checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: 1

Bond precision: C-C = 0.0077 A   Wavelength=0.71075

Cell: a=8.471(5)   b=15.985(9)   c=20.939(12)
               alpha=108.824(11)   beta=94.302(7)   gamma=90.009(5)
Temperature: 103 K

	Calculated	Reported
Volume	2675(3)	2675(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26 H39 Al P, C26 H40 Al P, 0.5(C6 H14)	C26 H39 Al P, C26 H40 Al P, 0.5(C6 H14)
Sum formula	C55 H86 Al2 P2	C27.50 H43 Al P
Mr	863.14	431.57
Dx,g cm-3	1.072	1.072
Z	2	4
Mu (mm-1)	0.147	0.147
F000	944.0	944.0
F000'	944.91	
h,k,lmax	10,19,25	10,19,24
Nref	9681	9202
Tmin,Tmax	0.974,0.985	0.844,1.000
Tmin'	0.971	

Correction method= # Reported T Limits: Tmin=0.844 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.951   Theta(max)= 25.249

R(reflections)= 0.0887(6276)   wR2(reflections)= 0.2231(9202)

S = 1.067   Npar= 557

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 C

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PLAT220_ALERT_2_C Non-Solvent  Resd 2  C   Ueq(max)/Ueq(min) Range        5.7 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 2  H   Uiso(max)/Uiso(min) Range        5.4 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C016     --C01J    .        0.16 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C016 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of    C01N Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      C01L    0.104 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.00775 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   18.614 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    2.866 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       470 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..      1 Check
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⬤ Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum:   C27.5 H43 Al1 P1
            Atom count from _chemical_formula_moiety:C55 H86 Al2 P2
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     8.29 Why ?
PLAT328_ALERT_4_G Possible Missing H on sp3? Phosphorus ..........     P001 Check
PLAT328_ALERT_4_G Possible Missing H on sp3? Phosphorus ..........     P002 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C00I Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       57 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .  Please Do !
PLAT898_ALERT_4_G Second Reported H-M Symbol in CIF Ignored ......        ! Check
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still     47% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       3 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...       2 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       1 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by       2 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 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
   6 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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* or *IUCrData*, 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 07/08/2019; check.def file version of 30/07/2019

NOMOVE FORCED

Prob = 50
Temp = 103

55 Y

PLATON-Oct 16 02:34:59 2019 - (70316)

Z -28   1   P -1   R = 0.09   RES=   0   142 X