

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rucs

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: rucs

Bond precision:	C-C = 0.0090 A	Wavelength=0.71073
Cell:	a=31.732(2) b=10.7145(7) c=17.6302(14)	
	alpha=90 beta=116.019(3) gamma=90	
Temperature:	296 K	
	Calculated	Reported
Volume	5386.6(7)	5386.5(7)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C23 H35 B Ru2 S5	?
Sum formula	C23 H35 B Ru2 S5	C23 H35 B Ru2 S5
Mr	684.76	684.76
Dx,g cm-3	1.689	1.689
Z	8	8
Mu (mm-1)	1.520	1.520
F000	2768.0	2768.0
F000'	2753.26	
h,k,lmax	37,12,20	37,12,20
Nref	4746	4742
Tmin,Tmax	0.796,0.859	
Tmin'	0.796	

Correction method= Not given

Data completeness= 0.999 Theta(max)= 24.999

R(reflections)= 0.0409(3414) wR2(reflections)= 0.0880(4742)

S = 1.016 Npar= 283

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

```
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Ru1      --S1      .      5.6 s.u.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..... 0.00895 Ang.
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.      0 Info
```

● Alert level G

```
PLAT128_ALERT_4_G Alternate Setting for Input Space Group      C2/c      I2/a Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C6 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C10 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C9 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C8 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C7 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C20 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C19 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C18 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C17 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C16 Check
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still      51% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).      3 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....      1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...      2 Note
```

```
0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
15 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
4 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
```

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_PLAT232_rucs
;
PROBLEM: Hirshfeld Test Diff (M-X)  Ru1      --S1      .      5.6 s.u.
RESPONSE: ...
;
_vrf_PLAT342_rucs
;
PROBLEM: Low Bond Precision on  C-C Bonds ..... 0.00895 Ang.
RESPONSE: ...
;
_vrf_PLAT978_rucs
;
PROBLEM: Number C-C Bonds with Positive Residual Density.      0 Info
RESPONSE: ...
;
# end Validation Reply Form
```

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 19/10/2018; check.def file version of 15/10/2018

