checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2-THF

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: 2-THF

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Bond precision:   C-C = 0.0105 A           Wavelength=0.71073

Cell:           a=13.7126(5)      b=14.0731(6)          c=20.7186(10)
                alpha=90          beta=99.150(4)      gamma=90
Temperature:    150 K

                Calculated                 Reported
Volume          3947.4(3)                  3947.4(3)
Space group     P 21/n                     P 1 21/n 1
Hall group      -P 2yn                     -P 2yn
Moiety formula  C28 H68 I N2 O Si4 U       C28 H68 I N2 O Si4 U
Sum formula     C28 H68 I N2 O Si4 U       C28 H68 I N2 O Si4 U
Mr              926.13                     926.13
Dx,g cm-3       1.558                      1.558
Z               4                          4
Mu (mm-1)       5.037                      5.037
F000            1836.0                     1836.0
F000'           1797.48
h,k,lmax        16,16,24                   16,16,24
Nref            7222                       7188
Tmin,Tmax       0.658,0.735                0.782,1.000
Tmin'           0.022

Correction method= # Reported T Limits: Tmin=0.782 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.995          Theta(max)= 25.347

R(reflections)= 0.0470( 5248)     wR2(reflections)= 0.0701( 7188)

S = 0.987                    Npar= 352
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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 C

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PLAT220_ALERT_2_C Non-Solvent Resd 1  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C8AA Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01047 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         29 Report
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on         U2      1.48 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H1AA            -0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H9              -0.45 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H16B            -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8AB            -0.42 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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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       37 Report
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....     0.76 mm
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records        1 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       32 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      306 Note
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        2 Note
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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
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   7 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   4 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.

PLATON version of 09/11/2017; check.def file version of 08/11/2017