

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: phw1120

Bond precision: O- C = 0.0090 A Wavelength=0.71070

Cell: a=15.5134(6) b=10.8600(4) c=18.0560(12)
alpha=90 beta=106.470(6) gamma=90
Temperature: 110 K

	Calculated	Reported
Volume	2917.2(3)	2917.2(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C12 H38.53 Cl0.47 O8.53 Ru2 S6, C H4 O, Cl, H2 O	C12 H38.53 Cl0.47 O8.53 Ru2 S6, C H4 O, Cl, H2 O
Sum formula	C13 H44.53 Cl1.47 O10.53 Ru2 S6	C13 H44.53 Cl1.47 O10.53 Ru2 S6
Mr	816.09	816.02
Dx,g cm-3	1.858	1.858
Z	4	4
Mu (mm-1)	1.643	1.643
F000	1662.9	1663.0
F000'	1657.24	
h,k,lmax	21,15,25	21,14,25
Nref	8629	7625
Tmin,Tmax	0.812,0.865	0.963,0.987
Tmin'	0.627	

Correction method= ANALYTICAL

Data completeness= 0.884 Theta(max)= 30.150

R(reflections)= 0.0420(6222) wR2(reflections)= 0.0767(7625)

S = 1.181 Npar= 355

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

PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms .. Please Check

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2	Note	
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please	Do !	
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	5	Why ?	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	10.15		
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3		
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru2 -- S5 ..	5.3	su	
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =	7	Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder	Percentage =	50	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	5		
	C1			
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	1	Note	

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
4 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*, 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 18/09/2013; check.def file version of 12/09/2013

Datablock phw1120 - ellipsoid plot

