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: 1x

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Bond precision:  C-C = 0.0110 A          Wavelength=0.71073

Cell:           a=24.2935(9)    b=12.6330(5)        c=17.7632(6)
                alpha=90        beta=113.007(1)     gamma=90
Temperature:    100 K
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	Calculated	Reported
Volume	5017.9(3)	5017.9(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C22 H17 Cu I N3 O, 0.179(C14 H10 N2), 0.642(C7 H6 N)	C22 H17 Cu I N3 O, 0.36(C7 H5 N), 0.64(C7 H6 N)
Sum formula	C29 H22.64 Cu I N4 O	C29 H22.64 Cu I N4 O
Mr	633.60	633.59
Dx,g cm-3	1.677	1.677
Z	8	8
Mu (mm-1)	2.131	2.131
F000	2517.1	2517.0
F000’	2516.59	
h,k,lmax	29,15,21	29,15,21
Nref	4613	4606
Tmin,Tmax	0.533,0.587	0.521,0.745
Tmin’	0.470	

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Correction method= # Reported T Limits: Tmin=0.521 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 25.367

R(reflections)= 0.0662( 3920)     wR2(reflections)= 0.1907( 4606)

S = 1.047                 Npar= 321
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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

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
dull

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -4.974
Test value = -3.975

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density	-4.97	eA-3
PLAT230_ALERT_2_C Hirshfeld Test Diff for N2 --C7 .	5.4	s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C26B --C27B .	0.19	Ang.
PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of	N2	Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.1	Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.5	Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.01095	Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	2	Note
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
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.10	Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	83.01	Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c	I2/a	Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	8	Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 --Cu1 .	5.8	s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 --Cu1_a .	8.3	s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of N4B Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C23A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C24A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C25A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C26A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C27A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C28A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C29A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H24A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H27A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28A Constrained at	0.3584	Check
PLAT300_ALERT_4_G Atom Site Occupancy of N4A Constrained at	0.6416	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C23B Constrained at	0.6416	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C24B Constrained at	0.6416	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C25B Constrained at	0.6416	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C26B Constrained at	0.6416	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C27B Constrained at	0.6416	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C28B Constrained at	0.6416	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C29B Constrained at	0.6416	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23B Constrained at	0.6416	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H24B Constrained at	0.6416	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25B Constrained at	0.6416	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H27B Constrained at	0.6416	Check

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PLAT300_ALERT_4_G Atom Site Occupancy of H29A       Constrained at     0.6416 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29B       Constrained at     0.6416 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
PLAT431_ALERT_2_G Short Inter HL..A Contact  I1       ..N4A      .       2.82 Ang.
                                        1/2-x,1/2+y,3/2-z  =      4_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C12      ..C28B             2.79 Ang.
                                          x,1-y,-1/2+z  =      6_565 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C13      ..C28B             2.89 Ang.
                                          x,1-y,-1/2+z  =      6_565 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          1 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
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  45 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 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
  33 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 22/12/2019; check.def file version of 13/12/2019

Datablock 1x - ellipsoid plot