

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) prueba_3_sq

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: prueba_3_sq

Bond precision: C-C = 0.0105 A

Wavelength=0.71070

Cell: a=12.058(2) b=14.584(3) c=17.487(3)
 alpha=74.21(3) beta=71.28(2) gamma=72.92(2)
Temperature: 293 K

	Calculated	Reported
Volume	2729.8(10)	2729.8(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C45 H28 O13 P2 Ru4 S4 [+ solvent]	?
Sum formula	C45 H28 O13 P2 Ru4 S4 [+ solvent]	C46.50 H31 Cl1.50 O13 P2 Ru4 S4
Mr	1371.14	1445.35
Dx, g cm ⁻³	1.668	1.758
Z	2	2
Mu (mm ⁻¹)	1.353	1.429
F000	1344.0	1419.0
F000'	1335.80	
h,k,lmax	15,18,22	14,17,22
Nref	12619	9350
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.741

Theta(max)= 27.573

R(reflections)= 0.0498(7057)

wR2(reflections)= 0.1545(9350)

S = 1.103

Npar= 629

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 A

EXPT005_ALERT_1_A _exptl_crystal_description is missing
Crystal habit description.
The following tests will not be performed.
CRYSR_01

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.896 Note

PLAT183_ALERT_1_A Missing _cell_measurement_reflms_used value Please Do !

PLAT184_ALERT_1_A Missing _cell_measurement_theta_min value Please Do !

PLAT185_ALERT_1_A Missing _cell_measurement_theta_max value Please Do !

🟡 Alert level B

CHEMW03_ALERT_2_B WARNING: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.95 <> 1.05

From the CIF: _cell_formula_units_Z 2

From the CIF: _chemical_formula_weight 1445.35

TEST: Calculate formula weight from _atom_site*

atom	mass	num	sum
C	12.01	45.00	540.49
H	1.01	28.00	28.22
P	30.97	2.00	61.95
O	16.00	13.00	207.99
S	32.07	4.00	128.26
Ru	101.07	4.00	404.28
Cl	35.45	0.00	0.00

Calculated formula weight 1371.20

PLAT911_ALERT_3_B Missing # FCF Refl Between THmin & STh/L= 0.600 1028 Report

PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 1 Check

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers 3 Check

PLAT973_ALERT_2_B Check Calcd Positive Residual Density on Ru1 1.76 eA-3

🟢 Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT230_ALERT_2_C Hirshfeld Test Diff for C14 -- C15 .. 5.3 s.u.

PLAT234_ALERT_4_C Large Hirshfeld Difference O1 -- C33 .. 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C11 -- C12 .. 0.18 Ang.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C15 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C14 Check

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01046 Ang.

PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check

PLAT973_ALERT_2_C Check Calcd Positive Residual Density on Ru2 1.42 eA-3

PLAT973_ALERT_2_C Check Calcd Positive Residual Density on Ru4 1.36 eA-3

PLAT973_ALERT_2_C Check Calcd Positive Residual Density on Ru3 1.33 eA-3

PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Note

🟠 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:C46.5 H31 Cl1.5 O13 P2 Ru4 S4
 Atom count from the _atom_site data: C45 H28 O13 P2 Ru4 S4
 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 2
 From the CIF: _chemical_formula_sum C46.50 H31 Cl1.50 O13 P2 Ru4 S4
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	93.00	90.00	3.00
H	62.00	56.00	6.00
Cl	3.00	0.00	3.00
O	26.00	26.00	0.00
P	4.00	4.00	0.00
Ru	8.00	8.00	0.00
S	8.00	8.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	25	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	10	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 .	5.33	%
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	5	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	2	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	5	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru4 -- C45 ..	5.2	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)..	7	% Note
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT793_ALERT_4_G	The Model has Chirality at P2 (Centro SPGR)	S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	184	Note
PLAT869_ALERT_4_G	ALERTS Related to the use of SQUEEZE Suppressed	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2034	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note

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

16 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 13 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 11 ALERT type 4 Improvement, methodology, query or suggestion
 0 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_EXPT005_prueba_3_sq
;
PROBLEM: _exptl_crystal_description is missing
RESPONSE: ...
;
_vrf_DIFF003_prueba_3_sq
;
PROBLEM: _diffrn_measurement_device_type is missing
RESPONSE: ...
;
_vrf_PLAT029_prueba_3_sq
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .      0.896 Note
RESPONSE: ...
;
_vrf_PLAT183_prueba_3_sq
;
PROBLEM: Missing _cell_measurement_reflns_used value ....    Please Do !
RESPONSE: ...
;
_vrf_PLAT184_prueba_3_sq
;
PROBLEM: Missing _cell_measurement_theta_min value .....    Please Do !
RESPONSE: ...
;
_vrf_PLAT185_prueba_3_sq
```

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;
PROBLEM: Missing _cell_measurement_theta_max value ..... Please Do !
RESPONSE: ...
;
_vrf_PLAT052_prueba_3_sq
;
PROBLEM: Info on Absorption Correction Method Not Given Please Do !
RESPONSE: ...
;
_vrf_PLAT053_prueba_3_sq
;
PROBLEM: Minimum Crystal Dimension Missing (or Error) ... Please Check
RESPONSE: ...
;
_vrf_PLAT054_prueba_3_sq
;
PROBLEM: Medium Crystal Dimension Missing (or Error) ... Please Check
RESPONSE: ...
;
_vrf_PLAT055_prueba_3_sq
;
PROBLEM: Maximum Crystal Dimension Missing (or Error) ... Please Check
RESPONSE: ...
;
_vrf_PLAT230_prueba_3_sq
;
PROBLEM: Hirshfeld Test Diff for C14 -- C15 .. 5.3 s.u.
RESPONSE: ...
;
_vrf_PLAT234_prueba_3_sq
;
PROBLEM: Large Hirshfeld Difference O1 -- C33 .. 0.16 Ang.
RESPONSE: ...
;
_vrf_PLAT241_prueba_3_sq
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of C15 Check
RESPONSE: ...
;
_vrf_PLAT242_prueba_3_sq
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of C14 Check
RESPONSE: ...
;
_vrf_PLAT342_prueba_3_sq
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.01046 Ang.
RESPONSE: ...
;
_vrf_PLAT918_prueba_3_sq
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
RESPONSE: ...
;
_vrf_PLAT973_prueba_3_sq
;
PROBLEM: Check Calcd Positive Residual Density on Ru2 1.42 eA-3
RESPONSE: ...
;
_vrf_PLAT978_prueba_3_sq
;

```

PROBLEM: Number C-C Bonds with Positive Residual Density.

0 Note

RESPONSE: ...

;

end Validation Reply Form

PLATON version of 24/11/2016; check.def file version of 23/11/2016

Datablock prueba_3_sq - ellipsoid plot

