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: isa341_newref

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Bond precision:  C-C = 0.0069 A          Wavelength=1.54178

Cell:            a=9.9554(5)    b=9.3037(4)        c=25.2695(12)
                 alpha=90       beta=94.670(3)     gamma=90
Temperature:     98 K

                Calculated                Reported
Volume          2332.74(19)               2332.74(19)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C18 H18 Cu3 N6 O12, H2 O  C6 H6 Cu N2 O4, 1/3(H2 O)
Sum formula     C18 H20 Cu3 N6 O13        C6 H6.67 Cu N2 O4.33
Mr              719.05                    239.67
Dx,g cm-3       2.047                     2.047
Z               4                         12
Mu (mm-1)       3.949                     3.949
F000            1444.0                    1444.0
F000'           1424.68
h,k,lmax        11,10,29                  11,10,29
Nref            3960                      3947
Tmin,Tmax       0.789,0.980               0.648,0.753
Tmin'           0.648

Correction method= # Reported T Limits: Tmin=0.648 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 65.054

R(reflections)= 0.0497( 2956)     wR2(reflections)= 0.1422( 3947)

S = 1.079                 Npar= 370
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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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THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
          Calculated sin(theta_max)/wavelength =    0.5881
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.25 Report
PLAT213_ALERT_2_C Atom C13             has ADP max/min Ratio .....        4.0 prolat
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00692 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H6       ..O4       .       2.65 Ang.
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Alert level G

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CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
          From the CIF: _cell_formula_units_Z   12
          From the CIF: _chemical_formula_sum  C6 H6.67 Cu N2 O4.33
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         72.00     72.00    0.00
          H         80.04     80.00    0.04
          Cu        12.00     12.00    0.00
          N         24.00     24.00    0.00
          O         51.96     52.00   -0.04
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.33 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       7.89 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1W      ..C1              3.00 Ang.
                                                    x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          2 Note
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Cu1      --Cu2       ..       4.11 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Cu1      --Cu1       ..       5.22 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Cu1      --Cu3       ..       5.52 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Cu1      --Cu1       ..       5.69 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Cu2      --Cu3       ..       5.18 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Cu2      --Cu3       ..       5.52 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.11 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2       (II)      .       2.14 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu3       (II)      .       2.14 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          3 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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  21 ALERT level G = General information/check it is not something unexpected

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   5 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 22/03/2021; check.def file version of 19/03/2021

Datablock isa341_newref - ellipsoid plot