

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shen01-5h

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: shen01-5h

Bond precision:	Si- O = 0.0035 A	Wavelength=0.71073	
Cell:	a=8.9687 (4)	b=5.77714 (19)	c=10.2272 (5)
	alpha=90	beta=114.927 (6)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	480.54 (4)	480.54 (4)	
Space group	P 21/m	P 21/m	
Hall group	-P 2yb	-P 2yb	
Moiety formula	Al3.17 Ce Fe2.31 H2 La0.52 Mn0.08 Nd0.16 O26 Pr0.14 Si6 Ti0.22,	?	
Sum formula	Al3.17 Ca2 Ce Fe2.31 H2 La0.52 Mn0.08 Nd0.16 O26 Pr0.14 Si6 Ti0	Al1.58 H Ca Ce0.50 Fe1.15 La0.26 Mn0.04 Nd0.08 O13 Pr0.07 Si3 T	
Mr	1150.16	574.69	
Dx, g cm ⁻³	3.974	3.972	
Z	1	2	
Mu (mm ⁻¹)	7.249	7.239	
F000	547.1	547.0	
F000'	548.93		
h, k, lmax	13, 9, 15	13, 8, 15	
Nref	2062	1850	
Tmin, Tmax	0.256, 0.235		
Tmin'	0.216		

Correction method= Not given

Data completeness= 0.897

Theta (max)= 33.675

R(reflections)= 0.0307(1692)

wR2(reflections)=
0.0879(1850)

S = 1.244

Npar= 128

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
PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density		2.19 Report
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)		02 Check
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)		03 Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.80A	From Nd2	1.92 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.60A	From O10	1.67 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.74A	From O2	0.59 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.75A	From O10	0.51 eA-3

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		2 Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3 Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.50 Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records		5 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		5 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		1 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	(K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	(K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Nd2	Constrained at	0.08 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Pr2	Constrained at	0.07 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ce2	Constrained at	0.416 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of La2	Constrained at	0.26 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mn3	Constrained at	0.04 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ti3	Constrained at	0.11 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	Constrained at	0.08 Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	28% 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
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		1 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		213 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.6 Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

10 **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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
14 ALERT type 4 Improvement, methodology, query or suggestion
2 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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