

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: 1

Bond precision:	C-C = 0.0038 A	Wavelength=0.71073
Cell:	a=9.7053(19) alpha=90	b=9.795(2) beta=97.43(3)
Temperature:	298 K	c=30.303(6) gamma=90
	Calculated	Reported
Volume	2856.5(10)	2856.5(10)
Space group	P 2/c	P 2/c
Hall group	-P 2yc	-P 2yc
Moiety formula	C20 H22 N6 Ni O2, C8 H4 O4, 2(H2 O)	C20 H22 N6 Ni O2, C8 H4 O4, 2(H2 O)
Sum formula	C28 H30 N6 Ni O8	C28 H30 N6 Ni O8
Mr	637.27	637.29
Dx,g cm-3	1.482	1.482
Z	4	4
Mu (mm-1)	0.741	0.741
F000	1328.0	1328.0
F000'	1329.93	
h,k,lmax	11,12,37	11,12,37
Nref	5609	5603
Tmin,Tmax	0.683,0.743	0.662,0.777
Tmin'	0.625	

Correction method= # Reported T Limits: Tmin=0.662 Tmax=0.777
AbsCorr = GAUSSIAN

Data completeness= 0.999 Theta(max)= 26.022

R(reflections)= 0.0395(4892) wR2(reflections)= 0.0920(5603)

S = 1.121 Npar= 420

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

PLAT420_ALERT_2_B D-H Without Acceptor 07 -- H34 ... Please 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 gaussian

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.3 Note

 Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report

PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size 0.62 mm

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4).. 100 % Note

PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #
H2 O 5 Note

PLAT860_ALERT_3_G Number of Least-Squares Restraints 4 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

3 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

3 ALERT type 4 Improvement, methodology, query or suggestion

2 ALERT type 5 Informative message, check

Datablock: 2

Bond precision: C-C = 0.0032 A Wavelength=0.71073

Cell: a=9.7461(19) b=9.797(2) c=30.287(6)

 alpha=90 beta=97.40(3) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	2867.8(10)	2867.9(10)
Space group	P 2/c	P 2/c
Hall group	-P 2yc	-P 2yc
Moiety formula	C20 H22 Co N6 O2, C8 H4 O4, 2(H2 O)	C20 H22 Co N6 O2, C8 H4 O4, 2(H2 O)
Sum formula	C28 H30 Co N6 O8	C28 H30 Co N6 O8
Mr	637.51	637.51
Dx, g cm-3	1.477	1.477
Z	4	4
Mu (mm-1)	0.660	0.659
F000	1324.0	1324.0
F000'	1325.97	
h, k, lmax	12, 12, 37	12, 12, 37
Nref	5637	5630
Tmin, Tmax	0.854, 0.924	0.991, 1.000
Tmin'	0.854	

Correction method= # Reported T Limits: Tmin=0.991 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.019

R(reflections)= 0.0354(5260) wR2(reflections)= 0.0851(5630)

S = 1.152 Npar= 420

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

PLAT420_ALERT_2_B D-H Without Acceptor 07 -- H33 ... Please 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
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.1 Note



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4).. 100 % Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints 4 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

- 1 **ALERT level B** = A potentially serious problem, consider carefully
 - 2 **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
-
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 3 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
 - 1 ALERT type 4 Improvement, methodology, query or suggestion
 - 2 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.



