checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PdH-2L

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: PdH-2L

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Bond precision:   C-C = 0.0245 A          Wavelength=0.71073

Cell:               a=9.3718(8)      b=22.849(2)      c=11.831(1)
                    alpha=90         beta=90          gamma=90
Temperature:        150 K

                Calculated                  Reported
Volume          2533.5(4)                   2533.4(4)
Space group     P n 21 a                    Pn21a
Hall group      P -2ac -2n                  ?
Moiety formula  C30 H30 N2 O4 Pd            ?
Sum formula     C30 H30 N2 O4 Pd            C30 H30 N2 O4 Pd
Mr              588.96                      588.96
Dx,g cm-3       1.544                       1.544
Z               4                           4
Mu (mm-1)       0.773                       0.773
F000            1208.0                      1208.0
F000'           1204.48
h,k,lmax        12,30,15                    12,29,14
Nref            6085[ 3118]                 5138
Tmin,Tmax       0.870,0.904                 0.430,1.000
Tmin'           0.870

Correction method= # Reported T Limits: Tmin=0.430 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.65/0.84        Theta(max)= 27.965

R(reflections)= 0.0799( 3489)                wR2(reflections)=
                                             0.2065( 5138)
S = 1.078                  Npar= 341
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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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.60Ang From Pd1 4.52 eA-3

Author Response: this is a "ghost" peak due to the presence of the Pd cation

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Alert level B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02448 Ang.

Author Response: This is likely related to the weak diffraction of the crystal

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note

Author Response: This is likely due to beam-stop

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.78Ang From Pd1 2.73 eA-3

Author Response: this is a "ghost" peak due to the presence of the Pd cation

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Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.480
From the CIF: _refine_ls_abs_structure_Flack_su 0.030

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.44 Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	4.60 eA-3
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C18 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	6 Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check

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Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6 Note
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group Pn21a	Pna21 Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	1 Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Pd1 (II) .	2.22 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	5 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	297 Note

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PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage         79 %
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
   3 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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
   6 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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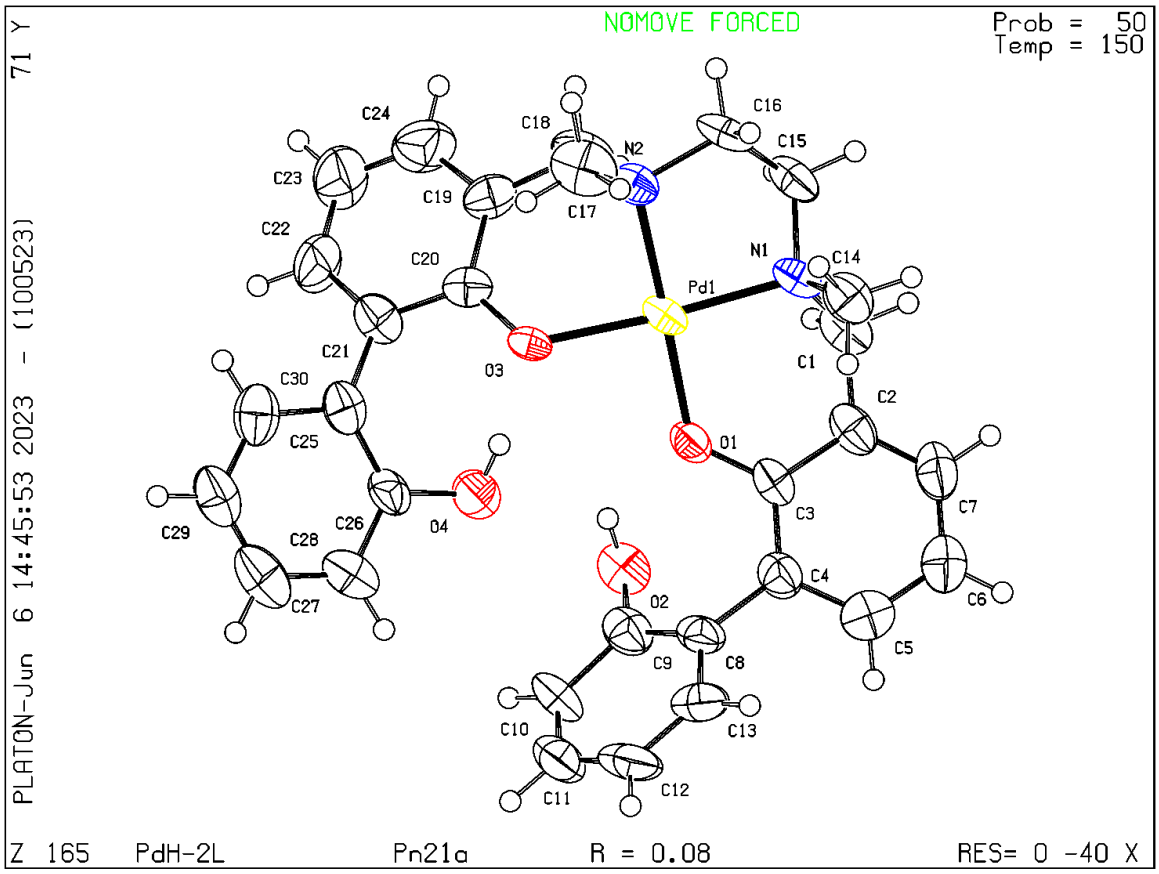
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 10/05/2023; check.def file version of 10/05/2023

Datablock PdH-2L - ellipsoid plot