

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: d451

Bond precision: C-C = 0.0062 A

Wavelength=0.71073

Cell: a=9.4955(7) b=12.1979(7) c=13.4593(9)
 alpha=70.556(6) beta=81.564(6) gamma=82.607(6)
Temperature: 294 K

	Calculated	Reported
Volume	1448.77(18)	1448.76(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H50 Cl4 N4 Ni3 O14, 2(C3 H8 O)	C44 H50 Cl4 N4 Ni3 O14, 2(C3 H8 O)
Sum formula	C50 H66 Cl4 N4 Ni3 O16	C50 H66 Cl4 N4 Ni3 O16
Mr	1296.94	1297.00
Dx, g cm ⁻³	1.487	1.487
Z	1	1
Mu (mm ⁻¹)	1.217	1.217
F000	674.0	674.0
F000'	675.87	
h,k,lmax	11,15,16	11,15,16
Nref	5698	5688
Tmin,Tmax	0.710,0.747	0.986,1.000
Tmin'	0.696	

Correction method= # Reported T Limits: Tmin=0.986 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max)= 26.020

R(reflections)= 0.0492(4219)

wR2(reflections)= 0.1239(5688)

S = 1.038

Npar= 359

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

PLAT417_ALERT_2_B Short Inter D-H..H-D H6 ..H7A .. 1.95 Ang.

Alert level C

PLAT213_ALERT_2_C Atom C11 has ADP max/min Ratio 3.3 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C24 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C23 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00624 Ang.
PLAT354_ALERT_3_C Short O-H (X0.82,N0.98A) O7 - H7A . 0.70 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C23 - C24 . 1.36 Ang.

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 !
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.006 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2 111.1 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 111.2 Degree
PLAT860_ALERT_3_G Number of Least-Squares Restraints 3 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
8 **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
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 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 09/11/2017; check.def file version of 08/11/2017

