checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Bi8TlAlCl43_RT_P63m

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: Bi8TlAlCl43_RT_P63m

Bond precision: Cl-Al = 0.0057 A Wavelength=0.71073

Cell: a=13.0332(10) b=13.0332(10) c=10.3986(5)
alpha=90 beta=90 gamma=120
Temperature: 296 K

	Calculated	Reported
Volume	1529.7(3)	1529.7(2)
Space group	P 63/m	P 63/m
Hall group	-P 6c	-P 6c
Moiety formula	0.667(Bi9), 3(Al Cl4), 2(Bi), Tl	?
Sum formula	Al3 Bi8 Cl12 Tl	Al3 Bi8 Cl12 Tl
Mr	2382.46	2382.55
Dx,g cm-3	5.173	5.173
Z	2	2
Mu (mm-1)	52.206	52.209
F000	1975.9	1976.0
F000’	1916.81	
h,k,lmax	16,16,12	16,16,12
Nref	1080	1077
Tmin,Tmax	0.011,0.048	0.097,0.250
Tmin’	0.003	

Correction method= # Reported T Limits: Tmin=0.097 Tmax=0.250
AbsCorr = NUMERICAL

Data completeness= 0.997 Theta(max)= 26.154

R(reflections)= 0.0392(799) wR2(reflections)= 0.0953(1077)

S = 1.040 Npar= 63

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

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of Al1 Check

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Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 14.40 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of Bi1 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Bi3 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Bi4 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Bi2 Constrained at 0.6667 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 3 0.33 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 4 0.17 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Tl1 (I) . 0.67 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al1 (III) . 3.17 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 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
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
7 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 18/02/2019; check.def file version of 18/02/2019

Datablock Bi8TlAlCl43_RT_P63m - ellipsoid plot