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

Bond precision:  C-C = 0.0065 Å  Wavelength=0.7107 Å

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

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

| Alert ID         | Description                                                                 | Type     | Level |
|------------------|-----------------------------------------------------------------------------|----------|-------|
| PLAT220_ALERT_2_C | NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range                                | ALERT 2  | C     |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for C29 --C30                                           | ALERT 2  | C     |
| PLAT241_ALERT_2_C | High ‘MainMol’ Ueq as Compared to Neighbors of O3 Check                     | ALERT 2  | C     |
| PLAT241_ALERT_2_C | High ‘MainMol’ Ueq as Compared to Neighbors of O5 Check                     | ALERT 2  | C     |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of Cu2 Check                     | ALERT 2  | C     |
| PLAT334_ALERT_2_C | Small Aver. Benzene C-C Dist C3 --C8                                        | ALERT 2  | C     |
| PLAT341_ALERT_3_C | Low Bond Precision on C-C Bonds                                              | ALERT 3  | C     |
| PLAT480_ALERT_4_C | Long H...A H-Bond Reported H2A ..O6 .5.63 Ang.                              | ALERT 4  | C     |

### Alert level G

| Alert ID         | Description                                                                 | Type     | Level |
|------------------|-----------------------------------------------------------------------------|----------|-------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite                           | ALERT 2  | G     |
| PLAT004_ALERT_5_G | Polymeric Structure Found with Maximum Dimension                           | ALERT 5  | G     |
| PLAT013_ALERT_1_G | No _shelx_hkl_checksum Found in CIF                                        | ALERT 1  | G     |
| PLAT154_ALERT_1_G | The s.u.’s on the Cell Angles are Equal ..(Note)                           | ALERT 1  | G     |
| PLAT172_ALERT_4_G | The CIF-Embedded .res File Contains DFIX Records                            | ALERT 4  | G     |
| PLAT301_ALERT_3_G | Main Residue Disorder ..............(Resd 1 )                               | ALERT 3  | G     |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Cu2 (II)                                        | ALERT 5  | G     |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints ..................................           | ALERT 3  | G     |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity ........................................... | ALERT 3  | G     |

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
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
