

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SB3

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: SB3

Bond precision: C-C = 0.0280 A Wavelength=0.71073

Cell: a=11.3251 (10) b=13.9376 (16) c=15.4756 (17)
 alpha=90 beta=103.189 (4) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	2378.3 (4)	2378.3 (4)
Space group	C c	C c
Hall group	C -2yc	C -2yc
Moiety formula	C20 H32 B3 Ru2 S	?
Sum formula	C20 H32 B3 Ru2 S	C20 H37 B3 Ru2 S
Mr	539.09	544.12
Dx, g cm ⁻³	1.506	1.520
Z	4	4
Mu (mm ⁻¹)	1.359	1.360
F000	1084.0	1104.0
F000'	1074.60	
h, k, lmax	13, 17, 19	13, 17, 19
Nref	4660 [2334]	4439
Tmin, Tmax	0.878, 0.934	0.680, 0.820
Tmin'	0.794	

Correction method= # Reported T Limits: Tmin=0.680 Tmax=0.820
AbsCorr = MULTI-SCAN

Data completeness= 1.90/0.95 Theta (max)= 25.995

R(reflections)= 0.0487 (3479)

wR2(reflections)=
0.1216 (4439)

S = 1.043

Npar= 368

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**

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds 0.028 Ang.

Author Response: This could be because of the disorder of Cp*.

 **Alert level C**

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: `_refine_ls_abs_structure_Flack` 0.500
From the CIF: `_refine_ls_abs_structure_Flack_su` 0.200
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 5.03 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) 6.33 Note
PLAT234_ALERT_4_C Large Hirshfeld Difference S1 --B2 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference S1' --B2 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference S1' --B3 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1 --C5 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C2 --C7 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C4 --C9 . 0.20 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Ru1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & Sth/L= 0.600 2 Report

 **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`: C20 H37 B3 Ru2 S1
Atom count from the `_atom_site` data: C20 H32 B3 Ru2 S1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: `_cell_formula_units_Z` 4
From the CIF: `_chemical_formula_sum` C20 H37 B3 Ru2 S
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	80.00	80.00	0.00
H	148.00	128.00	20.00
B	12.00	12.00	0.00
Ru	8.00	8.00	0.00
S	4.00	4.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 38 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 36 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 11.01 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 7 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 6 Report

PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	5	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	1	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0100	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for SecondPar	0.0200	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0300	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	46%	Note
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C9 Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H8A ..H17A .	2.13	Ang.
	-1/2+x,1/2-y,1/2+z =	4_455	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	893	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.5	Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	52.0	Degree
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
 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
 31 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 8 ALERT type 2 Indicator that the structure model may be wrong or deficient
 14 ALERT type 3 Indicator that the structure quality may be low
 16 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.

