

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_2776_sq

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: exp_2776_sq

Bond precision: C-C = 0.0145 Å Wavelength=1.54184

Cell: a=14.3028 (4) b=17.0485 (5) c=22.8204 (6)
 alpha=100.119 (2) beta=108.070 (2) gamma=103.957 (2)
Temperature: 101 K

	Calculated	Reported
Volume	4941.1 (3)	4941.1 (2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C188 H194 N14 Ni2 Pd2 [+ solvent]	C188 H194 N14 Ni2 Pd2
Sum formula	C188 H194 N14 Ni2 Pd2 [+ solvent]	C188 H194 N14 Ni2 Pd2
Mr	2979.76	2979.78
Dx, g cm ⁻³	1.001	1.001
Z	1	1
Mu (mm ⁻¹)	2.011	2.011
F000	1568.0	1568.0
F000'	1565.85	
h, k, lmax	17, 20, 27	17, 20, 27
Nref	17435	17419
Tmin, Tmax	0.574, 0.818	0.729, 1.000
Tmin'	0.521	

Correction method= # Reported T Limits: Tmin=0.729 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 66.601

R(reflections)= 0.1079(14724)

wR2(reflections)=
0.2932(17419)

S = 1.065

Npar= 982

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 C

PLAT082_ALERT_2_C	High R1 Value	0.11	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.29	Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.17	Report
PLAT213_ALERT_2_C	Atom C82 has ADP max/min Ratio	3.3	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	5.0	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	6.0	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C55 --C58 .	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C86 --C87 .	0.16	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C52	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C55	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C93	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01455	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.502	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.025	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	15	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.23Ang From C86	2.37	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.92Ang From Pd1	1.95	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.96Ang From Pd1	1.93	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.95Ang From C30	1.80	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.32Ang From Pd1	1.63	eA-3



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.11	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	38.33	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	18	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	3	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	3%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H51 ..H60A .	2.02	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H53 ..H61C .	1.90	Ang.
	x,y,z =	1_555	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pd1 (II) .	2.39	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni1 (II) .	2.13	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	66	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	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	76%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note

PLAT930_ALERT_2_G	FCF-based Twin Law (0 0 1)	Est.d BASF	0.16	Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (0 0 1)	Est.d BASF	0.20	Check
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		6	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.9	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 21 ALERT type 2 Indicator that the structure model may be wrong or deficient
 11 ALERT type 3 Indicator that the structure quality may be low
 8 ALERT type 4 Improvement, methodology, query or suggestion
 3 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.

