

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: I

| | | |
|-----------------|-------------------|---------------------------------------|
| Bond precision: | C-C = 0.0140 Å | Wavelength=0.71073 |
| Cell: | a=7.8897(9) | b=8.8950(14) c=10.4485(16) |
| | alpha=75.433(14) | beta=87.129(12) gamma=70.233(12) |
| Temperature: | 293 K | |
| | Calculated | Reported |
| Volume | 667.38(18) | 667.38(17) |
| Space group | P -1 | P-1 |
| Hall group | : -P 1 | ? |
| Moiety formula | C28 H36 N2 Ni O10 | Ni(L2)(EtOh)2(MeOh)2 |
| Sum formula | C28 H36 N2 Ni O10 | C28 H36 N2 Ni O10 |
| Mr | 619.28 | 619.30 |
| Dx,g cm-3 | 1.541 | 1.541 |
| Z | 1 | 1 |
| Mu (mm-1) | 0.791 | 0.791 |
| F000 | 326.0 | 326.0 |
| F000' | 326.50 | |
| h,k,lmax | 9,10,12 | 9,10,12 |
| Nref | 2352 | 1895 |
| Tmin,Tmax | 0.867,0.946 | 0.867,0.946 |
| Tmin' | 0.776 | |

Correction method= # Reported T Limits: Tmin=0.867 Tmax=0.946
AbsCorr = MULTI-SCAN

Data completeness= 0.806 Theta(max)= 25.030

R(reflections)= 0.0944(1686) wR2(reflections)= 0.2428(1895)

S = 1.059 Npar= 187

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 A

| | | | | | | |
|-------------------|-------------------------------------|------------|--------|---|-------|-------|
| PLAT029_ALERT_3_A | _diffn_measured_fraction_theta_full | value | Low | . | 0.806 | Why? |
| PLAT412_ALERT_2_A | Short Intra XH3 .. XHn | H12C | ..H14B | . | 1.40 | Ang. |
| | | -x,-y,1-z | = | | 2_556 | Check |
| PLAT413_ALERT_2_A | Short Inter XH3 .. XHn | H10A | ..H12B | . | 1.55 | Ang. |
| | | x,y,-1+z | = | | 1_554 | Check |
| PLAT413_ALERT_2_A | Short Inter XH3 .. XHn | H12A | ..H14B | . | 1.73 | Ang. |
| | | x,1+y,z | = | | 1_565 | Check |
| PLAT413_ALERT_2_A | Short Inter XH3 .. XHn | H12A | ..H12B | . | 1.74 | Ang. |
| | | -x,1-y,1-z | = | | 2_566 | Check |
| PLAT413_ALERT_2_A | Short Inter XH3 .. XHn | H12A | ..H12C | . | 1.76 | Ang. |
| | | -x,1-y,1-z | = | | 2_566 | Check |
| PLAT413_ALERT_2_A | Short Inter XH3 .. XHn | H12B | ..H12C | . | 1.79 | Ang. |
| | | -x,1-y,1-z | = | | 2_566 | Check |

Alert level B

| | | | | | | |
|-------------------|----------------------|-----|---------|---|-------|--------------|
| PLAT415_ALERT_2_B | Short Inter D-H..H-X | H4B | ..H10A | . | 1.94 | Ang. |
| | | | x,y,1+z | = | 1_556 | Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O3 | --H3B | . | | Please Check |

Alert level C

| | | | | | | |
|-------------------|--|-----------|--------|---|-------|-------------|
| PLAT094_ALERT_2_C | Ratio of Maximum / Minimum Residual Density | | | | 2.12 | Report |
| PLAT125_ALERT_4_C | No '_symmetry_space_group_name_Hall' Given | | | | | Please Do ! |
| PLAT220_ALERT_2_C | Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range | | | | 3.1 | Ratio |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for C4 --C5 | . | | | 6.5 | s.u. |
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X) Nil --O3 | . | | | 6.3 | s.u. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C2 --C3 | . | | | 0.22 | Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C7 --C8 | . | | | 0.16 | Ang. |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | | | | C3 | Check |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | | | | C4 | Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | | | | Nil | Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | | | | C2 | Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | | | | C5 | Check |
| PLAT341_ALERT_3_C | Low Bond Precision on C-C Bonds | | | | 0.014 | Ang. |
| PLAT361_ALERT_2_C | Long C(sp3)-C(sp3) Bond C12 - C13 | .. | | | 1.67 | Ang. |
| PLAT368_ALERT_2_C | Short C(sp2)-C(sp2) Bond C2 - C3 | . | | | 1.20 | Ang. |
| PLAT369_ALERT_2_C | Long C(sp2)-C(sp2) Bond C4 - C5 | . | | | 1.55 | Ang. |
| PLAT413_ALERT_2_C | Short Inter XH3 .. XHn | H10A | ..H12A | . | 2.12 | Ang. |
| | | -x,1-y,-z | = | | 2_565 | Check |
| PLAT414_ALERT_2_C | Short Intra D-H..H-X | H4B | ..H12B | . | 1.91 | Ang. |
| | | | x,y,z | = | 1_555 | Check |

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: C28 H36 N2 Nil O10
Atom count from _chemical_formula_moiety:

| | | | | | | |
|-------------------|--|--|--|--|-------|--------------|
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | | | | 1 | Report |
| PLAT005_ALERT_5_G | No Embedded Refinement Details Found in the CIF | | | | | Please Do ! |
| PLAT007_ALERT_5_G | Number of Unrefined Donor-H Atoms | | | | 3 | Report |
| PLAT042_ALERT_1_G | Calc. and Reported MoietyFormula Strings Differ | | | | | Please Check |
| PLAT066_ALERT_1_G | Predicted and Reported Tmin&Tmax Range Identical | | | | ? | Check |
| PLAT072_ALERT_2_G | SHELXL First Parameter in WGHT Unusually Large | | | | 0.17 | Report |
| PLAT093_ALERT_1_G | No s.u.'s on H-positions, Refinement Reported as | | | | mixed | Check |
| PLAT199_ALERT_1_G | Reported _cell_measurement_temperature (K) | | | | 293 | Check |
| PLAT200_ALERT_1_G | Reported _diffn_ambient_temperature (K) | | | | 293 | Check |
| PLAT335_ALERT_2_G | Check Large C6 Ring C-C Range C1 -C6 | | | | 0.35 | Ang. |

| | | | |
|-------------------|--|-------|-------|
| PLAT380_ALERT_4_G | Incorrectly? Oriented X(sp2)-Methyl Moiety | C10 | Check |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact C12 ..C12 | 2.16 | Ang. |
| | -x,1-y,1-z = | 2_566 | Check |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Nil (II) . | 2.00 | Info |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | 6 | Note |
| PLAT899_ALERT_4_G | SHELXL97 is Deprecated and Succeeded by SHELXL | 2018 | Note |

7 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
18 **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
26 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
 _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
 _publ_contact_author_phone are all missing.
 At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
 e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
 Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
 empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
```

```

RESPONSE: ...
;
_vrf_PLAT029_I
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .      0.806 Why?
RESPONSE: ...
;
_vrf_PLAT412_I
;
PROBLEM: Short Intra XH3 .. XHn      H12C      ..H14B      .      1.40 Ang.
RESPONSE: ...
;
_vrf_PLAT413_I
;
PROBLEM: Short Inter XH3 .. XHn      H10A      ..H12B      .      1.55 Ang.
RESPONSE: ...
;
# end Validation Reply Form

```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 19/10/2018; check.def file version of 15/10/2018

