

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1, 2

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: 1

Bond precision:	C-C = 0.0038 A	Wavelength=0.71069
Cell:	a=9.5916(10)	b=33.666(3) c=13.3219(13)
	alpha=90	beta=105.255(3) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	4150.2(7)	4150.2(7)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C10 H12 N4 Ni	C10 H12 N4 Ni
Sum formula	C10 H12 N4 Ni	C10 H12 N4 Ni
Mr	246.93	246.95
Dx,g cm-3	1.581	1.581
Z	16	16
Mu (mm-1)	1.839	1.839
F000	2048.0	2048.0
F000'	2053.75	
h,k,lmax	11,40,16	11,40,16
Nref	3952	3910
Tmin,Tmax	0.916,0.964	0.650,0.746
Tmin'	0.576	

Correction method= # Reported T Limits: Tmin=0.650 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 25.680

R(reflections)= 0.0308(3204) wR2(reflections)= 0.0793(3910)

S = 1.038 Npar= 275

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 G

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni2 --N7 . 5.2 s.u.
PLAT883_ALERT_1_G No Info for _atom_sites_solution_primary Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
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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
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: 2

Bond precision: C-C = 0.0046 Å Wavelength=0.71069
Cell: a=9.4362(7) b=10.7558(7) c=17.0271(12)
alpha=103.204(2) beta=94.650(2) gamma=93.872(2)
Temperature: 150 K

	Calculated	Reported
Volume	1670.3(2)	1670.3(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H42 N4 Ni Yb, C7 H8	C30 H42 N4 Ni Yb, C7 H8
Sum formula	C37 H50 N4 Ni Yb	C37 H50 N4 Ni Yb
Mr	782.54	782.56
Dx,g cm-3	1.556	1.556
Z	2	2
Mu (mm-1)	3.377	3.377
F000	796.0	796.0
F000'	796.11	
h,k,lmax	11,13,21	11,13,21
Nref	6840	6781
Tmin,Tmax	0.573,0.713	0.605,0.746
Tmin'	0.385	

Correction method= # Reported T Limits: Tmin=0.605 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 26.369

R(reflections)= 0.0236(6241) wR2(reflections)= 0.0588(6781)

S = 0.945

Npar= 404

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

PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.2	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.7	Note
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn H9C ..H10A .	1.85	Ang.
	x,y,z =	1_555	Check

● Alert level G

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C31 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C32 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C33 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C34 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C35 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C36 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C37 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H33 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H34 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H35 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37C Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C38 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C39 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C40 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C41 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C42 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C43 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C44 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44C Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 2	7.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 3	7.50	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	98	Check
	N1 -C4 -YB1 1.555 1.555 1.555	43.13	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	104	Check
	N2 -C5 -YB1 1.555 1.555 1.555	43.04	Deg.
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	30	Check
PLAT883_ALERT_1_G	No Info for _atom_sites_solution_primary		Please Do !
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	4	Note

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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.



