

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=0.71359
Cell:	a=6.8313 (5)	b=7.0454 (5) c=6.5105 (5)
	alpha=90	beta=103.565 (6) gamma=90
Temperature:	?	
	Calculated	Reported
Volume	304.60 (4)	304.60 (4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yabc
	As0.19 Ce1.80 Gd0.08 La0.76	
Moiety formula	Nd0.77 O16 P3.73 Pr0.21 ?	
	Sm0.14 Th0.	
	As0.19 Ca0.12 Ce1.80 Gd0.08	As0.047 Ca0.029 Ce0.451
Sum formula	La0.76 Nd0.77 O16 P3.73	Gd0.019 La0.19 Nd0.192 O4
	Pr0.21 Sm0.	P0.933 Pr0.05
Mr	945.14	236.30
Dx, g cm-3	5.153	5.153
Z	1	4
Mu (mm-1)	16.702	17.079
F000	421.6	422.0
F000'	420.69	
h, k, lmax	9, 9, 8	9, 9, 8
Nref	820	804
Tmin, Tmax		
Tmin'		
Correction method=	Not given	
Data completeness=	0.980	Theta (max)= 29.290

R(reflections)= 0.0559(767)

wR2(reflections)=
0.1904(804)

S = 8.248

Npar= 37

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

ABSMU01_ALERT_1_A The ratio of given/expected absorption coefficient lies
outside the range 0.90 <> 1.10

Calculated value of mu = 64.082

Value of mu given = 17.079

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 = 236.3000

GOODF01_ALERT_2_A The least squares goodness of fit parameter lies
outside the range 0.40 <> 6.00

Goodness of fit given = 8.248

PLAT087_ALERT_2_A Unsatisfactory S value (Too High) 8.25 Check

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 !

Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -7.030

Test value = -6.750

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

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 . 2.21 %

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

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -7.03 eA-3

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

PLAT213_ALERT_2_C Atom O1 has ADP max/min Ratio 3.8 oblate

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 01 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 04 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: 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
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

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

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

14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

44 **ALERT level G** = General information/check it is not something unexpected

40 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

8 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

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.

PLATON version of 13/05/2024; check.def file version of 04/05/2024

