checkCIF/PLATON report

Structure factors have been supplied for datablock(s) b

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: b

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Bond precision:    C-C = 0.0067 A              Wavelength=0.71073

Cell:              a=11.6267(7)      b=17.5415(11)       c=15.5668(10)
                   alpha=90          beta=96.244(4)      gamma=90
Temperature:       296 K

                   Calculated                  Reported
Volume             3156.0(3)                   3156.0(3)
Space group        I 2/c                       I 2/c
Hall group         -I 2yc                      -I 2yc
Moiety formula     C24 H20 Cu F6 N8 Si,  0.4(C6    ?
                   H12), 1.2(C3 H6)
Sum formula        C30 H32 Cu F6 N8 Si         C30 H32 Cu F6 N8 Si
Mr                 710.28                      710.26
Dx,g cm-3          1.495                       1.495
Z                  4                           4
Mu (mm-1)          0.801                       0.801
F000               1460.0                      1460.0
F000'              1462.26
h,k,lmax           13,20,18                    13,20,18
Nref               2773                        2771
Tmin,Tmax          0.887,0.901
Tmin'              0.887

Correction method= Not given

Data completeness= 0.999         Theta(max)= 24.997

R(reflections)= 0.0523( 2431)                  wR2(reflections)=
                                               0.1430( 2771)
S = 1.010                  Npar= 235
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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 B**
PLAT242_ALERT_2_B Low   'MainMol' Ueq as Compared to Neighbors of   Si1 Check

Author Response: These alerts are generated because there is disorder in the structure

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🟡 **Alert level C**
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given   Please Do !
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   F3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C3 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C11 Check

Author Response: These alerts are generated because there is disorder in the structure

PLAT260_ALERT_2_C Large Average Ueq of Residue Including   C13   0.188 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   C16   0.173 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C10   -C12_a   .   1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.00675 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.595   3 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.03Ang From C13   .   0.64 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.50Ang From C15   .   0.42 eA-3

⚪ **Alert level G**
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   6 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   6 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   18.90 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records   1 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)   100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3)   100% Note
PLAT411_ALERT_2_G Short Inter H...H Contact H9   ..H17   .   1.97 Ang.
                                     -1/2+x,1/2-y,z =   8_455 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn   H9   ..H18B   .   1.66 Ang.
                                     -1/2+x,1/2-y,z =   8_455 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn   H12   ..H18B   .   2.12 Ang.
                                     -1/2+x,1/2-y,z =   8_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact F2   ..C14   .   2.76 Ang.
                                        x,-1+y,z =   1_545 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact F2   ..C15   .   2.92 Ang.
                                        x,-1+y,z =   1_545 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact F4   ..C16   .   2.76 Ang.
                                     1-x,-1+y,1/2-z =   2_645 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact F4   ..C16   .   2.76 Ang.

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                                         x,-1+y,z  =      1_545 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C16      --C16        2.02 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1      (II)      .   2.20 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters    1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............   42 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still  76% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........  4.0 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.    2 Info
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  0 ALERT level A = Most likely a serious problem – resolve or explain
  1 ALERT level B = A potentially serious problem, consider carefully
 12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 26 ALERT level G = General information/check it is not something unexpected

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