checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 7Th

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: 7Th

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Bond precision:   C-C = 0.0170 A              Wavelength=0.71073

Cell:             a=55.079(2)      b=13.3829(7)          c=18.9888(9)
                  alpha=90         beta=95.335(5)        gamma=90
Temperature:      150 K

                  Calculated                  Reported
Volume            13936.3(11)                 13936.3(11)
Space group       C 2/c                       C 1 2/c 1
Hall group        -C 2yc                      -C 2yc
Moiety formula    C48 H118 Cl2 N4 Si8 Th2     C48 H118 Cl2 N4 Si8 Th2
Sum formula       C48 H118 Cl2 N4 Si8 Th2     C48 H118 Cl2 N4 Si8 Th2
Mr                1511.17                     1511.16
Dx,g cm-3         1.441                       1.440
Z                 8                           8
Mu (mm-1)         4.509                       4.509
F000              6080.0                      6080.0
F000'             5974.00
h,k,lmax          66,16,22                    66,16,22
Nref              12769                       12706
Tmin,Tmax         0.535,0.709                 0.937,0.983
Tmin'             0.326

Correction method= # Reported T Limits: Tmin=0.937 Tmax=0.983
AbsCorr = GAUSSIAN

Data completeness= 0.995           Theta(max)= 25.350

R(reflections)= 0.0707( 7130)      wR2(reflections)= 0.1713( 12706)

S = 1.012                    Npar= 684
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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

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on   Th1   3.70 eA-3

> **Author Response: No chemically sensible species can be assigned to this position. The residual density is located symmetrically either side of the Th atoms and is attributed to imperfect absorption correction. Face indexing of the crystal, combined with a smaller reduction mask as well as a strong absorber correction failed to account for the density. Finally, a larger frame scan range for the background was used, which also did not result in any reduction of the residual density.**

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on   Th2B   2.88 eA-3

> **Author Response: No chemically sensible species can be assigned to this position. The residual density is located symmetrically either side of the Th atoms and is attributed to imperfect absorption correction. Face indexing of the crystal, combined with a smaller reduction mask as well as a strong absorber correction failed to account for the density. Finally, a larger frame scan range for the background was used, which also did not result in any reduction of the residual density.**

🟠 Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).   34 Note

> **Author Response: Reduction of beam stop mask did not yield significant improvement. Most of those missing strong reflections appeared to be very strong and were treated as overflows.**

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.07A   From Th1   2.58 eA-3

🟡 Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
            Rint given   0.122
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ....   0.122 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C   Ueq(max)/Ueq(min) Range   3.4 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1 H   Uiso(max)/Uiso(min) Range   4.1 Ratio
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.01695 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   3.092 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   23 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....   4 Note
PLAT925_ALERT_1_C The Reported and Calculated Rho(max) Differ by .   1.39 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.05A   From Th1   2.32 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.00A   From Th2A   2.08 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.98A   From Th2B   2.08 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.00A   From Th1   1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.82A   From Th1   -1.89 eA-3

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.94A    From Th1          -1.66 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.88A    From Th1          -1.53 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.83A    From Th1          -1.51 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H14B            -0.40 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H18A            -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H26A            -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H34B            -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H47E            -0.38 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Info
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        43 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        74 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         8 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       16% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      1140 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         6 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         8 Note
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  23 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

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

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