

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: e__140224b_work_t

Bond precision: Cd-Br = 0.0045 Å Wavelength=0.71073

Cell: a=11.764(8) b=12.025(8) c=8.446(6)
 alpha=90 beta=90 gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	1194.8(14)	1194.8(14)
Space group	A m a 2	Ama2
Hall group	A 2 -2a	?
Moiety formula	Br2 Cd I2, 2(Rb)	?
Sum formula	Br2 Cd I2 Rb2	Br2 Cd I2 Rb2
Mr	696.95	696.96
Dx,g cm-3	3.875	3.874
Z	4	4
Mu (mm-1)	21.707	21.707
F000	1192.0	1192.0
F000'	1176.59	
h,k,lmax	14,14,10	14,14,10
Nref	1158[621]	1118
Tmin,Tmax	0.131,0.114	0.220,0.220
Tmin'	0.099	

Correction method= NONE

Data completeness= 1.80/0.97 Theta(max)= 25.410

R(reflections)= 0.0557(1002) wR2(reflections)= 0.1819(1118)

S = 1.103 Npar= Npar = 40

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

ABSTY03_ALERT_1_C The _exptl_absorpt_correction_type has been given as none.

However values have been given for Tmin and Tmax. Remove these if an absorption correction has not been applied.

From the CIF: _exptl_absorpt_correction_T_min 0.220

From the CIF: _exptl_absorpt_correction_T_max 0.220

PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
Br2 Cd I2

● Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.13 Why ?
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 148 Do !
CD1 -BR1 -RB2 -CD1 180.00 0.00 1.555 1.555 1.555 1.554
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 149 Do !
RB1 -BR1 -RB2 -CD1 -83.37 0.10 3.465 1.555 1.555 1.554
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 150 Do !
RB1 -BR1 -RB2 -CD1 83.37 0.10 1.555 1.555 1.555 1.554
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 164 Do !
RB2 -BR2 -RB2 -BR1 180.00 0.01 5.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 167 Do !
CD1 -BR2 -RB2 -BR2 0.00 0.01 1.555 1.555 1.555 5.544
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 168 Do !
RB2 -BR2 -RB2 -BR2 180.00 0.01 5.555 1.555 1.555 5.544
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 169 Do !
RB1 -BR2 -RB2 -BR2 -125.81 0.06 7.464 1.555 1.555 5.544
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 170 Do !
RB1 -BR2 -RB2 -BR2 125.81 0.06 5.554 1.555 1.555 5.544
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 172 Do !
RB2 -BR2 -RB2 -I1 -37.96 0.06 5.555 1.555 1.555 4.654
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 176 Do !
RB2 -BR2 -RB2 -I1 37.96 0.06 5.555 1.555 1.555 1.554
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 180 Do !
RB2 -BR2 -RB2 -I1 105.62 0.06 5.555 1.555 1.555 6.764
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 184 Do !
RB2 -BR2 -RB2 -I1 -105.62 0.06 5.555 1.555 1.555 7.464
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 188 Do !
RB2 -BR2 -RB2 -CD1 0.00 0.01 5.555 1.555 1.555 1.554
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 192 Do !
RB2 -BR2 -RB2 -RB1 54.19 0.06 5.555 1.555 1.555 5.554
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 195 Do !
RB2 -BR2 -RB2 -RB1 -54.19 0.06 5.555 1.555 1.555 7.464
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 198 Do !
RB2 -BR2 -RB2 -RB1 -59.65 0.15 5.555 1.555 1.555 3.464
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 202 Do !
RB2 -BR2 -RB2 -RB1 59.65 0.15 5.555 1.555 1.555 1.554
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
Rb
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1 (II) 2.17 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

21 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

1 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
19 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 05/02/2014; check.def file version of 05/02/2014

