

checkCIF/PLATON report

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

Bond precision: Si- O = 0.0070 Å Wavelength=0.71073

Cell: a=8.8238(13) b=5.7131(9) c=10.0034(16)
 alpha=90 beta=112.823(6) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	464.80(13)	464.80(13)
Space group	P 21/m	P 21/m
Hall group	-P 2yb	-P 2yb
Moiety formula	Al _{3.43} Ce _{1.93} H ₂ Mn _{4.07} O ₂₆ Si ₆ , 2(Ca _{0.25}), 0.066(Ca)	Al _{3.43} Ce _{1.93} H ₂ Mn _{4.07} O ₂₆ Si ₆ , 2(Ca _{0.25}), 0.066(Ca)
Sum formula	Al _{3.43} Ca _{0.57} Ce _{1.93} H ₂ Mn _{4.07} O ₂₆ Si ₆	Al _{3.43} Ca _{0.57} Ce _{1.93} H ₂ Mn _{4.07} O ₂₆ Si ₆
Mr	1196.49	1196.49
Dx, g cm ⁻³	4.275	4.275
Z	1	1
Mu (mm ⁻¹)	8.174	8.174
F000	563.9	564.0
F000'	565.84	
h, k, lmax	14, 9, 16	14, 9, 16
Nref	2232	2224
Tmin, Tmax	0.783, 0.849	0.819, 0.923
Tmin'	0.783	

Correction method= # Reported T Limits: Tmin=0.819 Tmax=0.923

AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 35.123

R(reflections)= 0.0575(1565)

wR2(reflections)=
0.1373(2224)

S = 1.028

Npar= 126

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 A

PLAT974_ALERT_2_A	Check Calcd Negative Resid. Density on	A2CE	-2.07 eA-3
PLAT974_ALERT_2_A	Check Calcd Negative Resid. Density on	A2CA	-2.07 eA-3

Alert level B

PLAT972_ALERT_2_B	Check Calcd Resid. Dens.	0.67Ang From A2CE	-2.60 eA-3
PLAT975_ALERT_2_B	Check Calcd Resid. Dens.	0.92Ang From O10	1.65 eA-3

Alert level C

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check	
PLAT927_ALERT_1_C	Reported and Calculated wR2 Differ by	-0.0013 Check	
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.81Ang From A2CE	2.10 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.86Ang From O6	1.66 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.92Ang From O10	1.65 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.21Ang From A2CE	1.62 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.73Ang From M3AL	1.59 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.52Ang From O9	1.51 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.65Ang From A2CE	-2.34 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.62Ang From A2CE	-2.21 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.63Ang From O8	1.49 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.73Ang From O6	1.12 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	1.07Ang From O8	-1.14 eA-3

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.38	Why ?
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	4	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder	27%	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
PLAT303_ALERT_2_G	Full Occupancy Atom H with # Connections	3.00	Check
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O9	136.2	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	9	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !	
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	8	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check	
PLAT982_ALERT_1_G	The Al-f' = 0.0560 Deviates from IT-value =	0.0645	Check
PLAT982_ALERT_1_G	The Ca-f' = 0.2030 Deviates from IT-value =	0.2262	Check

PLAT982_ALERT_1_G	The Ce-f' =	-0.5640	Deviates from	IT-value =	-0.2486	Check
PLAT982_ALERT_1_G	The Mn-f' =	0.2950	Deviates from	IT-value =	0.3368	Check
PLAT982_ALERT_1_G	The O-f' =	0.0080	Deviates from	IT-value =	0.0106	Check
PLAT982_ALERT_1_G	The Si-f' =	0.0720	Deviates from	IT-value =	0.0817	Check
PLAT983_ALERT_1_G	The Ce-f" =	2.6320	Deviates from	IT-Value =	2.6331	Check

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

12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 19 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
 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.

