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: 1

Bond precision: C-C = 0.0054 A Wavelength=1.54184

Cell: a=11.2744(5) b=11.6245(5) c=13.3452(7)
alpha=96.287(4) beta=108.779(4) gamma=101.405(4)
Temperature: 150 K

	Calculated	Reported
Volume	1594.70(14)	1594.70(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C46 H66 N8 Ni O6, 2(C4 H8 O2), 2(C H2 Cl2)	\ C46 H66 N8 Ni O6, 2(C4 H8 O2), 2(C H2 Cl2)C46 H66 N8 Ni O6, 2
Sum formula	C56 H86 Cl4 N8 Ni O10	C56 H86 Cl4 N8 Ni O10
Mr	1231.82	1231.83
Dx,g cm-3	1.283	1.283
Z	1	1
Mu (mm-1)	2.460	2.460
F000	654.0	654.0
F000’	654.11	
h,k,lmax	13,14,16	13,14,16
Nref	6138	5981
Tmin,Tmax	0.565,0.726	0.633,0.731
Tmin’	0.490	

Correction method= # Reported T Limits: Tmin=0.633 Tmax=0.731
AbsCorr = MULTI SCAN

Data completeness= 0.974 Theta(max)= 70.772

R(reflections)= 0.0808(5318) wR2(reflections)= 0.2369(5981)

S = 1.032 Npar= 366

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

PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C8 Check

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Alert level C

PLAT213_ALERT_2_C Atom C9 has ADP max/min Ratio ..... 3.6 prolat
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 5.3 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) ... 5.4 Ratio
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C25 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C24 Check

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Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C56 H86 Cl4 N8 Ni1 O10
Atom count from _chemical_formula_moiety:
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.17 Report
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..... 0.00400 Degree
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1 Note

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

3 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
3 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*, 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 21/04/2015; check.def file version of 09/03/2015

Datablock 1 - ellipsoid plot