checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 22jnac984

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: 22jnac984

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Bond precision:    C-C = 0.0044 A            Wavelength=1.54178

Cell:           a=12.9272(4)        b=13.1727(4)      c=19.6298(6)
                alpha=104.372(1)    beta=94.015(2)    gamma=95.213(2)
Temperature:    298 K

                    Calculated                  Reported
Volume              3209.80(17)                 3209.80(17)
Space group         P -1                        P -1
Hall group          -P 1                        -P 1
Moiety formula      C38 H56 Cu4 N16 O22 [+      C38 H56 Cu4 N16 O22, 7[H2O]
                    solvent]
Sum formula         C38 H56 Cu4 N16 O22 [+      C38 H70 Cu4 N16 O29
                    solvent]
Mr                  1343.19                     1469.24
Dx,g cm-3           1.390                       1.520
Z                   2                           2
Mu (mm-1)           2.168                       2.396
F000                1376.0                      1516.0
F000'               1364.46
h,k,lmax            15,15,23                    15,15,23
Nref                11344                       10915
Tmin,Tmax           0.787,0.806                 0.714,1.000
Tmin'               0.787

Correction method= # Reported T Limits: Tmin=0.714 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.962            Theta(max)= 66.591
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R(reflections)= 0.0354(9698)

wR2(reflections)= 0.0986(10915)

S = 1.038   Npar= 742

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**
PLAT420_ALERT_2_B D-H Bond Without Acceptor O62   --H62A   .   Please Check

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🟡 **Alert level C**
ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies
                 outside the range 0.99 <> 1.01
            Calculated value of mu =   2.301
            Value of mu given   =   2.396
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .   0.962 Why?
PLAT220_ALERT_2_C NonSolvent   Resd 1 C   Ueq(max)/Ueq(min) Range   3.3 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1 N   Ueq(max)/Ueq(min) Range   5.3 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1 O   Ueq(max)/Ueq(min) Range   3.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1   H   Uiso(max)/Uiso(min) Range   5.4 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C6 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor N32   --H32A   .   Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor N32   --H32B   .   Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor N72   --H72B   .   Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor N76   --H76A   .   Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.595   429 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....   10 Note
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..   1 Check

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⚪ **Alert level G**
FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C38 H70 Cu4 N16 O29
            Atom count from the _atom_site data: C38 H56 Cu4 N16 O22
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z   2
           From the CIF: _chemical_formula_sum C38 H70 Cu4 N16 O29
           TEST: Compare cell contents of formula and atom_site data

           atom   Z*formula cif sites diff
           C   76.00   76.00   0.00
           H   140.00   112.00   28.00
           Cu   8.00   8.00   0.00
           N   32.00   32.00   0.00
           O   58.00   44.00   14.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   4 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   14 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .   9.53 %

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PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --O12    .      6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu2      --O51    .      6.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu3      --O54    .      5.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu3      --O60    .      5.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu3      --O62    .     19.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu4      --O15    .      6.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu4      --N18    .      5.5 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )      3% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H46A     ..H49A   .     2.07 Ang.
                                            x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H52B     ..H50B   .     1.95 Ang.
                                            x,y,z  =      1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........      ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)     .     2.26 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu3       (II)     .     2.27 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu4       (II)     .     2.17 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      1 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed      ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .  Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still     79% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........    2.1 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      3 Info
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   0 ALERT level A = Most likely a serious problem – resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  28 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  21 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   4 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.

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