

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision:	C-C = 0.0092 Å	Wavelength=0.71073	
Cell:	a=16.604 (8)	b=24.002 (13)	c=14.571 (8)
	alpha=90	beta=103.381 (12)	gamma=90
Temperature:	295 K		

	Calculated	Reported
Volume	5649(5)	5649(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	?
Moiety formula	C28 H18 Br4 N2 Ni O4	C28 H18 Br4 N2 Ni1 O4
Sum formula	C28 H18 Br4 N2 Ni O4	C28 H18 Br4 N2 Ni1 O4
Mr	824.73	824.79
Dx, g cm ⁻³	1.939	1.939
Z	8	8
Mu (mm ⁻¹)	6.383	6.383
F000	3200.0	3200.0
F000'	3195.22	
h, k, lmax	20, 29, 17	20, 29, 17
Nref	10892	10738
Tmin, Tmax	0.415, 0.496	0.460, 0.500
Tmin'	0.369	

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Correction method= # Reported T Limits: Tmin=0.460 Tmax=0.500
AbsCorr = NUMERICAL
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Data completeness= 0.986 Theta (max)= 25.820

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R(reflections)= 0.0381( 7018)      wR2(reflections)=
S = 1.000                        0.1187( 7018)
Npar= 703
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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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings	Differ	Please Check
	Calc: C28 H18 Br4 N2 Ni O4			
	Rep.: C28 H18 Br4 N2 Ni1 O4			
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula	Strings	Differ	Please Check
	Calc: C28 H18 Br4 N2 Ni O4			
	Rep.: C28 H18 Br4 N2 Ni1 O4			
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds			0.00918 Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).			6 Note
	1 0 0, 1 1 0, 0 2 0, 1 2 0, -1 1 1,			0 1 1,
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		20 Report
	2 1 0, 2 2 0, 1 3 0, -2 1 1, 1 1 1,			-2 2 1,
	1 2 1, -1 3 1, 0 3 1, -2 0 2, -1 0 2,			-2 1 2,
	-1 1 2, 0 1 2, -2 0 4, -12 19 10, -11 20 10,			-14 15 11,
	8 15 11, -13 15 12,			



Alert level G

PLAT769_ALERT_4_G	CIF Embedded Explicitly Supplied Scattering Data	Please Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni1 (II) .	2.03 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni2 (II) .	2.00 Info
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please Check
PLAT882_ALERT_1_G	No Datum for _diffn_reflms_av_unetI/netI	Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	136 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1 Note
	-2 0 4,	
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked	! Info
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	195 Check
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	6.27 Note
	Predicted wR2: Based on SigI**2 1.36 or SHELX Weight 11.13	

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
5 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.

Datablock 1 - ellipsoid plot

