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: RbSe3B2O9OH

Bond precision: O-B = 0.0212 AWavelength=0.71073 Cell: a=4.6591(3) b=11.9288(8) c=16.3321(10)alpha=90 beta=90 gamma=90 Temperature: 293 K Calculated Reported Volume 907.70(10) 907.70(10)P 21 21 21 Space group P2(1)2(1)2(Hall group P 2ac 2ab ? Moiety formula B4 H2 O20 Se6, 2(Rb) ? B4 H2 O20 Rb2 Se6 Sum formula H B2 010 Rb Se3 Mr 1009.96 504.98 3.695 3.695 Dx,q cm-3 Ζ 2 4 Mu (mm-1) 17.525 17.525 F000 920.0 920.0 916.13 F000′ h,k,lmax 5,14,19 5,14,19 1603[974] Nref 1386 0.239,0.496 0.115,1.000 Tmin,Tmax Tmin' 0.004 Correction method= # Reported T Limits: Tmin=0.115 Tmax=1.000 AbsCorr = MULTI-SCAN Data completeness= 1.42/0.86 Theta(max) = 24.990R(reflections) = 0.0572(1106) wR2(reflections) = 0.1497(1386) S = 1.053Npar= 135

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

CHEMS01_ALERT_1_B The sum formula contains elements in the wrong order. H precedes B Sequence must be alphabetical for inorganic structures.

🏓 Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field. Absorption correction given as multi-scan Flack test results are ambiguous. STRVA01_ALERT_4_C From the CIF: _refine_ls_abs_structure_Flack 0.490 From the CIF: _refine_ls_abs_structure_Flack_su 0.050 PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check PLAT090 ALERT 3 C Poor Data / Parameter Ratio (Zmax > 18) 7.21 Note PLAT213_ALERT_2_C Atom 04 has ADP max/min Ratio 3.9 prolat PLAT220_ALERT_2_C Non-Solvent Resd 1 0 Ueq(max)/Ueq(min) Range 3.6 Ratio PLAT234_ALERT_4_C Large Hirshfeld Difference Se1 --O5_h 0.19 Ang. PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 04 Check

Alert level G

2	Report
2	Info
Please	Do !
1	Report
0.490	Note
0.50	Check
293	Check
293	Check
119.8	Degree
120.7	Degree
121.1	Degree
120.7	Degree
123.3	Degree
125.0	Degree
12	Note
2017	Note
	2 2 Please 1 0.490 0.50 293 293 119.8 120.7 121.1 120.7 123.3 125.0 12 2017

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0 ALERT level A = Most likely a serious problem - resolve or explain
1 ALERT level B = A potentially serious problem, consider carefully
8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
16 ALERT level G = General information/check it is not something unexpected
6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 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
3 ALERT type 5 Informative message, check
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Datablock: CsSe3B2O9OH

Bond precision: O-B = 0.0075 A

Wavelength=0.71073

a=4.6710(17) Cell: b=12.236(5) c=16.417(6) alpha=90 beta=90 gamma=90 298 K Temperature: Calculated Reported Volume 938.3(6) 938.4(6) Space group P 21 21 21 P2(1)2(1)2(Hall group P 2ac 2ab ? Moiety formula B4 H2 O20 Se6, 2(Cs) ? H B2 Cs 010 Se3 Sum formula B4 Cs2 H2 O20 Se6 1104.84 552.42 Mr Dx,g cm-3 3.911 3.910 Ζ 2 4 Mu (mm-1) 15.624 15.623 992.0 F000 992.0 F000′ 990.26 h,k,lmax 6,15,21 6,15,21 Nref 2133[1277] 2130 Tmin,Tmax 0.338,0.535 0.115,1.000 Tmin′ 0.019 Correction method= # Reported T Limits: Tmin=0.115 Tmax=1.000 AbsCorr = MULTI-SCAN Data completeness= 1.67/1.00 Theta(max)= 27.480 R(reflections) = 0.0261(2064) wR2(reflections) = 0.0570(2130) S = 1.088Npar= 131

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 CHEMS01_ALERT_1_B The sum formula contains elements in the wrong order. H precedes B Sequence must be alphabetical for inorganic structures.

Alert level C

PLAT230_	ALERT_	_2_C	Hirshfeld	Test	Diff	for	Se1		05_h	6.0	s.u.
PLAT907_	ALERT_	_2_C	Flack x >	0.5,	Struc	cture	Needs	to b	e Inverted?	0.56	Check

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Alert level G
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...
                                                                         1 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension
                                                                        2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF
                                                                    Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....
                                                                        1 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .
                                                                    0.557 Note
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...
                                                                     0.50 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2
                                                                     121.5 Degree
                                  Angle From 120 for O3
PLAT395_ALERT_2_G Deviating X-O-Y
                                                                    120.7 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4
                                                                    121.3 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O6
                                                                    119.2 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for 07
                                                                    122.3 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for 09
                                                                    124.3 Degree
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
                                                                        6 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL
                                                                    2017 Note
  0 ALERT level A = Most likely a serious problem - resolve or explain
  1 ALERT level B = A potentially serious problem, consider carefully
  7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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14 ALERT level G = General information/check it is not something unexpected

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

PLATON version of 13/12/2017; check.def file version of 12/12/2017



