

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo221108a_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: mo221108a_sq

Bond precision: C-C = 0.0153 Å Wavelength=0.71073

Cell: a=11.184(3) b=19.316(6) c=23.366(7)
 alpha=83.286(7) beta=84.457(7) gamma=75.853(6)
Temperature: 296 K

	Calculated	Reported
Volume	4849(2)	4849(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C47 H43 Cl2 Ni O2 P2 Si [+ solvent]	C47 H43 Cl2 Ni O2 P2 Si
Sum formula	C47 H43 Cl2 Ni O2 P2 Si [+ solvent]	C47 H43 Cl2 Ni O2 P2 Si
Mr	859.43	859.45
Dx, g cm ⁻³	1.177	1.177
Z	4	4
Mu (mm ⁻¹)	0.634	0.634
F000	1788.0	1788.0
F000'	1792.18	
h, k, lmax	13, 23, 28	13, 23, 28
Nref	18061	18055
Tmin, Tmax	0.941, 0.963	0.886, 1.000
Tmin'	0.939	

Correction method= # Reported T Limits: Tmin=0.886 Tmax=1.000

AbsCorr = MULTII-SCAN

Data completeness= 1.000

Theta(max)= 25.497

R(reflections)= 0.0869(5659)

wR2(reflections)=
0.2429(18055)

S = 0.839

Npar= 969

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 B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18

Rint given 0.185

PLAT020_ALERT_3_B	The Value of Rint is Greater Than 0.12	0.185	Report
PLAT026_ALERT_3_B	Ratio Observed / Unique Reflections (too) Low ..	31%	Check
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of	C2	Check
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of	C50	Check
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of	C61	Check
PLAT331_ALERT_2_B	Small Aver Phenyl C-C Dist C65 --C70 .	1.36	Ang.
PLAT341_ALERT_3_B	Low Bond Precision on C-C Bonds	0.01528	Ang.

● Alert level C

PLAT213_ALERT_2_C	Atom C50	has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	5.1	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 2 C	Ueq(max)/Ueq(min) Range	5.9	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H	Uiso(max)/Uiso(min) Range	4.7	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 2 H	Uiso(max)/Uiso(min) Range	5.9	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C14	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C16	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C17	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C26	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C49	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C60	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C87	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C88	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C91	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C93	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si1	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C1	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C5	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C12	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C15	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si2	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	O4	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C51	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C59	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C63	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C65	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C83	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C89	Check	
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C2 - C5 .	1.54	Ang.	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	16.507	Check	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.978	Check	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.740	Check	
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & Sth/L= 0.600	5	Report	

● **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	6	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	4	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	5	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1	143.1	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O4	145.2	Degree
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT793_ALERT_4_G	Model has Chirality at P2 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at Si1 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at Si2 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C3 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C49 (Centro SPGR)	R	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	882	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	7	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.3	Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	51.0	Degree
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
8 **ALERT level B** = A potentially serious problem, consider carefully
33 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
20 **ALERT level G** = General information/check it is not something unexpected

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

