checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2

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: 2

Bond precision: C-C = 0.0143 A Wavelength=0.71073

Cell: a=31.9947(6) b=9.10191(15) c=14.9567(3)
alpha=90 beta=90 gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	4355.58(14)	4355.57(14)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C24 H48 Br6 Cs3 O12 Sb	2(C12 H24 Cs O6), Br6 Cs Sb
Sum formula	C24 H48 Br6 Cs3 O12 Sb	C24 H48 Br6 Cs3 O12 Sb
Mr	1528.52	1528.56
Dx,g cm-3	2.331	2.331
Z	4	4
Mu (mm-1)	8.656	8.656
F000	2856.0	2856.0
F000’	2844.13	
h,k,lmax	48,13,22	48,13,22
Nref	16107[8317]	15190
Tmin,Tmax		0.074,0.107
Tmin’		

Correction method= # Reported T Limits: Tmin=0.074 Tmax=0.107
AbsCorr = SPHERE

Data completeness= 1.83/0.94 Theta(max)= 32.763

R(reflections)= 0.0423(13815) wR2(reflections)= 0.0971(15190)

S = 1.106 Npar= 416

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

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.494
From the CIF: _refine_ls_abs_structure_Flack_su 0.014
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01433 Ang.

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.90 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br2 . 10.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br3 . 5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br4 . 7.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br5 . 6.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1 --Br6 . 6.0 s.u.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.13 Ratio
PLAT774_ALERT_1_G Check X-Y Bond in CIF: Cs3 --Sb1 .. 4.54 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Sb1 (III) . 2.65 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 269 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
5 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* 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 22/04/2020; check.def file version of 09/03/2020

Datablock 2 - ellipsoid plot