checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

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Bond precision:  N- C = 0.0043 A         Wavelength=0.71070

Cell:           a=8.5598(14)    b=14.825(4)          c=10.853(2)
                alpha=90        beta=108.570(13)     gamma=90
Temperature:    300 K

                Calculated                Reported
Volume          1305.5(5)                 1305.5(5)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C3 Cu2 N3, C6 H14 N3      Cu2 C3 N3, C6 H14 N3
Sum formula     C9 H14 Cu2 N6             C9 H14 Cu2 N6
Mr              333.36                    333.34
Dx,g cm-3       1.696                     1.698
Z               4                         4
Mu (mm-1)       3.245                     3.249
F000            672.0                     672.0
F000'           674.63
h,k,lmax        11,19,14                  11,19,14
Nref            3049                      3009
Tmin,Tmax       0.527,0.595               0.400,0.600
Tmin'           0.517

Correction method= # Reported T Limits: Tmin=0.400 Tmax=0.600
AbsCorr = REFDELF

Data completeness= 0.987          Theta(max)= 27.673

R(reflections)= 0.0336( 2120)     wR2(reflections)= 0.0932( 3009)

S = 1.070                 Npar= 178
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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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PLAT230_ALERT_2_C Hirshfeld Test Diff for    N10      --C12      .        6.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N13      --C12      .        6.0 s.u.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N11 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C12 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2 Note
PLAT420_ALERT_2_C D-H Without Acceptor       N10      --H10A     .     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N10      --H10B     .     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.030 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
PLAT923_ALERT_1_C S    Values in the CIF and FCF Differ by .......      0.013 Check
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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
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          4 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 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
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          6 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          6 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of N1         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3A        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         75% Note
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  2  )         22% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H16A     ..H15C     .       1.86 Ang.
                                                    x,y,z  =      1_555 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         48 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         38 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 ...........        1.1 Low
PLAT964_ALERT_2_G SHELXL WEIGHT Parameter in CIF & RES Differ ....     Please 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
 11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 32 ALERT level G = General information/check it is not something unexpected

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

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 18/09/2020; check.def file version of 20/08/2020

Datablock I - ellipsoid plot