

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) niphen

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: niphen

Bond precision: C-C = 0.0108 Å Wavelength=0.71073

Cell: a=12.2327(3) b=13.0491(3) c=20.7742(5)
 alpha=72.935(1) beta=77.210(1) gamma=89.982(1)
Temperature: 100 K

	Calculated	Reported
Volume	3084.00(13)	3084.00(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C67 H49 N10 Ni2 O2, 3(C H4 O), Cl [+ solvent]	C67 H49 N10 Ni2 O2, Cl, 3(C H4 O)
Sum formula	C70 H61 Cl N10 Ni2 O5 [+ solvent]	C70 H61 Cl N10 Ni2 O5
Mr	1275.12	1275.15
Dx, g cm ⁻³	1.373	1.373
Z	2	2
Mu (mm ⁻¹)	0.715	0.715
F000	1328.0	1328.0
F000'	1330.07	
h, k, lmax	14, 15, 24	14, 15, 24
Nref	10872	10859
Tmin, Tmax	0.830, 0.867	0.209, 0.266
Tmin'	0.830	

Correction method= # Reported T Limits: Tmin=0.209 Tmax=0.266

AbsCorr = MULTII-SCAN

Data completeness= 0.999

Theta(max)= 24.999

R(reflections)= 0.0811(5967)

wR2(reflections)=
0.2702(10859)

S = 1.100

Npar= 811

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 0.199

Author Response: The best available crystal was too small and had low reflective power.

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 0.199 Report

Author Response: The best available crystal was too small and had low reflective power.

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density 5.08 Report

Author Response: The chlorine anion is disordered in two positions, that are too close to resolve it correctly.



Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT018_ALERT_1_C	_diffn_measured_fraction_theta_max .NE. *_full	! Check
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.27 Report
PLAT234_ALERT_4_C	Large Hirshfeld Difference C57 --C58 .	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C60 --C61 .	0.16 Ang.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0108 Ang.
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O1S - H1S .	1.04 Ang.
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O2S - H2S .	1.02 Ang.
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O3S - H3S .	1.02 Ang.
PLAT414_ALERT_2_C	Short Intra D-H..H-X H1S ..H1SC .	1.99 Ang.
	x,y,z = 1_555	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	15.944 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.807 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.134 Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	5 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	9 Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.27Ang From Cl03	2.24 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 ... 1 Report

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	3	Report
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT014_ALERT_1_G	No _shelx_fab_checksum Found in CIF		Please Check
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.16	Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	4%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact C22 ..C22 .	3.16	Ang.
	1-x,1-y,1-z =	2_666	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	232	A**3
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	12	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni01 (II) .	2.11	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni02 (II) .	2.09	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	9	Note
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	33%	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	4	Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	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
 3 **ALERT level B** = A potentially serious problem, consider carefully
 16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 24 **ALERT level G** = General information/check it is not something unexpected

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

