

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: mo_20141029d496_0m-sr_sq

Bond precision: C-C = 0.0096 A Wavelength=0.71073

Cell: a=9.289(8) b=11.63(1) c=14.042(12)
 alpha=67.599(10) beta=76.686(10) gamma=87.161(12)

Temperature: 293 K

	Calculated	Reported
Volume	1364(2)	1364(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H42 Cl4 N4 Ni3 O14 [+ solvent]	C40 H42 Cl4 N4 Ni3 O14
Sum formula	C40 H42 Cl4 N4 Ni3 O14 [+ solvent]	C40 H42 Cl4 N4 Ni3 O14
Mr	1120.65	1120.70
Dx, g cm ⁻³	1.364	1.365
Z	1	1
Mu (mm ⁻¹)	1.279	1.279
F000	574.0	574.0
F000'	575.83	
h,k,lmax	11,14,17	11,14,17
Nref	5665	5502
Tmin,Tmax	0.724,0.784	0.732,0.793
Tmin'	0.710	

Correction method= # Reported T Limits: Tmin=0.732 Tmax=0.793
AbsCorr = MULTI-SCAN

Data completeness= 0.971 Theta(max)= 26.492

R(reflections)= 0.0747(3164) wR2(reflections)= 0.2102(5502)

S = 1.041 Npar= 297

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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full value Low .	0.977	Why?
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C5 --C7 ..	5.6	s.u.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00959	Ang.



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.10	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1	110.4	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2	111.0	Degree
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	7	Note

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

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

PLATON version of 09/11/2017; check.def file version of 08/11/2017

