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=6.9044(9)      b=6.9044(9)      c=6.0629(8)
                   alpha=90         beta=90          gamma=90
Temperature:       531 K

                   Calculated                  Reported
Volume             289.02(8)                   289.02(7)
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 As0.1 Dy0.07 Er0.04 Gd0.04
Sum formula        Ho0.15 O16 P3.58 Y3.07      Ho0.04 O4 P0.88 Y0.73
                   Yb0.14                      Yb0.03
Mr                 824.33                      199.80
Dx,g cm-3          4.736                       4.591
Z                  1                           4
Mu (mm-1)          23.282                      23.369
F000               377.4                       377.0
F000'              369.45
h,k,lmax           9,9,8                       9,9,8
Nref               115                         116
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness= 1.009          Theta(max)= 29.110
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R(reflections)= 0.0217(113)   wR2(reflections)=
                                                    wR= 0.0293(116)

S = 2.860   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
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
ABSMU01_ALERT_1_B The ratio of given/expected absorption coefficient lies
                outside the range 0.95 <> 1.05
            Calculated value of mu =   22.134
            Value of mu given   =   23.369
PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by ..   25.13 Check

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🟡 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 =   2.860
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
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.: As0.1 Dy0.07 Er0.04 Gd0.04 Ho0.04 O4 P0.88 Y0.
                73 Yb0.03
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 -I 4bd;-2 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.1 Dy.07 Er.04 Gd.04 Ho.04 O4
            Atom count from the _atom_site data: As0.106 Dy.0734 Er.0408 Gd.0464
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.

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          From the CIF: _cell_formula_units_Z     4
          From the CIF: _chemical_formula_sum  As0.1 Dy0.07 Er0.04 Gd0.04 Ho0.04
          TEST: Compare cell contents of formula and atom_site data

          atom     Z*formula  cif sites diff
          As          0.40        0.42   -0.02
          Dy          0.28        0.29   -0.01
          Er          0.16        0.16   -0.00
          Gd          0.16        0.19   -0.03
          Ho          0.16        0.15    0.01
          O          16.00       16.00    0.00
          P           3.52        3.58   -0.06
          Y           2.92        3.07   -0.15
          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
PLAT120_ALERT_1_G Reported I41/amd   Inconsistent with Explicit      I41/amd 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 !
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 Dy-f'=   -0.1320 Deviates from  IT-value =      -0.1892 Check
PLAT982_ALERT_1_G The Er-f'=   -0.2056 Deviates from  IT-value =      -0.2586 Check
PLAT982_ALERT_1_G The Gd-f'=   -0.0996 Deviates from  IT-value =      -0.1653 Check
PLAT982_ALERT_1_G The Ho-f'=   -0.1634 Deviates from  IT-value =      -0.2175 Check
PLAT982_ALERT_1_G The  P-f'=    0.1048 Deviates from  IT-value =       0.1023 Check
PLAT982_ALERT_1_G The  Y-f'=   -2.9793 Deviates from  IT-value =      -2.7962 Check
PLAT982_ALERT_1_G The Yb-f'=   -0.3326 Deviates from  IT-value =      -0.3850 Check
PLAT983_ALERT_1_G The As-f"=    2.0283 Deviates from  IT-Value =       2.0058 Check
PLAT983_ALERT_1_G The Dy-f"=    4.4885 Deviates from  IT-Value =       4.4098 Check
PLAT983_ALERT_1_G The Er-f"=    5.0438 Deviates from  IT-Value =       4.9576 Check
PLAT983_ALERT_1_G The Gd-f"=    3.9799 Deviates from  IT-Value =       3.9035 Check
PLAT983_ALERT_1_G The Ho-f"=    4.7604 Deviates from  IT-Value =       4.6783 Check
PLAT983_ALERT_1_G The  P-f"=    0.0969 Deviates from  IT-Value =       0.0942 Check
PLAT983_ALERT_1_G The  Y-f"=    3.5765 Deviates from  IT-Value =       3.5667 Check
PLAT983_ALERT_1_G The Yb-f"=    5.6460 Deviates from  IT-Value =       5.5486 Check
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   5 **ALERT level A** = Most likely a serious problem – resolve or explain
   2 **ALERT level B** = A potentially serious problem, consider carefully
   9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  37 **ALERT level G** = General information/check it is not something unexpected

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

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2 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
9 ALERT type 4 Improvement, methodology, query or suggestion
5 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.

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

Datablock I - ellipsoid plot