

## 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

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Bond precision:	= 0.0000 A	Wavelength=0.71359	
Cell:	a=6.7795 (5)	b=7.0058 (5)	c=6.4543 (5)
	alpha=90	beta=103.551 (6)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	298.02 (4)	298.02 (4)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yabc	
Moiety formula	As0.19 Ce1.80 Gd0.08 La0.76 Nd0.77 O16 P3.73 Pr0.21 Sm0.14 Th0.	?	
Sum formula	As0.19 Ca0.12 Ce1.80 Gd0.08 La0.76 Nd0.77 O16 P3.73 Pr0.21 Sm0.	As0.047 Ca0.029 Ce0.451 Gd0.019 La0.19 Nd0.192 O4 P0.933 Pr0.05	
Mr	945.14	236.40	
Dx, g cm-3	5.266	5.269	
Z	1	4	
Mu (mm-1)	17.071	17.477	
F000	421.6	422.0	
F000'	420.69		
h, k, lmax	9, 9, 8	9, 9, 8	
Nref	799	784	
Tmin, Tmax			
Tmin'			
Correction method=	Not given		
Data completeness=	0.981	Theta (max)= 29.240	

R(reflections)= 0.0289( 771)

wR2(reflections)=  
0.0883( 784)

S = 4.029

Npar= 37

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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.

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### Alert level A

EXPT005\_ALERT\_1\_A \_exptl\_crystal\_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR\_01

ABSMU01\_ALERT\_1\_A The ratio of given/expected absorption coefficient lies  
outside the range 0.90 <> 1.10

Calculated value of mu = 65.497

Value of mu given = 17.477

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 = 462.6085

Formula weight given = 236.4000

PLAT183\_ALERT\_1\_A Missing \_cell\_measurement\_reflns\_used Value .... Please Do !

PLAT184\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_min Value ..... Please Do !

PLAT185\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_max Value ..... Please Do !

PLAT699\_ALERT\_1\_A Missing \_exptl\_crystal\_description Value ..... Please Do !

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### Alert level B

GOODF01\_ALERT\_2\_B The least squares goodness of fit parameter lies  
outside the range 0.60 <> 4.00

Goodness of fit given = 4.029

PLAT087\_ALERT\_2\_B Unsatisfactory S value (Too High) ..... 4.03 Check

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### Alert level C

RADNW01\_ALERT\_1\_C The radiation wavelength lies outside the expected range  
for the supplied radiation type. Expected range 0.71065-0.71075

Wavelength given = 0.71359

PLAT051\_ALERT\_1\_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.32 %

PLAT052\_ALERT\_1\_C Info on Absorption Correction Method Not Given Please Do !

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

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### 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: As.047 Ca.029 Ce0.451 Gd.019 La0

Atom count from the \_atom\_site data: As.0471 Ca.0291 Ce0.4505 Gd.019

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 !
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
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	0.0208 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Gd	Constrained at	0.019 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Sm	Constrained at	0.034 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Nd	Constrained at	0.1923 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Pr	Constrained at	0.0536 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ce	Constrained at	0.4505 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of La	Constrained at	0.1897 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Y	Constrained at	0.0111 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of As	Constrained at	0.0471 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of P	Constrained at	0.9335 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca	Constrained at	0.0291 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
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 !
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0	Sig(I)
PLAT982_ALERT_1_G	The As-f' = 0.0511 Deviates from IT-value =	0.0499	Check
PLAT982_ALERT_1_G	The Ca-f' = 0.2304 Deviates from IT-value =	0.2262	Check
PLAT982_ALERT_1_G	The Ce-f' = -0.1940 Deviates from IT-value =	-0.2486	Check
PLAT982_ALERT_1_G	The Gd-f' = -0.0996 Deviates from IT-value =	-0.1653	Check
PLAT982_ALERT_1_G	The La-f' = -0.2291 Deviates from IT-value =	-0.2871	Check
PLAT982_ALERT_1_G	The Nd-f' = -0.1365 Deviates from IT-value =	-0.1943	Check
PLAT982_ALERT_1_G	The P-f' = 0.1048 Deviates from IT-value =	0.1023	Check
PLAT982_ALERT_1_G	The Pr-f' = -0.1628 Deviates from IT-value =	-0.2180	Check
PLAT982_ALERT_1_G	The Sm-f' = -0.1026 Deviates from IT-value =	-0.1638	Check
PLAT982_ALERT_1_G	The Th-f' = -7.2113 Deviates from IT-value =	-7.2400	Check
PLAT982_ALERT_1_G	The Y-f' = -2.9793 Deviates from IT-value =	-2.7962	Check
PLAT983_ALERT_1_G	The As-f" = 2.0283 Deviates from IT-Value =	2.0058	Check
PLAT983_ALERT_1_G	The Ca-f" = 0.3135 Deviates from IT-Value =	0.3064	Check
PLAT983_ALERT_1_G	The Ce-f" = 2.6828 Deviates from IT-Value =	2.6331	Check
PLAT983_ALERT_1_G	The Gd-f" = 3.9799 Deviates from IT-Value =	3.9035	Check
PLAT983_ALERT_1_G	The La-f" = 2.5026 Deviates from IT-Value =	2.4523	Check
PLAT983_ALERT_1_G	The Nd-f" = 3.0744 Deviates from IT-Value =	3.0179	Check
PLAT983_ALERT_1_G	The P-f" = 0.0969 Deviates from IT-Value =	0.0942	Check
PLAT983_ALERT_1_G	The Pr-f" = 2.8740 Deviates from IT-Value =	2.8214	Check
PLAT983_ALERT_1_G	The Sm-f" = 3.5061 Deviates from IT-Value =	3.4418	Check
PLAT983_ALERT_1_G	The Th-f" = 9.0375 Deviates from IT-Value =	8.8979	Check
PLAT983_ALERT_1_G	The Y-f" = 3.5765 Deviates from IT-Value =	3.5667	Check

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- 7 **ALERT level A** = Most likely a serious problem - resolve or explain  
 2 **ALERT level B** = A potentially serious problem, consider carefully  
 8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 46 **ALERT level G** = General information/check it is not something unexpected
- 41 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 3 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  
 14 ALERT type 4 Improvement, methodology, query or suggestion  
 4 ALERT type 5 Informative message, check

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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

