

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) armellinoite-Ce

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: armellinoite-Ce

Bond precision: = 0.0000 A Wavelength=0.71073

Cell: a=10.749(2) b=10.749(2) c=12.030(2)
 alpha=90 beta=90 gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	1390.0(6)	1390.0(6)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	As14.82 Ce4.34 O64 P1.18, 4(H2 O), 15.664(Ca)	?
Sum formula	As14.82 Ca15.66 Ce4.34 H8 O68 P1.18	As1.85 H Ca1.96 Ce0.54 O8.50 P0.15
Mr	3478.12	434.71
Dx, g cm ⁻³	4.155	4.155
Z	1	8
Mu (mm ⁻¹)	13.872	13.871
F000	1623.5	1623.0
F000'	1627.78	
h, k, lmax	16, 16, 18	16, 11, 18
Nref	1274	1275
Tmin, Tmax	0.095, 0.125	0.091, 0.120
Tmin'	0.072	

Correction method= # Reported T Limits: Tmin=0.091 Tmax=0.120

AbsCorr = MULTI-SCAN

Data completeness= 1.001

Theta(max)= 32.557

R(reflections)= 0.0227(1136)

wR2(reflections)=
0.0523(1275)

S = 1.167

Npar= 71

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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.144 Check
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.52A	From O5	1.00 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.87A	From O5	0.57 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.50A	From O5	0.52 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.52A	From O5	0.49 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.52A	From O5	0.49 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.52A	From O5	0.49 eA-3

● Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
From the CIF: _cell_formula_units_Z 8
From the CIF: _chemical_formula_sum As1.85 H Ca1.96 Ce0.54 O8.50 P0.15
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
As	14.80	14.82	-0.02
H	8.00	8.00	0.00
Ca	15.68	15.66	0.02
Ce	4.32	4.34	-0.02
O	68.00	68.00	0.00
P	1.20	1.18	0.02

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT017_ALERT_1_G	Check Scattering Type Consistency of AAas	CA	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of AB as	CE	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of BA as	CE	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of BBas	CA	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of TA as	AS	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of TB as	P	
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.12	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	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	9.33	Why ?
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	3	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O5 Constrained at	0.25	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	32%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	6	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info

PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.9	Low
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ		5	Units

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

12 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
3 ALERT type 3 Indicator that the structure quality may be low
9 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.

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