

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) NiL2_200K

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: NiL2_200K

Bond precision: C-C = 0.0034 Å Wavelength=0.71073

Cell: a=13.276(3) b=8.2907(17) c=12.530(3)
 alpha=90 beta=93.021(6) gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	1377.2(5)	1377.2(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C30 H34 N4 Ni O2	C30 H34 N4 Ni O2
Sum formula	C30 H34 N4 Ni O2	C30 H34 N4 Ni O2
Mr	541.30	541.32
Dx,g cm-3	1.305	1.305
Z	2	2
Mu (mm-1)	0.738	0.738
F000	572.0	572.0
F000'	572.85	
h,k,lmax	19,11,18	18,11,17
Nref	4307	3805
Tmin,Tmax	0.796,0.915	0.380,0.863
Tmin'	0.796	

Correction method= # Reported T Limits: Tmin=0.380 Tmax=0.863
AbsCorr = MULTI-SCAN

Data completeness= 0.883 Theta(max)= 30.807

R(reflections)= 0.0535(2653) wR2(reflections)= 0.1562(3805)

S = 1.007 Npar= 169

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

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.408	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	10	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	6	Note



Alert level G

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Nil --N2 .	5.3	s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Nil (III) .	3.04	Info
PLAT882_ALERT_1_G	No Datum for _diffrn_reflms_av_unetI/netI		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	484	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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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
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
1 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

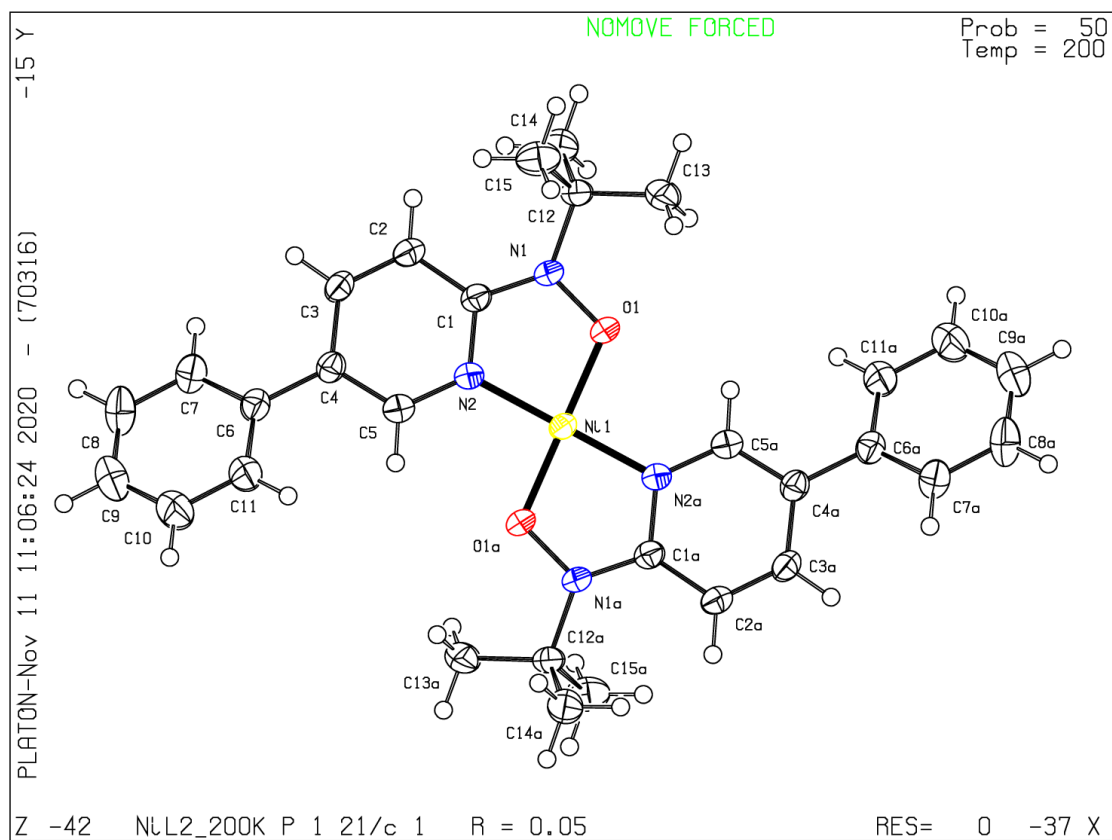
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* 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 18/09/2020; check.def file version of 20/08/2020

Datablock NiL2_200K - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) NiL2I3_200K

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Datablock: NiL2I3_200K

Bond precision: C-C = 0.0046 A

Wavelength=0.71073

Cell: a=11.828(3) b=11.963(4) c=12.703(4)
 alpha=111.438(14) beta=100.692(13) gamma=91.250(14)
Temperature: 200 K

	Calculated	Reported
Volume	1636.1(9)	1636.2(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H34 N4 Ni O2, I3	C30 H34 N4 Ni O2, I3
Sum formula	C30 H34 I3 N4 Ni O2	C30 H34 I3 N4 Ni O2
Mr	922.00	922.04
Dx,g cm-3	1.872	1.871
Z	2	2
Mu (mm-1)	3.456	3.457
F000	890.0	890.0
F000'	888.10	
h,k,lmax	15,15,16	15,15,16
Nref	7526	7418
Tmin,Tmax	0.710,0.764	0.589,0.764
Tmin'	0.623	

Correction method= # Reported T Limits: Tmin=0.589 Tmax=0.764
AbsCorr = MULTI-SCAN

Data completeness= 0.986

Theta(max)= 27.484

R(reflections)= 0.0330(5382)

wR2(reflections)= 0.0743(7418)

S = 1.055

Npar= 361

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test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).	11 Note
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Alert level C

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	61 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF	19 Note
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check

Alert level G

PLAT794_ALERT_5_G Tentative Bond Valency for Nil (III) .	3.25 Info
PLAT882_ALERT_1_G No Datum for _diffrn_reflms_av_unetI/netI	Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	36 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	3.7 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	1 Info

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