

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 = 0.0040 A

Wavelength=0.71073

Cell: a=13.718(1) b=14.030(2) c=14.908(2)
 alpha=115.285(12) beta=116.477(11) gamma=92.967(10)
Temperature: 130 K

	Calculated	Reported
Volume	2215.8(7)	2215.8(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C20 H14 N2 Ni O2), 3(C H ? Cl3)	
Sum formula	C43 H31 Cl9 N4 Ni2 O4	C43 H31 Cl9 N4 Ni2 O4
Mr	1104.15	1104.19
Dx,g cm-3	1.655	1.655
Z	2	2
Mu (mm-1)	1.441	1.441
F000	1116.0	1116.0
F000'	1120.31	
h,k,lmax	19,19,20	18,18,19
Nref	12362	10314
Tmin,Tmax	0.745,0.794	0.682,0.827
Tmin'	0.473	

Correction method= # Reported T Limits: Tmin=0.682 Tmax=0.827
AbsCorr = ANALYTICAL

Data completeness= 0.834

Theta(max)= 29.513

R(reflections)= 0.0394(8211)

wR2(reflections)= 0.0892(10314)

S = 1.027

Npar= 559

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

PLAT048_ALERT_1_C	MoietyFormula Not Given (or Incomplete)	Please Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C31 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C51 Check



Alert level G

PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	2 Units
PLAT794_ALERT_5_G	Tentative Bond Valency for NilA (III) .	3.00 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for NilB (III) .	3.01 Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.8 Low

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
5 **ALERT level G** = General information/check it is not something unexpected

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

checkCIF publication errors



Alert level A

PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

1 **ALERT level A** = Data missing that is essential or data in wrong format
0 **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_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 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.

