checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20012

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: 20012

```
Bond precision:    C-C = 0.0083 A             Wavelength=0.71073

Cell:              a=8.471(4)      b=17.550(9)          c=18.443(9)
                   alpha=90        beta=99.605(11)      gamma=90
Temperature:       150 K

                   Calculated                 Reported
Volume             2703(2)                    2703(2)
Space group        P 21/c                     P 1 21/c 1
Hall group         -P 2ybc                    -P 2ybc
Moiety formula     C27 H24 Cu N3 O S, F6 P    C27 H24 Cu N3 O S, F6 P
Sum formula        C27 H24 Cu F6 N3 O P S     C27 H24 Cu F6 N3 O P S
Mr                 647.07                     647.06
Dx,g cm-3          1.590                      1.590
Z                  4                          4
Mu (mm-1)          1.013                      1.013
F000               1316.0                     1316.0
F000'              1318.85
h,k,lmax           10,21,22                   10,21,22
Nref               5315                       5307
Tmin,Tmax          0.854,0.960                0.568,0.843
Tmin'              0.615

Correction method= # Reported T Limits: Tmin=0.568 Tmax=0.843
AbsCorr = EMPIRICAL

Data completeness= 0.998          Theta(max)= 25.999

R(reflections)= 0.0636( 2647)     wR2(reflections)= 0.1426( 5307)

S = 0.886                    Npar= 498
```

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

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
          Rint given    0.122
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00829 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H19      ..H20     .      1.99 Ang.
                                             x,y,z  =      1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   18.321 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    3.886 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         4 Report
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         27 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         27 Report
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........     0.122 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         8 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT244_ALERT_4_G Low     'Solvent' Ueq as Compared to Neighbors of       P1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1          Constrained at     0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1A         Constrained at      0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1B         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2          Constrained at     0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2A         Constrained at      0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2B         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3          Constrained at     0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3A         Constrained at      0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3B         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4          Constrained at     0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4A         Constrained at      0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4B         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5          Constrained at     0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5A         Constrained at      0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5B         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6          Constrained at     0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6A         Constrained at      0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6B         Constrained at     0.25 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       9% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )      86% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H19      ..H24C    .      2.14 Ang.
                                             x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F3B      ..C12            2.79 Ang.
                                             x,y,z  =      1_555 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         7 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      1249 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       4.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  35 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
  25 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 18/09/2020; check.def file version of 20/08/2020