checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_20221250_0m

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_20221250_0m

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Bond precision:   C-C = 0.0049 A          Wavelength=1.54178

Cell:              a=9.6891(4)      b=15.0403(6)      c=18.0395(7)
                   alpha=90         beta=90           gamma=90
Temperature:       298 K

                 Calculated                Reported
Volume           2628.84(18)               2628.84(18)
Space group      P 21 21 21                P 21 21 21
Hall group       P 2ac 2ab                 P 2ac 2ab
Moiety formula   C23 H32 F3 N5 O4          4(C23 H32 F3 N5 O4)
Sum formula      C23 H32 F3 N5 O4          C92 H124 F12 N16 O20
Mr               499.54                    2002.06
Dx,g cm-3        1.262                     1.265
Z                4                         1
Mu (mm-1)        0.862                     0.882
F000             1056.0                    1056.0
F000'            1059.74
h,k,lmax         12,18,22                  11,18,22
Nref             5379[ 3040]               5247
Tmin,Tmax        0.809,0.916               0.545,0.754
Tmin'            0.768

Correction method= # Reported T Limits: Tmin=0.545 Tmax=0.754
AbsCorr = NONE

Data completeness= 1.73/0.98        Theta(max)= 74.547

R(reflections)= 0.0457( 4272)                wR2(reflections)=
                                             0.1183( 5247)
S = 1.076                  Npar= 348
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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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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       0.98 Check
PLAT057_ALERT_3_C Correction for Absorption Required   RT(exp) ...       1.13 Do !
PLAT234_ALERT_4_C Large Hirshfeld Difference F2       --C1       .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F3       --C1       .       0.22 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00495 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         26 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....         15 Note
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Alert level G

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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:   C92 H124 F12 N16 O20
           Atom count from _chemical_formula_moiety:C92 H128 F12 N20 O16
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:C92 H124 F12 N16 O20
           Atom count from the _atom_site data:  C92 H128 F12 N20 O16
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    1
          From the CIF: _chemical_formula_sum  C92 H124 F12 N16 O20
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         92.00     92.00    0.00
          H        124.00    128.00   -4.00
          F         12.00     12.00    0.00
          N         16.00     20.00   -4.00
          O         20.00     16.00    4.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          2 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...          4 Check
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F00M       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F00T       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F00U       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1         Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2         Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3         Constrained at       0.25 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )          9% Note
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C1       - C2       .       1.51 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          3 Note
PLAT791_ALERT_4_G Model has Chirality at C3          (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C10         (Sohnke SpGr)          S Verify
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PLAT791_ALERT_4_G Model has Chirality at C11         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C12         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C17         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C20         (Sohnke SpGr)          S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        12 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        25 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         1 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         2 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
   9 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
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  17 ALERT type 4 Improvement, methodology, query or suggestion
   2 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_20221250_0m - ellipsoid plot