

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) averievite-PKBr

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: averievite-PKBr

Bond precision:	P- O = 0.0075 A	Wavelength=0.71073
Cell:	a=10.9738(5) b=6.3067(3) c=15.7610(5)	
	alpha=90 beta=95.424(4) gamma=90	
Temperature:	296 K	
	Calculated	Reported
Volume	1085.91(8)	1085.91(8)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	Br2 Cu10 O20 P4, 2(K)	Br, 0.25(Cu20 K4 O40 P8)
Sum formula	Br2 Cu10 K2 O20 P4	Br Cu5 K O10 P2
Mr	1317.38	658.65
Dx,g cm-3	4.029	4.029
Z	2	4
Mu (mm-1)	14.032	14.032
F000	1236.0	1236.0
F000'	1243.50	
h,k,lmax	15,8,22	15,8,22
Nref	1585	3738
Tmin,Tmax	0.066,0.431	0.757,1.000
Tmin'	0.042	

Correction method= # Reported T Limits: Tmin=0.757 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 2.358 Theta(max)= 29.996

R(reflections)= 0.0552(3572) wR2(reflections)= 0.1427(3738)

S = 1.126 Npar= 93

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

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.458	Check
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	2	Check
PLAT939_ALERT_3_C	Large Value of Not (SHELXL) Weight Optimized S .	15.97	Check

● 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
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	56.12	Why ?
PLAT300_ALERT_4_G	Atom Site Occupancy of K1 Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1	Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law [1-1 0] Est.d BASF	0.25	Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law [1-1 0] Est.d BASF	0.25	Check
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.4	Low
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	1	Check

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 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

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.

