

checkCIF/PLATON (full publication check)

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.

Please wait while processing

[CIF dictionary](#)

[Interpreting this report](#)

Datablock: I

Bond precision:	C-C = 0.0134 A	Wavelength=0.71073	
Cell:	a=14.717(2)	b=16.851(3)	c=21.227(3)
	alpha=90	beta=90	gamma=90
Temperature:	173 K		
	Calculated	Reported	
Volume	5264.2(14)	5264.3(15)	
Space group	P 21 21 21	P2(1)2(1)2(1)	
Hall group	P 2ac 2ab	?	
Moiety formula	C40 H76 N8 Ni2 O4, 2(Cl O4), O	?	
Sum formula	C40 H76 Cl2 N8 Ni2 O13	C40 H78 Cl2 N8 Ni2 O13	
Mr	1065.37	1067.42	
Dx,g cm-3	1.344	1.347	
Z	4	4	
Mu (mm-1)	0.880	0.880	
F000	2264.0	2272.0	
F000'	2268.76		
h,k,lmax	18,21,27	18,21,27	
Nref	11628[6389]	11584	
Tmin,Tmax	0.674,0.831	0.688,0.837	
Tmin'	0.661		
Correction method=	MULTI-SCAN		
Data completeness=	1.81/1.00	Theta(max)=	27.100
R(reflections)=	0.0708(5038)	wR2(reflections)=	0.2098(11584)
S =	1.038	Npar=	598

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

[PLAT306_ALERT_2_B](#) Isolated Oxygen Atom (H-atoms Missing ?) [O1W Check](#)

Alert level C

[ABSTY02_ALERT_1_C](#) An _exptl_absorpt_correction_type has been given without

a literature citation. This should be contained in the

_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

[PLATO26_ALERT_3_C](#) Ratio Observed / Unique Reflections too Low 43 %

[PLATO41_ALERT_1_C](#) Calc. and Reported SumFormula Strings Differ Please Check

[PLATO48_ALERT_1_C](#) MoietyFormula Not Given Please Do !

[PLATO68_ALERT_1_C](#) Reported F000 Differs from Calcd (or Missing)... Please Check

[PLAT125_ALERT_4_C](#) No '_symmetry_space_group_name_Hall' Given Please Do !

[PLAT230_ALERT_2_C](#) Hirshfeld Test Diff for N1 -- C1 .. 6.4 su

PLAT230_ALERT_2_C Hirshfeld Test Diff for N8 -- C34 .. 5.6 su
 PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for Ni2 Check
 PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for N8 Check
 PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0134 Ang.
 PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C33 - C34 ... 1.43 Ang.

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and the formula from the _atom_site* data.
 Atom count from _chemical_formula_sum: C40 H78 Cl2 N8 Ni2 O13
 Atom count from the _atom_site data: C40 H76 Cl2 N8 Ni2 O13
 CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
 CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
 From the CIF: _cell_formula_units_Z 4
 From the CIF: _chemical_formula_sum C40 H78 Cl2 N8 Ni2 O13
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	160.00	160.00	0.00
H	312.00	304.00	8.00
Cl	8.00	8.00	0.00
N	32.00	32.00	0.00
Ni	8.00	8.00	0.00
O	52.00	52.00	0.00

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 47
 PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 8 Why ?
 PLAT093_ALERT_1_G No su's on H-positions, refinement reported as . mixed
 PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of Cl1 Check
 PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of Cl2 Check
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 31 Do !
 N3 -N11 -N1 -C1 -39.00 3.00 1.555 1.555 1.555 1.555

And 23 other PLAT710 Alerts

More ...

PLAT791_ALERT_4_G The Model has Chirality at N1 (Verify) S

And 11 other PLAT791 Alerts

More ...

PLAT860_ALERT_3_G Number of Least-Squares Restraints 686 Note

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

7 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
 3 ALERT type 3 Indicator that the structure quality may be low
 39 ALERT type 4 Improvement, methodology, query or suggestion
 2 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.

