

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ras1515SN

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: ras1515SN

Bond precision: C-C = 0.0022 Å Wavelength=1.54184

Cell: a=7.3033(1) b=19.2677(1) c=20.4218(1)
 alpha=90 beta=90 gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	2873.71(4)	2873.71(4)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C26 H36 N4 Ni O6, 2(Cl)	C26 H36 N4 Ni O6 2+, (Cl -)2
Sum formula	C26 H36 Cl2 N4 Ni O6	C26 H36 Cl2 N4 Ni O6
Mr	630.18	630.21
Dx, g cm-3	1.457	1.457
Z	4	4
Mu (mm-1)	3.079	3.079
F000	1320.0	1320.0
F000'	1314.26	
h, k, lmax	9, 23, 25	9, 23, 25
Nref	2829	2823
Tmin, Tmax	0.676, 0.719	0.640, 0.720
Tmin'	0.484	

Correction method= # Reported T Limits: Tmin=0.640 Tmax=0.720
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 72.417

R(reflections)= 0.0285(2777) wR2(reflections)= 0.0723(2823)

S = 1.022 Npar= 232

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

PLAT391_ALERT_3_C Deviating Methyl C5 H-C-H Bond Angle 118 Degree



Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing	0.00010 Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing	0.00010 Ang.
PLAT153_ALERT_1_G	The s.u.'s on the Cell Axes are Equal ..(Note)	0.0001 Ang.
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	16 Note
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ni1 --N1 .	6.7 s.u.
PLAT793_ALERT_4_G	Model has Chirality at C3 (Centro SPGR)	R Verify
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni1 (II) .	2.12 Info
PLAT882_ALERT_1_G	No Datum for _diffrn_reflns_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	5 Note
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	3 Check

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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
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check
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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.

