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: 1z

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Bond precision:  C-C = 0.0187 A          Wavelength=0.71073

Cell:            a=24.184(10)    b=12.642(6)         c=17.903(8)
                 alpha=90        beta=113.189(4)     gamma=90
Temperature:     100 K

                 Calculated                Reported
Volume           5031(4)                   5031(4)
Space group      C 2/c                     C 1 2/c 1
Hall group       -C 2yc                    -C 2yc
Moiety formula   C22 H17 Cu I N3 O, O      C22 H17 Cu I N3 O, O
Sum formula      C22 H17 Cu I N3 O2        C22 H17 Cu I N3 O2
Mr               545.84                    545.82
Dx,g cm-3        1.441                     1.441
Z                8                         8
Mu (mm-1)        2.114                     2.114
F000             2144.0                    2144.0
F000'            2143.42
h,k,lmax         29,15,21                  29,15,21
Nref             4724                      4667
Tmin,Tmax        0.621,0.655               0.582,0.745
Tmin'            0.609

Correction method= # Reported T Limits: Tmin=0.582 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.988          Theta(max)= 25.566

R(reflections)= 0.0729( 2052)     wR2(reflections)= 0.2534( 4667)

S = 1.023                 Npar= 272
```

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 A

PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 391 Ang**3

Author Response: The structure is porous in nature and in MOF structure the solvent accessable void are observed very frquently, in this structure the solvent gets removed when we expose our crystal in the air only few disorderd water molecule were modeled according to the Q peaks, we have CHN and TGA which strongly supports the presence of water in the crystal void rest is empty in nature.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.131
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.131 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 44% Check
PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of C4 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O2A 0.210 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O2B 0.154 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01867 Ang.

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.13 Report
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 --Cu1 . 5.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 --Cu1_a . 6.8 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O2A Constrained at 0.6733 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2B Constrained at 0.3267 Check
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
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) ..... O2A Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) ..... O2B Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
5 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 22/12/2019; check.def file version of 13/12/2019

Datablock 1z - ellipsoid plot