checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rod147_150k_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: rod147_150k_0m

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Bond precision:   C-C = 0.0035 A            Wavelength=1.54178

Cell:          a=8.0240(4)          b=9.4295(5)         c=23.8856(11)
               alpha=100.767(1)   beta=95.673(2)   gamma=97.244(2)
Temperature:   150 K

                  Calculated                     Reported
Volume            1747.30(15)                    1747.30(15)
Space group       P -1                           P -1
Hall group        -P 1                           -P 1
Moiety formula    C36 H33 Cu2 N3 O8, C H4 O      C72 H66 Cu4 N6 O16, 2(C H4
                                                 O)
Sum formula       C37 H37 Cu2 N3 O9              C74 H74 Cu4 N6 O18
Mr                794.80                         1589.55
Dx,g cm-3         1.511                          1.511
Z                 2                              1
Mu (mm-1)         2.008                          2.008
F000              820.0                          820.0
F000'             814.40
h,k,lmax          9,11,29                        9,11,29
Nref              6662                           6397
Tmin,Tmax         0.575,0.755                    0.585,0.753
Tmin'             0.521

Correction method= # Reported T Limits: Tmin=0.585 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.960            Theta(max)= 70.205

R(reflections)= 0.0366( 6197)        wR2(reflections)= 0.1038( 6397)

S = 1.053                     Npar= 477
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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.

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🟡 **Alert level C**

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PLAT220_ALERT_2_C NonSolvent    Resd 1  C   Ueq(max)/Ueq(min) Range      3.1 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        87 Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.49A    From O9           -0.61 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.43A    From O10          -0.57 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H37F            -0.36 eA-3
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⚪ **Alert level G**

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        3 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension        1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        2 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ   Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...    2.00 Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O9          Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O10         Constrained at    0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9A         Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37A        Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37B        Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37C        Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10A        Constrained at    0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37D        Constrained at    0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37E        Constrained at    0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37F        Constrained at    0.25 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )    50% Note
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H18A     ..H37F     .    2.14 Ang.
                                           -x,-y,2-z  =      2_557 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2      (II)      .    2.11 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       2 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600     177 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....       1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...       1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........     3.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      12 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by       6 Check
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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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  28 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
  14 ALERT type 4 Improvement, methodology, query or suggestion
   4 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 10/08/2020; check.def file version of 06/08/2020