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: d492

Bond precision: C-C = 0.0065 A Wavelength=0.71073

Cell: a=11.3008(8) b=11.3069(10) c=12.1027(10)
alpha=102.513(7) beta=100.115(7) gamma=94.689(7)
Temperature: 293 K

	Calculated	Reported
Volume	1474.7(2)	1474.7(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H48 Cl4 N6 Ni3 O14, 1.706(C3 H7 N O)	C44 H48 Cl4 N6 Ni3 O14, 1.71(C3 H7 N O)
Sum formula	C49.12 H59.94 Cl4 N7.71 Ni3 O15.71	C49.12 H59.94 Cl4 N7.71 Ni3 O15.71
Mr	1327.46	1327.65
Dx,g cm-3	1.495	1.495
Z	1	1
Mu (mm-1)	1.199	1.199
F000	686.2	686.0
F000’	688.11	
h,k,lmax	13,13,14	13,13,14
Nref	5799	5788
Tmin,Tmax	0.739,0.816	0.772,1.000
Tmin’	0.725	

Correction method= # Reported T Limits: Tmin=0.772 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 26.020

R(reflections)= 0.0524(4073) wR2(reflections)= 0.1422(5788)

S = 1.053 Npar= 373

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

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT193_ALERT_1_C Cell and Diffraction Temperatures Differ by .... 1 Degree
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C18 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00653 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H22C ..H25C 2.08 Ang.

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: C49.12 H59.94 Cl4 N7.71 Ni3
Atom count from _chemical_formula_moiety:C49.13 H59.97 Cl4 N7.71 Ni3
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.007 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 2 10.24 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2 112.2 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 110.3 Degree
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 36 Note

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
7 ALERT type 4 Improvement, methodology, query or suggestion
0 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 30/01/2018; check.def file version of 30/01/2018

Datablock d492 - ellipsoid plot