checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: BCu5

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Bond precision:   C-C = 0.0065 A             Wavelength=0.71073

Cell:          a=8.7723(18)      b=12.318(3)       c=13.833(3)
               alpha=101.77(3)   beta=105.28(3)    gamma=104.70(3)
Temperature:   170 K

                  Calculated                  Reported
Volume            1334.7(7)                   1334.7(6)
Space group       P -1                        P -1
Hall group        -P 1                        -P 1
Moiety formula    C60 H50 Cu3 F6 N2 O12       ?
Sum formula       C60 H50 Cu3 F6 N2 O12       C60 H50 Cu3 F6 N2 O12
Mr                1295.67                     1295.64
Dx,g cm-3         1.612                       1.612
Z                 1                           1
Mu (mm-1)         1.274                       1.274
F000              661.0                       661.0
F000'             662.30
h,k,lmax          12,17,19                    12,16,19
Nref              7405                        7268
Tmin,Tmax         0.775,0.844                 0.596,0.800
Tmin'             0.723

Correction method= # Reported T Limits: Tmin=0.596 Tmax=0.800
AbsCorr = NUMERICAL

Data completeness= 0.981          Theta(max)= 29.475

R(reflections)= 0.0471( 4531)     wR2(reflections)= 0.1256( 7268)

S = 0.945                    Npar= 390
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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 NonSolvent    Resd 1  C   Ueq(max)/Ueq(min) Range      3.6 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for     C29       --C30    .        6.7 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Cu2 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C3      -C8             1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.00648 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H2A      ..O6      .      2.63 Ang.
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         2 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT013_ALERT_1_G No      _shelx_hkl_checksum Found in CIF ......  Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)    0.03 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )        2% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2      (II)      .     2.13 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        1 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........     2.1 Low
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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
   8 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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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
   2 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 10/08/2020; check.def file version of 06/08/2020

Datablock BCu5 - ellipsoid plot