

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_14_br_0m_a

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_14_br_0m_a

Bond precision:	C-C = 0.0199 Å	Wavelength=1.54178
Cell:	a=19.9240 (8) alpha=90	b=27.1078 (10) beta=104.644 (2) c=25.9815 (9) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	13576.7 (9)	13576.7 (9)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C96 H90 Br4 N6 O8 Rh4, 2 (C F3 O3 S) [+ solvent]	C96 H90 Br4 N6 O8 Rh4, 2 (C F3 O3 S), 4 [CF3SO3]
Sum formula	C98 H90 Br4 F6 N6 O14 Rh4 S2 [+ solvent]	C102 H90 Br4 F18 N6 O26 Rh4 S6
Mr	2485.13	3081.43
Dx, g cm ⁻³	1.216	1.508
Z	4	4
Mu (mm ⁻¹)	5.995	6.875
F000	4952.0	6120.0
F000'	4957.82	
h, k, lmax	23, 32, 31	23, 32, 31
Nref	24495	24007
Tmin, Tmax	0.410, 0.357	0.500, 0.753
Tmin'	0.310	

Correction method= # Reported T Limits: Tmin=0.500 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.980 Theta (max)= 67.559

R(reflections)= 0.1383(10208)

wR2(reflections)=
0.3148(24007)

S = 1.085

Npar= 1071

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.135

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.135 Report

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 43% Check

PLAT082_ALERT_2_C High R1 Value 0.14 Report

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.31 Report

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Rh04 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C019 Check

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.1 Note

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 3) 2.4 Note

PLAT260_ALERT_2_C Large Average Ueq of Residue Including Rh01 0.107 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including S1 0.292 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including S3 0.197 Check

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01991 Ang.

PLAT362_ALERT_2_C Short C(sp3)-C(sp2) Bond C02R - C03B . 1.38 Ang.

PLAT410_ALERT_2_C Short Intra H...H Contact H01X ..H02B . 1.99 Ang.

x,y,z = 1_555 Check

PLAT410_ALERT_2_C Short Intra H...H Contact H015 ..H00T . 1.93 Ang.

x,y,z = 1_555 Check

PLAT410_ALERT_2_C Short Intra H...H Contact H021 ..H013 . 1.99 Ang.

x,y,z = 1_555 Check

PLAT410_ALERT_2_C Short Intra H...H Contact H016 ..H01T . 1.94 Ang.

x,y,z = 1_555 Check

PLAT420_ALERT_2_C D-H Bond Without Acceptor N00X --H00X . Please Check

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -37.050 Report

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -4.427 Report

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.599 484 Report

1 2 0, 2 2 0, 23 2 0, 23 3 0, 14 19 0, 17 22 0,
16 23 0, 14 24 0, 15 24 0, 14 25 0, 13 26 0, 0 32 0,
4 32 0, 1 0 1, 3 0 1, 1 1 1, 0 2 1, 0 3 1,
-23 5 1, 22 9 1, -21 14 1, -17 14 1, -16 16 1, 19 18 1,
18 20 1, -17 22 1, -16 23 1, -13 23 1, 16 23 1, -15 24 1,
14 24 1, 15 24 1, -14 25 1, 13 25 1, 14 25 1, -14 26 1,
-13 26 1, 13 26 1, -13 27 1, 10 29 1, -9 30 1, -7 31 1,
-4 32 1, 0 32 1, 3 32 1, 0 0 2, -1 1 2, 0 1 2,
2 1 2, -2 3 2, 3 3 2, -4 5 2, 21 12 2, 20 15 2,
-20 17 2, -19 19 2, -17 21 2, -17 22 2, -16 23 2, 15 23 2,
-15 24 2, -14 24 2, 14 24 2, 15 24 2, -15 25 2, -14 25 2,
14 25 2, -14 26 2, -13 26 2, 13 26 2, -13 27 2, -10 27 2,
12 27 2, -12 28 2, 11 28 2, -9 30 2, -7 31 2, 6 31 2,
-4 32 2, 0 32 2, 3 32 2, -1 0 3, 2 1 3, -3 4 3,
22 6 3, -23 7 3, -10 11 3, 21 11 3, -9 12 3, 18 19 3,
-18 21 3, -16 24 3, -15 24 3, 14 24 3, -15 25 3, -14 25 3,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.28Ang From Rh02 1.79 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.27Ang From Rh04 1.67 eA-3

