checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: Bi- O = 0.0719 A Wavelength=0.71073

Cell: a=5.5119(1) b=5.5119(1) c=29.0984(14)
alpha=90 beta=90 gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	884.04(5)	884.04(5)
Space group	P 21 c n	P 21 c n
Hall group	P -2n 2a	P -2n 2a
Moiety formula	Bi8 Nb2 O16, 2(Br)	Bi4 Br Nb O8
Sum formula	Bi8 Br2 Nb2 O16	Bi4 Br Nb O8
Mr	2273.46	1136.74
Dx,g cm-3	8.541	8.541
Z	2	4
Mu (mm-1)	85.150	85.150
F000	1888.0	1888.0
F000’	1820.83	
h,k,lmax	6,6,36	6,6,36
Nref	1798[995]	1978
Tmin,Tmax	0.002,0.154	0.011,0.227
Tmin’	0.000	

Correction method= # Reported T Limits: Tmin=0.011 Tmax=0.227
AbsCorr = GAUSSIAN

Data completeness= 1.99/1.10 Theta(max)= 26.359

R(reflections)= 0.0850(1681) wR2(reflections)= 0.2488(1978)

S = 1.179 Npar= 53

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

ATOM007_ALERT_1_A _atom_site_aniso_label is missing
Unique label identifying the atom site.

Alert level B

DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00
_refine_diff_density_min given = -12.094
Test value = -8.300
SYMMS02_ALERT_1_B The unit-cell lengths a and b should not be equal for an
orthorhombic cell
Cell 5.5119 5.5119 29.0984
Angles 90.0000 90.0000 90.0000
PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 11.45 eA-3
PLAT098_ALERT_2_B Large Reported Min. (Negative) Residual Density -12.09 eA-3
PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Ima2 Check
Note: (Pseudo) Lattice Translation Implemented

Alert level C

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro .... Please Do !
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 1 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
Bi8 Nb2 O16

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 283.58 Why ?
PLAT110_ALERT_2_G ADDSYM Detects Potential Lattice Translation ... ? Check
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem I 100 %Fit
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Nb1 (V) . 5.48 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT898_ALERT_4_G Second Reported H-M Symbol in CIF Ignored ..... ! Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT931_ALERT_5_G Found Twin Law (1 1 0)[ ] Est. BASF 0.52 Check
PLAT931_ALERT_5_G Found Twin Law ( )[1 1 0] Est. BASF 0.52 Check

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
4 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 30/01/2018; check.def file version of 30/01/2018

Datablock shelx - ellipsoid plot