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: isn163_130k_0m

Bond precision: C-C = 0.0107 A   Wavelength=1.54178

Cell: a=12.9120(7)   b=14.0896(8)   c=27.1332(13)
                alpha=90   beta=94.491(2)   gamma=90
Temperature: 130 K

	Calculated	Reported
Volume	4921.1(5)	4921.0(5)
Space group	P 2/c	P 1 2/c 1
Hall group	-P 2yc	-P 2yc
Moiety formula	C48 H34 Br2 Cu N2 O P2, F6 P [+ solvent]	C48 H34 Br2 Cu N2 O P2, F6 P, 0.8[CH2CL2], 0.9[H2O]
Sum formula	C48 H34 Br2 Cu F6 N2 O P3 [+ solvent]	C48.80 H37.40 Br2 Cl1.60 Cu F6 N2 O1.90 P3
Mr	1085.03	1169.20
Dx,g cm-3	1.464	1.578
Z	4	4
Mu (mm-1)	3.957	4.797
F000	2168.0	2338.0
F000'	2163.70	
h,k,lmax	15,17,33	15,17,32
Nref	9319	8930
Tmin,Tmax	0.497,0.825	0.591,0.753
Tmin'	0.421	

Correction method= # Reported T Limits: Tmin=0.591 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.958   Theta(max)= 69.862

R(reflections)= 0.0870(8307)   wR2(reflections)= 0.2516(8930)

S = 1.122   Npar= 556

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**
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   P3   0.174 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.01067 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: C48.8 H37.4 Br2 Cl1.6 Cu1 F6
           Atom count from _chemical_formula_moiety:C48.8 H35.6 Br2 Cl1.6 Cu1 F6
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:C48.8 H37.4 Br2 Cl1.6 Cu1 F6 N2
           Atom count from the _atom_site data: C48 H34 Br2 Cu1 F6 N2 O1 P3
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   4
           From the CIF: _chemical_formula_sum C48.80 H37.40 Br2 Cl1.60 Cu F6 N2
           TEST: Compare cell contents of formula and atom_site data

           atom   Z*formula cif sites diff
           C   195.20   192.00   3.20
           H   149.60   136.00   13.60
           Br   8.00   8.00   0.00
           Cl   6.40   0.00   6.40
           Cu   4.00   4.00   0.00
           F   24.00   24.00   0.00
           N   8.00   8.00   0.00
           O   7.60   4.00   3.60
           P   12.00   12.00   0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   13 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   6 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 .   17.51 %
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large   0.12 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   31.63 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records   1 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   P3   --F1   .   24.6 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   P3   --F2   .   9.4 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   P3   --F3   .   15.2 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   P3   --F4   .   24.6 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   P3   --F5   .   9.2 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   P3   --F6   .   15.6 s.u.
PLAT244_ALERT_4_G Low   Solvent Ueq as Compared to Neighbors of   P3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Br1   Constrained at   0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Br2   Constrained at   0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Br3   Constrained at   0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Br4   Constrained at   0.2 Check
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   4% Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure   651 A**3
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters   1 Info

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PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        123 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed         ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          6 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
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  31 ALERT level G = General information/check it is not something unexpected

   6 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
   3 ALERT type 3 Indicator that the structure quality may be low
  17 ALERT type 4 Improvement, methodology, query or suggestion
   0 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