

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sdk-k4

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: sdk-k4

Bond precision:	C-C = 0.0168 A	Wavelength=0.71073	
Cell:	a=39.516(5)	b=6.2571(11)	c=17.424(2)
	alpha=90	beta=102.668(12)	gamma=90
Temperature:	294 K		
	Calculated	Reported	
Volume	4203.3(10)	4203.4(10)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	2(C14 H9 Br N2 O4 V), H18 Na2 O9, 2(H2 O)	2(C14 H9 Br N2 O4 V), H18 Na2 O9, 2(H2 O)	
Sum formula	C28 H40 Br2 N4 Na2 O19 V2	C28 H40 Br2 N4 Na2 O19 V2	
Mr	1044.30	1044.32	
Dx,g cm-3	1.650	1.650	
Z	4	4	
Mu (mm-1)	2.443	2.443	
F000	2104.0	2104.0	
F000'	2105.41		
h,k,lmax	54,8,23	53,8,23	
Nref	11253	9936	
Tmin,Tmax	0.485,0.599	0.160,1.000	
Tmin'	0.212		

Correction method= # Reported T Limits: Tmin=0.160 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.883 Theta(max)= 29.055

R(reflections)= 0.1347(4281) wR2(reflections)= 0.3147(9936)

S = 1.065 Npar= 550

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**

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 0.402
Additional refinement cycles may be required.

Author Response: Crystal quality was not that good. But after several attempt this data

PLAT080_ALERT_2_A Maximum Shift/Error 0.40 Why ?

**Author Response: Alert comes due to non-convergent refinement as the
crystal quality wa**

PLAT203_ALERT_2_A Negative Isotropic ADP for H14A -0.001 Report

Author Response: Crystal quality was not that good. But after several attempt this data

PLAT355_ALERT_3_A Long O-H (X0.82,N0.98A) O13 - H13B . 1.22 Ang.

Author Response: same as above

PLAT417_ALERT_2_A Short Inter D-H..H-D H16A ..H19B .. 1.33 Ang.

Author Response: same as above

 **Alert level B**

PLAT110_ALERT_2_B ADDSYM Detects Potential Lattice Translation ... ? Check
PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem I 100 %Fit
PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group I2/c Check
Note: (Pseudo) Lattice Translation Implemented
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.01679 Ang.
PLAT355_ALERT_3_B Long O-H (X0.82,N0.98A) O14 - H14B . 1.10 Ang.

Author Response: same as above

PLAT417_ALERT_2_B Short Inter D-H..H-D H10A ..H16B .. 1.95 Ang.

Author Response: same as above

PLAT417_ALERT_2_B Short Inter D-H..H-D H10A ..H18B .. 2.04 Ang.

Author Response: same as above

PLAT417_ALERT_2_B Short Inter D-H..H-D H15B ..H19B .. 2.07 Ang.

Author Response: same as above

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 16 Note

● **Alert level C**

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	43%	Check
PLAT082_ALERT_2_C	High R1 Value	0.13	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.31	Report
PLAT213_ALERT_2_C	Atom C4 has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C	Atom C11 has ADP max/min Ratio	3.7	prolat
PLAT213_ALERT_2_C	Atom C14 has ADP max/min Ratio	3.5	oblate
PLAT223_ALERT_4_C	Solv./Anion Resd 3 H Ueq(max)/Ueq(min) Range	10.0	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C11 --C12	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C19 --C20	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C24 --C25	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C26 --C27	0.18	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C11	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C5	Check
PLAT245_ALERT_2_C	U(iso) H12A Smaller than U(eq) O12 by	0.030	Ang**2
PLAT245_ALERT_2_C	U(iso) H12B Smaller than U(eq) O12 by	0.015	Ang**2
PLAT245_ALERT_2_C	U(iso) H13A Smaller than U(eq) O13 by	0.034	Ang**2
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.5	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.1	Note
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist C15 -C20	1.37	Ang.
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O14 - H14A .	1.05	Ang.

Author Response: same as above

PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1	Note
	C14 H9 Br N2 O4 V		
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	81.206	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	11.698	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.857	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.164	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.326	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	9	Report
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 1.07A From O17	-0.45	eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Info

● **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	16	Report
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	0.63	mm
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	52.98	Why ?
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C15 -C20	0.15	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1	Note
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	3	Info
PLAT908_ALERT_2_G	Max. Perc. Data with I > 2*s(I) per Res.Shell .	65.56%	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1293	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2	Note

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

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

