checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3

Bond precision: C-C = 0.0051 A Wavelength=0.71073

Cell: a=32.220(6) b=23.844(5) c=22.496(5)
alpha=90 beta=133.81(3) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	12472(8)	12472(4)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	3(C24 H40 N2 Ni O2), 2(C25 H40 N Ni O2)	?
Sum formula	C122 H200 N8 Ni5 O10	C61 H100 N4 Ni2.50 O5
Mr	2232.35	1116.22
Dx,g cm-3	1.189	1.189
Z	4	8
Mu (mm-1)	0.797	0.797
F000	4832.0	4832.0
F000’	4840.19	
h,k,lmax	38,28,26	38,28,26
Nref	11039	10891
Tmin,Tmax	0.723,0.775	0.731,0.785
Tmin’	0.708	

Correction method= NONE

Data completeness= 0.987 Theta(max)= 25.050

R(reflections)= 0.0359(8099) wR2(reflections)= 0.1084(10891)

S = 0.740 Npar= 655

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
PLAT413_ALERT_2_A Short Inter XH3 .. XHn H10K .. H10K .. 1.80 Ang.

Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for C14 -- C41 .. 22.5 su

---

Alert level C

ABSTY03_ALERT_1_C The _exptl_absorpt_correction_type has been given as none.
However values have been given for Tmin and Tmax. Remove
these if an absorption correction has not been applied.
From the CIF: _exptl_absorpt_correction_T_min 0.731
From the CIF: _exptl_absorpt_correction_T_max 0.785
GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 0.740
PLAT230_ALERT_2_C Hirshfeld Test Diff for C14 -- C65 .. 5.3 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for C53 -- C76 .. 5.7 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ni2 -- C14 .. 6.9 su
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C41
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C20
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C25
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C37
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C14
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C48
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C65
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C51
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C53

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ?
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ..... 0.50 Ratio
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.1. Differ by ... 4 Units
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature 293 K
PLAT200_ALERT_1_G Check the Reported _diffrn_ambient_temperature 293 K

---

1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
14 **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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 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 05/11/2012; check.def file version of 05/11/2012

Datablock 3 - ellipsoid plot