checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Pd6L8

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: Pd6L8

Bond precision: C-C = 0.0120 A Wavelength=1.34050

Cell: a=36.6353(5) b=36.6353(5) c=36.6353(5)
alpha=90 beta=90 gamma=90
Temperature: 253 K

	Calculated	Reported
Volume	49170(2)	49170(2)
Space group	F m -3 m	F m -3 m
Hall group	-F 4 2 3	-F 4 2 3
Moiety formula	C264 H192 N24 O16 P4 Pd3 [+ solvent]	C264 H192 N24 O16 P4 Pd3
Sum formula	C264 H192 N24 O16 P4 Pd3 [+ solvent]	C264 H192 N24 O16 P4 Pd3
Mr	4399.50	4399.50
Dx,g cm-3	1.189	1.189
Z	8	8
Mu (mm-1)	1.677	1.677
F000	18160.0	18160.0
F000'	18205.00	
h,k,lmax	37,37,37	36,36,36
Nref	1399	1369
Tmin,Tmax	0.551,0.669	0.384,1.000
Tmin'	0.487	

Correction method= # Reported T Limits: Tmin=0.384 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.979 Theta(max)= 42.796

R(reflections)= 0.1406(1222) wR2(reflections)= 0.3848(1369)

S = 1.878 Npar= 113

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 = 0.5068

Author Response: PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550 RESPONSE: Author Response: The crystals of this giant supramolecular assembly Author Response: The crystals of this giant supramolecular assembly diffract very weekly in nature, possibly due to a large amount of amorphous solvents and highly-disordered counterions existing in the unit cell, which occupy as much as 55.4% of the unit cell based on PLATON calculation.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pd1 3.10 eA-3

Author Response: The positive residual electron density peak is located near the Pd1 atom and arises from residual Fourier features commonly observed around heavy metal centers. Palladium is a strong scatterer, and minor absorption and truncation effects can lead to such residual density. The coordination environment of Pd1 is chemically reasonable and well defined, and no chemically meaningful disorder could be identified.

Alert level B

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.38 Report
PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing). C11_1 Check

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Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
RADNW01_ALERT_1_C The radiation wavelength lies outside the expected range
for the supplied radiation type. Expected range 1.34130-1.34150

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           Wavelength given =    1.34050
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.979 Why?
PLAT082_ALERT_2_C High R1 Value ..................................       0.14 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       3.07 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.8 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C10_1    --C11_1    .       0.17 Ang.
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      N1_1 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours     C11_1 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours     C13_1 Check
PLAT242_ALERT_2_C Low   MainResAtom  Ueq as Compared to Neighbours        P2 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pd1      0.170 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........     O14_1 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............      0.012 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.507        23 Report
                  2  2  2,   0  4  4,   0  6  6,   1  1  7,   0  4  8,   2  4  8,
                  2  6  8,   0  8 10,   6  8 10,   8 14 14,   1  1 15,   0 10 16,
                  2 12 16,   7  9 17,   2  4 18,   5  7 21,   1 11 21,  20 22 22,
                  5 11 23,  20 20 24,  11 25 25,  10 10 34,   4  8 36,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         18 Check
                  1  1  1,   1  3  3,   3  3  3,   0  2  4,   2  2  4,   1  5  7,
                  5  5  7,   2  2  8,   1  3  9,   1  7  9,   2  8 10,   1  7 11,
                 10 10 12,   3  5 13,   0  2 14,   0  4 14,   0 10 14,   2  6 16,
PLAT977_ALERT_2_C Check Negative Difference Density on H13_1     .      -0.31 eA-3
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          4 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms         13 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1      --N1_1     .        8.4 s.u.
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
                  O14_1   C10_1   C12_1
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)         10% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    1)     251.50 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....      C1_3 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in  Crystal Structure         ! Info
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         22 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          2 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        123 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed         ! Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated   and Succeeded by SHELXL     2019/3 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         70% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
                  2  2  2,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         14 Note
                  1  1  7,   2  4  8,   2  6  8,   0  8 10,   6  8 10,   0 10 16,
                  1 11 21,   5 11 23,   8 14 14,   1  1 15,   2 12 16,   7  9 17,
                  2  4 18,   5  7 21,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     32.650 Note
              Predicted wR2: Based on SigI**2  1.18 or SHELX Weight 20.49
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PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
PLAT994_ALERT_1_G SHELXL .ins Contains no or MERG 0 Instruction ..          ! Note
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  26 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 ALERT type 2 Indicator that the structure model may be wrong or deficient
  10 ALERT type 3 Indicator that the structure quality may be low
  14 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 15/01/2026; check.def file version of 02/01/2026

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duplicate check

No duplication found

Datablock Pd6L8 - ellipsoid plot