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: H2O-HK3rd

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Bond precision:  C-C = 0.0083 A          Wavelength=0.63000

Cell:              a=26.282(3)      b=26.282(3)      c=26.282(3)
                   alpha=90         beta=90          gamma=90
Temperature:       298 K
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	Calculated	Reported
Volume	18154(6)	18155(6)
Space group	F m -3 m	F m -3 m
Hall group	-F 4 2 3	-F 4 2 3
Moiety formula	2(C3 H1.96 Cu0.50 O2.48), 0.32(H2 O)	C18 H6 Cu3 O12 2.88(H2 O), 0.96 (H2 O)
Sum formula	C6 H4.56 Cu O5.28	C18 H13.68 Cu3 O15.84
Mr	224.69	674.03
Dx,g cm-3	0.987	0.986
Z	48	16
Mu (mm-1)	1.032	1.032
F000	5366.4	5366.0
F000’	5384.46	
h,k,lmax	36,36,36	36,36,36
Nref	1333	1324
Tmin,Tmax	0.946,0.950	0.787,1.000
Tmin’	0.946	

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Correction method= # Reported T Limits: Tmin=0.787 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.993          Theta(max)= 25.981

R(reflections)= 0.0699( 668)      wR2(reflections)= 0.2522( 1324)

S = 0.996                 Npar= 53
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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 A

PLAT601_ALERT_2_A Unit Cell Contains Solvent Accessible VOIDS of . 5043 Ang**3

Author Response: This crystal have exposured into very small amount of water mist. It has observed that the unit cell contains large accesible voids in the crystal during the sturucture analysis. However, the structure solvent of water molecule have not fully occupied in the voids and it has still a large voids.

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.211

Author Response: The crystal was very small and weakly diffracting even after prolonged exposure time from challenging sample. However, the structure was determined and refined properly.

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.9865 Check

Author Response: Large voids account for the low density of the structure.

Alert level C

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cu1 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O2W 0.115 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C2 -C3_m 1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00833 Ang.

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C18 H13.68 Cu3 O15.84
Atom count from _chemical_formula_moiety:C18 H9.92 Cu3 O124.84
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0 0.995 Report
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.211 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 ... 3.00 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.63000 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report

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PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O1W        Constrained at       0.96 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1O1       Constrained at       0.96 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2W        Constrained at       0.08 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1O2       Constrained at       0.08 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2O2       Constrained at       0.08 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        22% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          3 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         3 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............        18 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          9 Note
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  1 ALERT level A = Most likely a serious problem - resolve or explain
  2 ALERT level B = A potentially serious problem, consider carefully
  4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 29 ALERT level G = General information/check it is not something unexpected

  9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  7 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
  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 22/03/2021; check.def file version of 19/03/2021

Datablock H2O-HK3rd - ellipsoid plot