checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Cu-Ho-valen-dca

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: Cu-Ho-valen-dca

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Bond precision:   C-C = 0.0167 A          Wavelength=0.71073

Cell:             a=8.8038(6)     b=16.3659(12)      c=19.8889(13)
                  alpha=90        beta=91.557(1)     gamma=90
Temperature:      298 K
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	Calculated	Reported
Volume	2864.6(3)	2864.6(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H28 Cl Cu Ho N6 O10 [+ solvent]	C22 H28 Cl Cu Ho N6 O10
Sum formula	C22 H28 Cl Cu Ho N6 O10 [+ solvent]	C22 H28 Cl Cu Ho N6 O10
Mr	800.43	800.42
Dx,g cm-3	1.856	1.856
Z	4	4
Mu (mm-1)	3.640	3.640
F000	1580.0	1580.0
F000'	1581.63	
h,k,lmax	10,19,23	10,19,23
Nref	5057	4984
Tmin,Tmax	0.190,0.233	0.190,0.233
Tmin'	0.160	

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Correction method= # Reported T Limits: Tmin=0.190 Tmax=0.233
AbsCorr = MULTI-SCAN

Data completeness= 0.986           Theta(max)= 25.019
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R(reflections)= 0.0901(2754) wR2(reflections)= 0.2156(4984)

S = 0.865 Npar= 346

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 B

PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set Please Do !

Author Response: It has been checked that all the atoms form a connected set. No action is taken.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.19Ang From O6 2.57 eA-3

Author Response: Small randomly oriented second fragment caused this difference Fourier peak not part of the correct crystal structure.

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Ho1 2.00 eA-3

Author Response: Ho1 is a heavy atom and this alert is often found for molecules of this type.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.126
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full ! Check
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.126 Report
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ho1 --O6 . 5.8 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ho1 --O9 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O8 --C21 . 0.22 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O5 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O6 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of N5 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Ho1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C20 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01667 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 71 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.48Ang From O1 2.44 eA-3

Author Response: Small randomly oriented second fragment caused this difference Fourier peak not part of the correct crystal structure.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From Ho1            1.99 eA-3
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Author Response: Small randomly oriented second fragment caused this difference Fourier peak not part of the correct crystal structure.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.03Ang From Ho1            1.70 eA-3
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Author Response: Small randomly oriented second fragment caused this difference Fourier peak not part of the correct crystal structure.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.16Ang From Ho1            1.70 eA-3
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Author Response: Small randomly oriented second fragment caused this difference Fourier peak not part of the correct crystal structure.

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From Ho1           -2.47 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.87Ang From Ho1           -2.45 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.14Ang From Ho1           -2.33 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.01Ang From Ho1           -2.21 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.01Ang From Ho1           -2.21 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.86Ang From O8      .      0.78 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.01Ang From O8      .     -0.90 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8B       .     -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H21C      .     -0.40 eA-3
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         1 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         4 Report
PLAT014_ALERT_1_G N.O.K.   _shelx_fab_checksum Found in CIF ......  Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical         ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    159.99 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         0 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (III)     .      2.64 Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          3 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         6 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed         ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .  Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        21 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       2.7 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged  Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..      50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  3 ALERT level B = A potentially serious problem, consider carefully
 29 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 19 ALERT level G = General information/check it is not something unexpected
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  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 29 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
  5 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 28/11/2022; check.def file version of 28/11/2022

Datablock Cu-Ho-valen-dca - ellipsoid plot