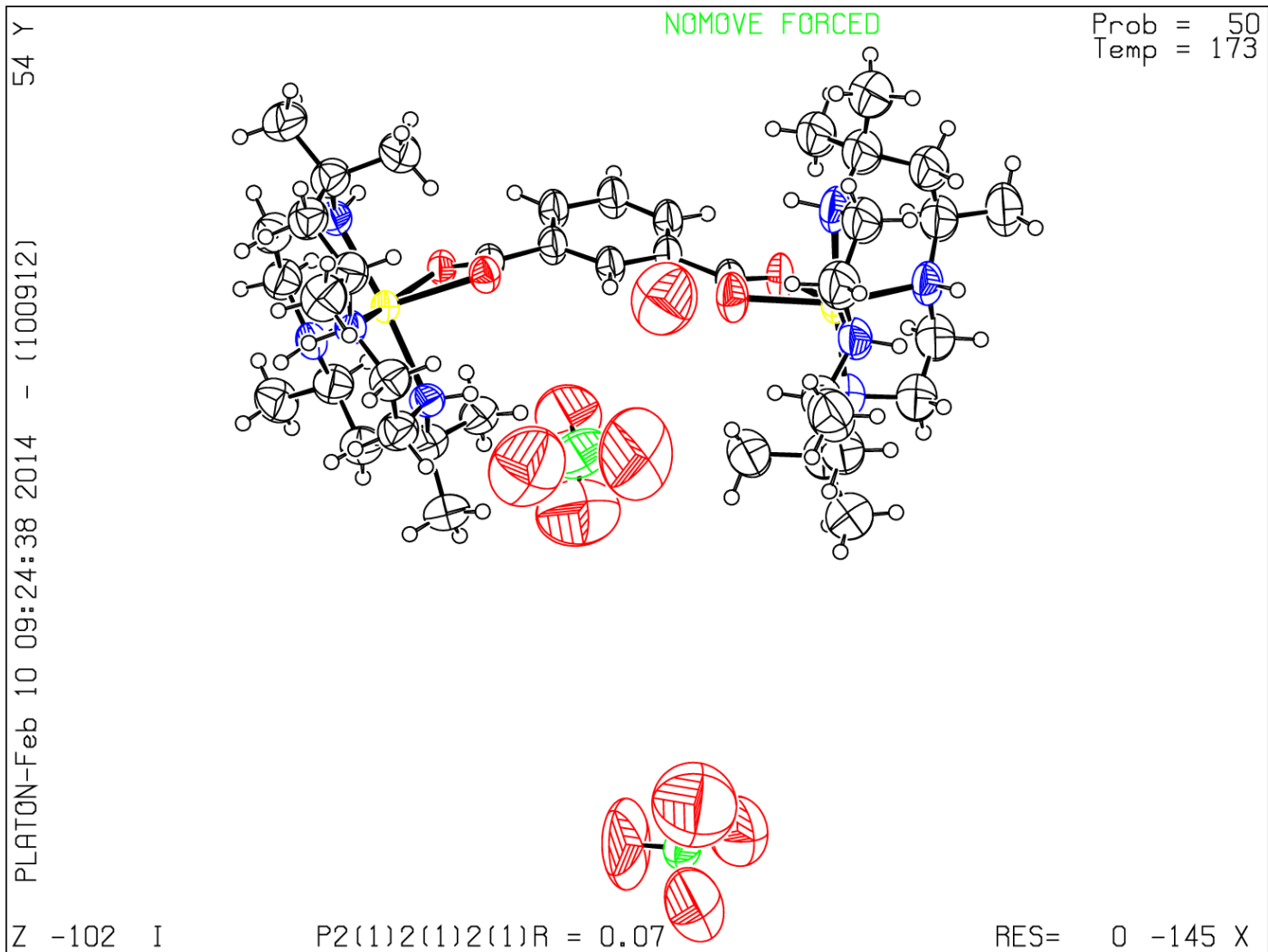
If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the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

```
# 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: ...
;
# 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 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 18/09/2013; check.def file version of 12/09/2013

Datablock I - ellipsoid plot



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