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: isn164_130k_0m

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Bond precision:  C-C = 0.0038 A          Wavelength=1.54178

Cell:          a=12.4032(9)      b=18.9805(14)    c=22.0591(17)
               alpha=70.330(3)   beta=77.791(3)   gamma=87.292(3)
Temperature:   130 K
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	Calculated	Reported
Volume	4777.9(6)	4777.9(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C48 H34 Br2 Cu N2 O P2, F6 P [+ solvent]	C48 H34 Br2 Cu N2 O P2, F6 P, 1[CH2CL2]
Sum formula	C48 H34 Br2 Cu F6 N2 O P3 [+ solvent]	C49 H36 Br2 Cl2 Cu F6 N2 O P3
Mr	1085.03	1169.97
Dx,g cm-3	1.508	1.626
Z	4	4
Mu (mm-1)	4.076	5.128
F000	2168.0	2336.0
F000’	2163.70	
h,k,lmax	15,23,26	14,23,26
Nref	18239	17481
Tmin,Tmax	0.457,0.599	0.671,0.753
Tmin’	0.312	

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Correction method= # Reported T Limits: Tmin=0.671 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.958          Theta(max)= 70.417

R(reflections)= 0.0327( 16297)    wR2(reflections)= 0.0834( 17481)

S = 1.008                 Npar= 1135
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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 B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .... 1 Report
O1

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for O2 --C79 . 6.6 s.u.
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.0 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.5 Note

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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:C49 H36 Br2 Cl2 Cu1 F6 N2 O1 P3
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 C49 H36 Br2 Cl2 Cu F6 N2 O P3
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	196.00	192.00	4.00
H	144.00	136.00	8.00
Br	8.00	8.00	0.00
Cl	8.00	0.00	8.00
Cu	4.00	4.00	0.00
F	24.00	24.00	0.00
N	8.00	8.00	0.00
O	4.00	4.00	0.00
P	12.00	12.00	0.00

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
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 . 20.52 %
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.23 Why ?
PLAT154_ALERT_1_G The s.u.’s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 --P1 . 5.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu2 --P4 . 5.7 s.u.
PLAT244_ALERT_4_G Low Solvent Ueq as Compared to Neighbors of P5 Check
PLAT244_ALERT_4_G Low Solvent Ueq as Compared to Neighbors of P6 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
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 ... 9 Note

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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
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
17 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  9 ALERT type 2 Indicator that the structure model may be wrong or deficient
  0 ALERT type 3 Indicator that the structure quality may be low
  5 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

Datablock isn164_130k_0m - ellipsoid plot