrosymmetric structure
           sine(theta)/lambda                0.5747
           Proportion of unique data used    1.0000
           Ratio reflections to parameters   7.9891
THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =    0.5747
PLAT088_ALERT_3_B Poor Data / Parameter Ratio ....................        7.99
PLAT220_ALERT_2_B Large Non-Solvent    F    Ueq(max)/Ueq(min) ...        4.31 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for    F25    -- C75     ..        9.91 su
PLAT241_ALERT_2_B Check High    Ueq as Compared to Neighbors for          O4
PLAT242_ALERT_2_B Check Low     Ueq as Compared to Neighbors for         C66
PLAT242_ALERT_2_B Check Low     Ueq as Compared to Neighbors for        C70B
PLAT242_ALERT_2_B Check Low     Ueq as Compared to Neighbors for        C72B
PLAT242_ALERT_2_B Check Low     Ueq as Compared to Neighbors for         C75
PLAT242_ALERT_2_B Check Low     Ueq as Compared to Neighbors for         C77
PLAT242_ALERT_2_B Check Low     Ueq as Compared to Neighbors for        C66B
PLAT301_ALERT_3_B Main Residue  Disorder .........................       32.00 Perc.
PLAT234_ALERT_4_B Large Hirshfeld Difference F14B   -- C71B    ..        0.20  Ang.
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🟡 Alert level C
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ABSTM02_ALERT_3_C  The ratio of expected to reported Tmax/Tmin(RR) is > 1.10
           Tmin and Tmax reported:      0.286     0.355
           Tmin and Tmax expected:      0.250     0.355
           RR =      1.141
           Please check that your absorption correction is appropriate.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......        0.97
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....        2.16
PLAT213_ALERT_2_C Atom F21     has ADP max/min Ratio .............        3.40 prola
PLAT213_ALERT_2_C Atom F31     has ADP max/min Ratio .............        3.20 prola
PLAT213_ALERT_2_C Atom F32     has ADP max/min Ratio .............        3.80 prola
PLAT213_ALERT_2_C Atom F33     has ADP max/min Ratio .............        3.20 prola
PLAT213_ALERT_2_C Atom F25B    has ADP max/min Ratio .............        3.10 prola
PLAT213_ALERT_2_C Atom C70     has ADP max/min Ratio .............        3.40 prola
PLAT213_ALERT_2_C Atom C71     has ADP max/min Ratio .............        3.40 prola
PLAT213_ALERT_2_C Atom C72     has ADP max/min Ratio .............        3.40 prola
PLAT220_ALERT_2_C Large Non-Solvent    C    Ueq(max)/Ueq(min) ...        2.97 Ratio
PLAT220_ALERT_2_C Large Non-Solvent    C    Ueq(max)/Ueq(min) ...        3.10 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F18B   -- C72B    ..        5.89 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F27    -- C75     ..        5.95 su
PLAT242_ALERT_2_C Check Low     Ueq as Compared to Neighbors for         Al1
PLAT242_ALERT_2_C Check Low     Ueq as Compared to Neighbors for         C67
PLAT242_ALERT_2_C Check Low     Ueq as Compared to Neighbors for        C71B
PLAT242_ALERT_2_C Check Low     Ueq as Compared to Neighbors for         C73
PLAT242_ALERT_2_C Check Low     Ueq as Compared to Neighbors for        C68B
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PLAT242_ALERT_2_C Check Low        Ueq as Compared to Neighbors for      C70
PLAT242_ALERT_2_C Check Low        Ueq as Compared to Neighbors for      C71
PLAT242_ALERT_2_C Check Low        Ueq as Compared to Neighbors for      C74B
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.87
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ...        10
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C28    -  C29    ...      1.42 Ang.
PLAT042_ALERT_1_C Calc. and Rep. MoietyFormula Strings Differ ....         ?
PLAT060_ALERT_4_C Ratio Tmax/Tmin (Exp-to-Rep) (too) Large .......      1.12
PLAT142_ALERT_4_C su on b - Axis Small or Missing (x 100000) .....        20 Ang.
PLAT143_ALERT_4_C su on c - Axis Small or Missing (x 100000) .....        20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Al1     -- O4      ..      0.12  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F3      -- C67     ..      0.16  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F4      -- C68     ..      0.18  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F9      -- C69     ..      0.19  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F11B    -- C70B    ..      0.15  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F17B    -- C72B    ..      0.19  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F30     -- C76     ..      0.18  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C64B    -- C70B    ..      0.19  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C64B    -- C71B    ..      0.17  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C64B    -- C72B    ..      0.18  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C66     -- C76     ..      0.17  Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C66     -- C78     ..      0.17  Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #         5
                  C7 H8
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Alert level G
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PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......       885
PLAT302_ALERT_4_G Anion/Solvent Disorder ........................     33.00 Perc.
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  2 ALERT level A = In general: serious problem
 14 ALERT level B = Potentially serious problem
 43 ALERT level C = Check and explain
  2 ALERT level G = General alerts; check


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

Datablock sw139 - ellipsoid plot