

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) attalinite-Ce = [letnikovite-\(Ce\)](#)

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: attalinite-Ce

Bond precision:	Si- O = 0.0156 A	Wavelength=0.71073
Cell:	a=7.4726 (3) b=22.9196 (9) c=13.9360 (6)	alpha=90 beta=105.550 (5) gamma=90
Temperature:	298 K	
	Calculated	Reported
Volume	2299.44 (17)	2299.43 (17)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	Ce7.21 F4 O72 Si28, 15.471(F), 10.4(O), 0.162(Cs), 7.22(Ca), 1.	?
Sum formula	Ca7.22 Ce7.21 Cs0.16 F19.47 Mg1.44 Na4 O82.40 Si28	Ca1.805 Ce1.803 Cs0.04 F4.87 Mg0.36 O20.60 Si7
Mr	3922.59	981.93
Dx, g cm-3	2.833	2.833
Z	1	4
Mu (mm-1)	4.516	4.516
F000	1859.0	1859.0
F000'	1862.36	
h, k, lmax	9, 29, 17	9, 29, 17
Nref	2596	2580
Tmin, Tmax	0.869, 0.905	0.868, 0.905
Tmin'	0.809	

Correction method= # Reported T Limits: Tmin=0.868 Tmax=0.905
AbsCorr = MULTII-SCAN

Data completeness= 0.994

Theta(max)= 26.999

R(reflections)= 0.0420 (2126)

wR2(reflections)=
0.1164 (2580)

S = 1.124

Npar= 183

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

SHFSU01_ALERT_2_B The absolute value of parameter shift to su ratio > 0.10
Absolute value of the parameter shift to su ratio given 0.183
Additional refinement cycles may be required.

PLAT080_ALERT_2_B Maximum Shift/Error 0.18 Why ?
O3 O8 O10

PLAT213_ALERT_2_B Atom O1 has ADP max/min Ratio 5.0 prolat
PLAT213_ALERT_2_B Atom O4 has ADP max/min Ratio 4.6 prolat
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) W1 Check

● Alert level C

CHEMW01_ALERT_1_C The ratio of given/expected molecular weight as calculated
from the _chemical_formula_sum lies outside
the range 0.99 <> 1.01
Calculated formula weight = 957.7586
Formula weight given = 981.9296

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 5.12 Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 2 Check
X1 W1

PLAT213_ALERT_2_C Atom O5 has ADP max/min Ratio 3.3 prolat
PLAT214_ALERT_2_C Atom A2 (Anion/Solvent) ADP max/min Ratio 4.6 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 5.1 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si4 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 13 Report

● Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: Cal.805 Ce1.803 Cs.04 F4.87 Mg0.
Atom count from the _atom_site data: Cal.805 Ce1.802 Cs.0406 F4.8677

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT017_ALERT_1_G Check Scattering Type Consistency of M1 as CE
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2as CA
PLAT017_ALERT_1_G Check Scattering Type Consistency of M3as CA
PLAT017_ALERT_1_G Check Scattering Type Consistency of M4 as MG
PLAT017_ALERT_1_G Check Scattering Type Consistency of A1as NA
PLAT017_ALERT_1_G Check Scattering Type Consistency of A2 as CS
PLAT017_ALERT_1_G Check Scattering Type Consistency of X1 as F
PLAT017_ALERT_1_G Check Scattering Type Consistency of X2 as F
PLAT017_ALERT_1_G Check Scattering Type Consistency of X3 as F
PLAT017_ALERT_1_G Check Scattering Type Consistency of X4 as F

PLAT017_ALERT_1_G	Check Scattering Type Consistency of W1	as	0	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of W2	as	0	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of W3	as	0	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of W4	as	0	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of W5	as	0	
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.250	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical		?	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		33.41	Why ?
PLAT300_ALERT_4_G	Atom Site Occupancy of X1	Constrained at	0.9244	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of X3	Constrained at	0.9811	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of X4	Constrained at	0.9811	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of W2	Constrained at	0.44	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of W3	Constrained at	0.19	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of W4	Constrained at	0.16	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of W5	Constrained at	0.23	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of A2	Constrained at	0.0406	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	6%	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
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 6)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 7)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 8)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 9)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 10)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 11)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 13)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 14)	100%	Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	W2	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	W3	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	W4	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	W5	Check
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O1	.	128.2	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O4	.	136.0	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O8	.	134.9	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Si1 ..X4 .	3.36	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Si4 ..W3 .	2.87	Ang.
		1/2+x,1/2-y,z =	8_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Si4 ..W3 .	2.87	Ang.
		1/2+x,-1/2+y,z =	3_545	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Si4 ..W5 .	2.96	Ang.
		1/2+x,-1/2+y,z =	3_545	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Si4 ..W5 .	2.96	Ang.
		1/2+x,1/2-y,z =	8_555	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	X2 ..X4 .	2.66	Ang.
		x,y,z =	1_555	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	X2 ..X4 .	2.66	Ang.
		1-x,y,1-z =	2_656	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		15	Note
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters		1	Info
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		!	Info
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..		!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3	Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (0 0 1) Est.d BASF		0.48	Check
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		1	Note

PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 54.0 Degree

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

21 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
28 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
23 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.

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