

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) plumbogaidonnayite

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: plumbogaidonnayite

Bond precision: Si- O = 0.0130 A Wavelength=1.54184

Cell: a=11.7690(4) b=12.9867(3) c=6.66165(16)

 alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	1018.17(5)	1018.17(5)
Space group	P 21 n b	P 21 n b
Hall group	P -2bc 2a	P -2bc 2a
Moiety formula	Ca0.72 K0.56 O44 Pb2.63 Si12 Zr4	Ca0.18 K0.14 O11 Pb0.66 Si3 Zr
Sum formula	Ca0.72 K0.56 O44 Pb2.63 Si12 Zr4	Ca0.18 K0.14 O11 Pb0.66 Si3 Zr
Mr	2001.24	500.40
Dx, g cm ⁻³	3.264	3.264
Z	1	4
Mu (mm ⁻¹)	34.702	34.716
F000	920.5	921.0
F000'	915.26	
h, k, lmax	14, 16, 8	14, 16, 8
Nref	2166[1138]	1859
Tmin, Tmax	0.524, 0.499	0.400, 1.000
Tmin'	0.476	

Correction method= # Reported T Limits: Tmin=0.400 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.63/0.86

Theta(max)= 77.550

R(reflections) = 0.0559 (1788)

wR2(reflections) =
0.1355 (1859)

S = 1.114

Npar = 182

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 B

PLAT213_ALERT_2_B	Atom	has ADP max/min Ratio	4.3	prolat
PLAT241_ALERT_2_B	High	'MainMol' Ueq as Compared to Neighbors of	011	Check
PLAT987_ALERT_1_B	The Flack x is >> 0 -	Do a BASF/TWIN Refinement		Please Check

Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings	Differ		Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms	..		Please Check
PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	6.19	Note
PLAT220_ALERT_2_C	NonSolvent Resd 1 0	Ueq(max)/Ueq(min) Range	6.0	Ratio
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		Si3 Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		09 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.265	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		2 Report
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.99Ang From O11		0.96 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.05Ang From O2		0.70 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	1.05Ang From O6		-0.66 eA-3

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		2	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor	...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)	...		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	17.92	Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group	P21nb		Pna21 Note
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	6%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O2		135.1	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O3		133.0	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O6		135.2	Degree
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		10 Note
PLAT915_ALERT_3_G	No Flack x Check Done: Low Friedel Pair Coverage		71	%
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		3	Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
11 **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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

13 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
3 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.

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