checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_BruecknerJK_153F40_0m

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: cu_BruecknerJK_153F40_0m

```
Bond precision:  C-C = 0.0031 A          Wavelength=1.54178

Cell:             a=19.678(3)     b=37.0229(9)      c=4.7720(4)
                  alpha=90        beta=90           gamma=90
Temperature:      102 K

                Calculated                Reported
Volume          3476.6(6)                 3476.6(7)
Space group     P 21 21 2                 P 21 21 2
Hall group      P 2 2ab                   P 2 2ab
Moiety formula  2(C38 H38 O12), C H4 O    ?
Sum formula     C77 H80 O25               C38.50 H40 O12.50
Mr              1405.41                   702.70
Dx,g cm-3       1.343                     1.343
Z               2                         4
Mu (mm-1)       0.838                     0.838
F000            1484.0                    1484.0
F000'           1489.09
h,k,lmax        25,47,6                   24,47,5
Nref            7449[ 4339]               7338
Tmin,Tmax       0.904,0.967               0.770,0.929
Tmin'           0.832

Correction method= # Reported T Limits: Tmin=0.770 Tmax=0.929
AbsCorr = MULTI-SCAN

Data completeness= 1.69/0.99      Theta(max)= 78.476

R(reflections)= 0.0364( 7290)     wR2(reflections)= 0.0919( 7338)

S = 1.198                 Npar= 479
```

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

```
PLAT035_ALERT_1_B _chemical_absolute_configuration Info  Not Given     Please Do !
```

Alert level C

```
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H13      ..H19B     .       2.14 Ang.
                                                x,y,-1+z  =      1_554 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          1 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O13        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C39        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H39A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H39B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H39C       Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        100% Note
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O3             109.2 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2       ..C17             2.91 Ang.
                                       -1/2+x,1/2-y,-z  =      4_455 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          6 Check
PLAT791_ALERT_4_G Model has Chirality at C1          (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C2          (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C13         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C20         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C21         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C32         (Sohnke SpGr)          S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          5 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         16 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         23 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          1 Check
```

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

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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT035_cu_Brueckner JK_153F40_0m
;
PROBLEM: _chemical_absolute_configuration Info  Not Given     Please Do !
RESPONSE: ...
;
# end Validation Reply Form
```

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 16/07/2020; check.def file version of 12/07/2020

Datablock cu_BrueckerJK_153F40_0m - ellipsoid plot