checkCIF/PLATON report

Structure factors have been supplied for datablock(s) TPP_Al_azpMe2_90K

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: TPP_Al_azpMe2_90K

Bond precision: C-C = 0.0046 A   Wavelength=0.71073

Cell: a=11.8738(19)   b=13.224(2)   c=16.406(3)
                 alpha=81.934(2)   beta=81.586(2)   gamma=64.230(2)
Temperature: 90 K

	Calculated	Reported
Volume	2286.4(7)	2286.4(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C28 H24 Al N4 O4, C24 H20 P, C H4 O, O	?
Sum formula	C53 H48 Al N4 O6 P	C53 H48 Al N4 O6 P
Mr	894.90	894.93
Dx,g cm-3	1.300	1.300
Z	2	2
Mu (mm-1)	0.136	0.136
F000	940.0	940.0
F000'	940.71	
h,k,lmax	15,16,20	15,16,20
Nref	9688	9378
Tmin,Tmax	0.973,0.984	0.970,0.990
Tmin'	0.960	

Correction method= # Reported T Limits: Tmin=0.970 Tmax=0.990
AbsCorr = ?

Data completeness= 0.968   Theta(max)= 26.730

R(reflections)= 0.0703(7563)   wR2(reflections)= 0.2036(9378)

S = 1.039   Npar= 739

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 B**

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density   1.87 eA-3

> **Author Response: The structure refinement is converged using the composition determined by the elemental analysis. Further assignment of electron density was not performed.**

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O7 Check

> **Author Response: The oxygen atom is an isolated water molecule.**

🟡 **Alert level C**

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
              The relevant atom site should be identified.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .   0.968 Why?
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given   Please Do !
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.28 Report
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O2 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   O7   0.203 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.00461 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X   H53B   ..H105   .   1.93 Ang.
                                             x,y,z =   1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   2.083 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   177 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .   1 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.91Ang From O7   1.80 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.00Ang From O7   .   1.42 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.76Ang From O7   .   1.41 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.40Ang From O7   .   -0.82 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.48Ang From O7   .   -0.79 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.63Ang From O5   .   -0.61 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.63Ang From O7   .   -0.56 eA-3
PLAT992_ALERT_5_C Repd & Actual _reflns_number_gt Values Differ by   23 Check

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⚪ **Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   32 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   81 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   1 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical   ? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large   0.10 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.002 Degree
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records   2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   7 Report

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PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Al1      --O1       .     6.3 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )     43% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      3 Note
PLAT767_ALERT_4_G INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters      1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............    887 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).      3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600    131 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........    1.3 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      6 Info
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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   2 **ALERT level B** = A potentially serious problem, consider carefully
  20 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  21 **ALERT level G** = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  19 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
   8 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check

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 19/02/2022; check.def file version of 19/02/2022