

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=0.41029 | |
| Cell: | a=6.9176(3) | b=6.9176(3) | c=6.0644(2) |
| | alpha=90 | beta=90 | gamma=90 |
| Temperature: | 293 K | | |
| | Calculated | Reported | |
| Volume | 290.20(3) | 290.20(2) | |
| Space group | I 41/a m d: | I 41/a m d | |
| Hall group | I 4bw 2bw - | -I 4bd;-2 | |
| | As0.42 Dy0.29 Er0.16 Gd0.19 | | |
| Moiety formula | Ho0.15 O16 P3.58 Y3.07 | ? | |
| | Yb0.14 | | |
| | As0.42 Dy0.29 Er0.16 Gd0.19 | As0.11 Dy0.07 Er0.05 Gd0.05 | |
| Sum formula | Ho0.15 O16 P3.58 Y3.07 | Ho0.04 O4 P0.89 Y0.77 | |
| | Yb0.14 | Yb0.03 | |
| Mr | 824.33 | 207.70 | |
| Dx, g cm ⁻³ | 4.717 | 4.753 | |
| Z | 1 | 4 | |
| Mu (mm ⁻¹) | 5.426 | 5.549 | |
| F000 | 377.4 | 377.0 | |
| F000' | 377.66 | | |
| h, k, lmax | 11, 11, 10 | 5, 10, 10 | |
| Nref | 215 | 131 | |
| Tmin, Tmax | | 0.621, 1.000 | |
| Tmin' | | | |

Correction method= # Reported T Limits: Tmin=0.621 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.609

Theta(max)= 20.550

R(reflections)= 0.0214(125)

wR2(reflections)=

wR= 0.0281(131)

S = 2.180

Npar= 11

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.830 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 = 2.180

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

Calc: As0.11 Dy0.07 Er0.04 Gd0.05 Ho0.04 O4 P0.89 Y0.77 Yb0.03

Rep.: As0.11 Dy0.07 Er0.05 Gd0.05 Ho0.04 O4 P0.89 Y0

.77 Yb0.03

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 6.47 Check

PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.22 %

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 -I 4bd;-2 Check

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.

From the CIF: _cell_formula_units_Z 4

From the CIF: _chemical_formula_sum As0.11 Dy0.07 Er0.05 Gd0.05 Ho0.04

TEST: Compare cell contents of formula and atom_site data

| atom | Z*formula | cif sites | diff |
|------|-----------|-----------|-------|
| As | 0.44 | 0.42 | 0.02 |
| Dy | 0.28 | 0.29 | -0.01 |
| Er | 0.20 | 0.16 | 0.04 |
| Gd | 0.20 | 0.19 | 0.01 |
| Ho | 0.16 | 0.15 | 0.01 |
| O | 16.00 | 16.00 | 0.00 |
| P | 3.56 | 3.58 | -0.02 |
| Y | 3.08 | 3.07 | 0.01 |
| Yb | 0.12 | 0.14 | -0.02 |

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 |
| PLAT092_ALERT_4_G | Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka | 0.41029 | Ang. |
| PLAT120_ALERT_1_G | Reported I41/amd Inconsistent with Explicit | I41/amd | Check |
| 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 Yb | Constrained at | 0.0343 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Er | Constrained at | 0.0408 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Ho | Constrained at | 0.038 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Dy | Constrained at | 0.0734 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Gd | Constrained at | 0.0464 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Y | Constrained at | 0.7671 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of As | Constrained at | 0.106 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of P | Constrained at | 0.894 Check |
| PLAT301_ALERT_3_G | Main Residue Disorder(Resd 1) | 80% | Note |
| 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 | 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 As-f' = 0.2876 Deviates from the B&C-Value | 0.2862 | Check |
| PLAT984_ALERT_1_G | The Dy-f' = -0.7013 Deviates from the B&C-Value | -0.6931 | Check |
| PLAT984_ALERT_1_G | The Er-f' = -0.6345 Deviates from the B&C-Value | -0.6220 | Check |
| PLAT984_ALERT_1_G | The Gd-f' = -0.7818 Deviates from the B&C-Value | -0.7795 | Check |
| PLAT984_ALERT_1_G | The Ho-f' = -0.6662 Deviates from the B&C-Value | -0.6559 | Check |
| PLAT984_ALERT_1_G | The Y-f' = 0.2101 Deviates from the B&C-Value | 0.2121 | Check |
| PLAT984_ALERT_1_G | The Yb-f' = -0.5816 Deviates from the B&C-Value | -0.5663 | Check |
| PLAT985_ALERT_1_G | The As-f" = 0.7656 Deviates from the B&C-Value | 0.7629 | Check |
| PLAT985_ALERT_1_G | The Dy-f" = 1.7265 Deviates from the B&C-Value | 1.7135 | Check |
| PLAT985_ALERT_1_G | The Er-f" = 1.9539 Deviates from the B&C-Value | 1.9391 | Check |
| PLAT985_ALERT_1_G | The Gd-f" = 1.5201 Deviates from the B&C-Value | 1.5073 | Check |
| PLAT985_ALERT_1_G | The Ho-f" = 1.8377 Deviates from the B&C-Value | 1.8236 | Check |
| PLAT985_ALERT_1_G | The Yb-f" = 2.2018 Deviates from the B&C-Value | 2.1850 | Check |

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

31 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
6 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 I - ellipsoid plot