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.06Ang From O3 . 0.78 eA-3
 PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.61Ang From O5 . -0.61 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H035 . -0.31 eA-3

● 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: C102 H90 Br4 F18 N6 O26 Rh4 S6

Atom count from the _atom_site data: C98 H90 Br4 F6 N6 O14 Rh4 S2

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 C102 H90 Br4 F18 N6 O26 Rh4 S6

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	408.00	392.00	16.00
H	360.00	360.00	0.00
Br	16.00	16.00	0.00
F	72.00	24.00	48.00
N	24.00	24.00	0.00
O	104.00	56.00	48.00
Rh	16.00	16.00	0.00
S	24.00	8.00	16.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 34 Note
 PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms 134 Report
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report

H00J H00X

PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check

Calc: C98 H90 Br4 F6 N6 O14 Rh4 S2

Rep.: C102 H90 Br4 F18 N6 O26 Rh4 S6

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: C96 H90 Br4 N6 O8 Rh4, 2(C F3 O3 S)

Rep.: C96 H90 Br4 N6 O8 Rh4, 2(C F3 O3 S), 4[CF3SO3]

PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 12.80 %

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 250.00 Why ?

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 10 Report

PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 10 Report

PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 1 Report

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 16 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 3 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report

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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report

PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C13 Check
 PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C18 Check
 PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
 PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 181 Note

Rh01	Rh02	Rh03	Rh04	Br05	Br06	Br07	Br08
O00A	O00B	O00C	O00D	O00E	O00G	O00H	O00I
N00J	H00J	N00K	C023	H023	C029	H029	C01S
C01X	H01X	C024	H024	N00L	C01B	H01B	C01M
H01M	C02A	C01N	H01N	C02D	H02D	N00P	C00Q
H00Q	C015	H015	C00V	C021	H021	C025	H025
C00S	C016	H016	C01U	H01U	C01F	C01J	C01G
H01G	N00X	H00X	C00Y	C00T	H00T	C01W	H01W
C02Q	C01Q	C013	H013	N012	C01P	H01P	C01T
H01T	C01I	C02N	H02N	C035	H035	C01A	C00R
C01O	C01K	C01Y	C01C	C01E	C02B	H02B	C018
H018	C011	C00Z	C014	H014	C01V	C00N	H00N
C00M	C00O	C026	H026	C02G	H02G	C019	C01L
C01H	C020	C010	C017	C02S	C02X	C02I	C02P
C033	C02T	C034	C02R	C00U	C01D	C02W	H02A
H02C	H02E	C02Y	H02F	H02H	H02I	C030	C028
C01Z	C02M	C02V	C031	H03A	H03B	H03C	C036
H03D	H03E	H03F	C03A	H03G	H03H	H03I	C03B
H03J	H03K	H03L	C03C	H03M	H03N	H03O	C03F
H03P	H03Q	H03R	C03G	H03S	H03T	H03U	C03O
H03V	H03W	H03X	C03Q	H03Y	Ha	C03R	H03Z
Hb	Hc	C03T	H03	Hd	He	C03U	Hf
Hg	C045	H04A	H04B	H04C			

PLAT860_ALERT_3_G Number of Least-Squares Restraints 1684 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 !
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
 -1 0 1, 0 1 1,
 PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
 1 2 0,
 PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 27 Note
 -4 5 2, -3 4 3, -2 3 2, -2 3 7, -1 0 1, -1 0 3,
 -1 1 2, -1 1 7, 0 0 2, 0 1 1, 0 1 2, 0 1 4,
 0 2 1, 0 3 1, 0 5 4, 1 0 1, 1 1 1, 1 2 0,
 2 1 2, 2 1 3, 2 2 0, 2 2 5, 2 3 6, 3 2 6,
 3 3 2, 3 3 4, 3 6 7,
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.3 Low
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.000 Note
 Predicted wR2: Based on SigI**2 10.50 or SHELX Weight 29.01
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 27 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 42 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 25 ALERT type 2 Indicator that the structure model may be wrong or deficient
 23 ALERT type 3 Indicator that the structure quality may be low
 13 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check

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.

