

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: I

Bond precision:	= 0.0000 A	Wavelength=0.29060	
Cell:	a=6.7878 (5)	b=7.0034 (13)	c=6.4691 (3)
	alpha=90	beta=103.554 (6)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	298.96 (6)	298.96 (6)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yabc	
	As0.17 Ce1.83 La0.84 Nd0.74		
Moiety formula	O16 P3.83 Pr0.20 Sm0.12	?	
	Th0.08, 0.1		
	As0.17 Ca0.19 Ce1.83 La0.84	Ce0.4566 La0.2104 Nd0.1848	
Sum formula	Nd0.74 O16 P3.83 Pr0.20	Pr0.0503 Ca0.0467 Th0.0199	
	Sm0.12 Th0.	Sm0.0312	
Mr	939.71	234.90	
Dx, g cm-3	5.220	5.220	
Z	1	4	
Mu (mm-1)	5.681	5.753	
F000	419.8	420.0	
F000'	411.64		
h, k, lmax	15, 15, 14	13, 9, 14	
Nref	3577	870	
Tmin, Tmax		0.821, 1.000	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.821 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.243 Theta (max)= 19.080

R(reflections)= 0.0425(805)

wR2(reflections)=

wR= 0.0530(870)

S = 3.030

Npar= 36

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

EXPT005_ALERT_1_A _exptl_crystal_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR_01

CHEMW01_ALERT_1_A The ratio of given/expected molecular weight as calculated

from the _chemical_formula_sum lies outside

the range 0.90 <> 1.10

Calculated formula weight = 167.8147

Formula weight given = 234.9000

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.470 Why?

PLAT699_ALERT_1_A Missing _exptl_crystal_description Value Please Do !

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies

outside the range 0.80 <> 2.00

Goodness of fit given = 3.030

PLAT027_ALERT_3_C _diffn_reflths_theta_full value (too) Low 9.92 Degree

PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 1.26 %

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -P 2yabc Check

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: Ca.0467 Ce0.4566 La0.2104 Nd0.18

Atom count from the _atom_site data: As.0416 Ca.0467 Ce0.4566 La0.210

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu

not performed for this radiation type.

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !

PLAT820_ALERT_5_G Internal PLATON Read Problem with ALERT Number . _820

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

PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.29060 Ang.

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Th Constrained at 0.0199 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Sm Constrained at 0.0312 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Nd Constrained at 0.1848 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Pr Constrained at 0.0503 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of Ce	Constrained at	0.4566	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of La	Constrained at	0.2104	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of As	Constrained at	0.0416	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of P	Constrained at	0.9584	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca	Constrained at	0.0467	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	33%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 2)	100%	Note
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters		1	Info
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please	Do !
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ		2	Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ		6	Units
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of		3.0	Sig(I)
PLAT984_ALERT_1_G	The Ce-f' = -2.0261	Deviates from the B&C-Value	-2.0173	Check
PLAT984_ALERT_1_G	The La-f' = -1.4695	Deviates from the B&C-Value	-1.4559	Check
PLAT984_ALERT_1_G	The Nd-f' = -3.1323	Deviates from the B&C-Value	-3.1595	Check
PLAT984_ALERT_1_G	The Pr-f' = -3.2550	Deviates from the B&C-Value	-3.2225	Check
PLAT984_ALERT_1_G	The Sm-f' = -2.0065	Deviates from the B&C-Value	-2.0091	Check
PLAT984_ALERT_1_G	The Th-f' = -0.9622	Deviates from the B&C-Value	-0.8911	Check
PLAT985_ALERT_1_G	The As-f" = 0.4019	Deviates from the B&C-Value	0.4005	Check
PLAT985_ALERT_1_G	The Ce-f" = 3.1615	Deviates from the B&C-Value	3.1748	Check
PLAT985_ALERT_1_G	The Nd-f" = 0.6212	Deviates from the B&C-Value	0.6180	Check
PLAT985_ALERT_1_G	The Pr-f" = 3.3462	Deviates from the B&C-Value	3.3560	Check
PLAT985_ALERT_1_G	The Sm-f" = 0.7152	Deviates from the B&C-Value	0.7111	Check
PLAT985_ALERT_1_G	The Th-f" = 3.4684	Deviates from the B&C-Value	3.4345	Check

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

26 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 2 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
 13 ALERT type 4 Improvement, methodology, query or suggestion
 8 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.

Datablock 1 - ellipsoid plot

