checkCIF/PLATON report

Structure factors have been supplied for datablock(s) DMAJ237

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: DMAJ237

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Bond precision:  C-C = 0.0152 A          Wavelength=0.71073

Cell:            a=16.9255(9)     b=16.9255(9)     c=29.689(2)
                 alpha=90         beta=90          gamma=120
Temperature:     150 K

                Calculated                Reported
Volume          7365.6(9)                 7365.7(10)
Space group     R -3                      R -3 :H
Hall group      -R 3                      -R 3
Moiety formula  C36 H30 N12 O18 Pd3, 2(O) ?
Sum formula     C36 H30 N12 O20 Pd3       C36 H34 N12 O20 Pd3
Mr              1269.92                   1273.95
Dx,g cm-3       1.718                     1.723
Z               6                         6
Mu (mm-1)       1.173                     1.173
F000            3768.0                    3792.0
F000'           3751.87
h,k,lmax        16,16,29                  16,16,29
Nref            1716                      1712
Tmin,Tmax       0.861,0.983               0.760,0.880
Tmin'           0.861

Correction method= # Reported T Limits: Tmin=0.760 Tmax=0.880
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 20.823

R(reflections)= 0.0406( 1490)     wR2(reflections)= 0.1292( 1712)

S = 1.153                 Npar= 216
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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.

Alert level A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5002

Author Response: The crystal was poorly diffracting at higher Bragg angles. Recrystallisation and fresh data collection did not improve the situation.

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio ..... 7.93 Note

Author Response: This is due to insufficient number of reflections available for refinement. Theta maximum is only 20.8 degrees.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O7 Check

Author Response: The oxygen atom sits on 3-fold axis. Fixing hydrogen atoms leads to symmetry generation meaningless extra hydrogen atoms.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O8 Check

Author Response: The oxygen atom sits on 3-fold axis. Fixing hydrogen atoms leads to symmetry generation meaningless extra hydrogen atoms.

PLAT601_ALERT_2_B Unit Cell Contains Solvent Accessible VOIDS of . 200 Ang**3

Author Response: If the lattice water molecules are asigned hydrogen atoms the voids may not be present.

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 4.03 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.72 Report
PLAT234_ALERT_4_C Large Hirshfeld Difference O4 --C11 . 0.16 Ang.
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O8 0.141 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0152 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.500 3 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.25A From O7 1.61 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.77A From O7 1.50 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.53A From O7 1.34 eA-3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the

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            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C36 H34 N12 O20 Pd3
            Atom count from the _atom_site data:  C36 H30 N12 O20 Pd3
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
           From the CIF: _cell_formula_units_Z    6
           From the CIF: _chemical_formula_sum  C36 H34 N12 O20 Pd3
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        216.00    216.00    0.00
           H        204.00    180.00   24.00
           N         72.00     72.00    0.00
           O        120.00    120.00    0.00
           Pd        18.00     18.00    0.00
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     102.77 Why ?
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )       0.33 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )       0.33 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1       (II)      .       2.20 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        81% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          3 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 18/09/2020; check.def file version of 20/08/2020

Datablock DMAJ237 - ellipsoid plot