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: xiao1

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Bond precision:   C-C = 0.0042 A            Wavelength=0.71073

Cell:            a=4.6530(1)     b=14.5305(4)         c=25.9934(7)
                 alpha=90        beta=98.735(2)       gamma=90
Temperature:     293 K

                 Calculated                  Reported
Volume           1737.04(8)                  1737.04(8)
Space group      P 21/c                      P 21/c
Hall group       -P 2ybc                     -P 2ybc
Moiety formula   C14 H13 Cu N4 O4, 2(H2 O)   C14 H13 Cu N4 O4, 2(H2 O)
Sum formula      C14 H17 Cu N4 O6            C14 H17 Cu N4 O6
Mr               400.87                      400.87
Dx,g cm-3        1.533                       1.533
Z                4                           4
Mu (mm-1)        1.295                       1.295
F000             824.0                       824.0
F000'            825.63
h,k,lmax         5,17,30                     5,17,31
Nref             3068                        3010
Tmin,Tmax        0.712,0.752                 0.797,0.845
Tmin'            0.698

Correction method= # Reported T Limits: Tmin=0.797 Tmax=0.845
AbsCorr = EMPIRICAL

Data completeness= 0.981          Theta(max)= 25.000

R(reflections)= 0.0412( 2930)     wR2(reflections)= 0.1171( 3010)

S = 1.044                  Npar= 233
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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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PLAT213_ALERT_2_C Atom N1              has ADP max/min Ratio .....        3.6 prolat
PLAT213_ALERT_2_C Atom C2              has ADP max/min Ratio .....        3.1 prolat
PLAT220_ALERT_2_C Non-Solvent   Resd 1  C   Ueq(max)/Ueq(min) Range      4.6 Ratio
PLAT220_ALERT_2_C Non-Solvent   Resd 1  N   Ueq(max)/Ueq(min) Range      5.8 Ratio
PLAT220_ALERT_2_C Non-Solvent   Resd 1  O   Ueq(max)/Ueq(min) Range      3.2 Ratio
PLAT222_ALERT_3_C Non-Solv.   Resd 1  H   Uiso(max)/Uiso(min) Range      4.3 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu1       --O2        .       8.6 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu1       --O4        .       8.6 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu1       --N2        .       6.2 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu1       --N3        .       6.4 s.u.
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.9 Note
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      6 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension      1 Info
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  P21/c    P21/n Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records      1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records      2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records      2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)    293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)     293 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .   1.18 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)     .    2.23 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      6 Note
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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
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   5 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 23/04/2018; check.def file version of 23/04/2018