

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=6.7926 (5) alpha=90 | b=7.0159 (5) beta=103.544 (6) | c=6.4676 (5) gamma=90 |
| Temperature: | 531 K | | |
| | Calculated | Reported | |
| Volume | 299.65 (4) | 299.65 (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 P0.934 Pr0.05 | |
| Mr | 945.14 | 236.40 | |
| Dx, g cm-3 | 5.238 | 5.239 | |
| Z | 1 | 4 | |
| Mu (mm-1) | 16.978 | 17.362 | |
| F000 | 421.6 | 422.0 | |
| F000' | 420.69 | | |
| h, k, lmax | 9, 9, 8 | 9, 9, 8 | |
| Nref | 804 | 789 | |
| Tmin, Tmax | | | |
| Tmin' | | | |
| Correction method= | Not given | | |
| Data completeness= | 0.981 | Theta (max)= 29.250 | |

R(reflections)= 0.0330(774)

wR2(reflections)=
0.1059(789)

S = 4.771

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 = 65.141

Value of mu given = 17.362

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 = 462.6394

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 !

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 = 4.771

PLAT087_ALERT_2_B Unsatisfactory S value (Too High) 4.77 Check

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 . 2.21 %

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

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: 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 |

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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
 44 **ALERT level G** = General information/check it is not something unexpected
- 39 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

