

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelxs

Bond precision: C-C = 0.0150 A Wavelength=0.71073

Cell: a=12.183(2) b=8.8520(18) c=19.674(4)
 alpha=90 beta=103.23(3) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	2065.4(7)	2065.4(7)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C10 H22 N4 Ni3 O18	?
Sum formula	C10 H22 N4 Ni3 O18	C5 H11 N2 Ni1.50 O9
Mr	662.39	331.22
Dx,g cm-3	2.130	2.130
Z	4	8
Mu (mm-1)	2.809	2.809
F000	1352.0	1352.0
F000'	1356.82	
h,k,lmax	14,10,23	14,10,23
Nref	1818	1742
Tmin,Tmax	0.481,0.714	0.467,0.729
Tmin'	0.403	

Correction method= MULTI-SCAN

Data completeness= 0.958 Theta(max)= 24.990

R(reflections)= 0.0937(1081) wR2(reflections)= 0.1544(1742)

S = 1.100 Npar= 172

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

PLAT029_ALERT_3_B	_diffrn_measured_fraction_theta_full	Low	0.96
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H3A	.. H5A ..	2.06 Ang.
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H4A	.. H5B ..	1.96 Ang.
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H6A	.. H6A ..	1.97 Ang.
PLAT731_ALERT_1_B	Bond Calc	0.85(6), Rep	0.848(10)	6.00 su-Ra
	07 -H7B	1.555 1.555	#	33

● Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.156
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 0.16
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.26
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 15
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT045_ALERT_1_C Calculated and Reported Z Differ by 0.50 Ratio
PLAT731_ALERT_1_C Bond Calc 0.85(3), Rep 0.848(10) 3.00 su-Ra
O5 -H5A 1.555 1.555 # 28
PLAT731_ALERT_1_C Bond Calc 0.85(3), Rep 0.847(10) 3.00 su-Ra
O5 -H5B 1.555 1.555 # 29
PLAT731_ALERT_1_C Bond Calc 0.85(4), Rep 0.850(10) 4.00 su-Ra
O7 -H7A 1.555 1.555 # 32

● Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 27.07
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 64
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature 293 K
PLAT200_ALERT_1_G Check the Reported _diffrn_ambient_temperature 293 K
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 25
N1 -N2 -NI2 -N2 11.00 0.00 1.555 1.555 1.555 7.657
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 26
C4 -N2 -NI2 -N2 8.00 0.00 1.555 1.555 1.555 7.657
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 37
C5 -O8 -NI2 -O8 11.00 0.00 1.555 1.555 1.555 7.657
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 42
O6 -NI1 -O2 -C1 148.00 3.00 1.555 1.555 1.555 1.555
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Ni2 2.12

0 **ALERT level A** = In general: serious problem
5 **ALERT level B** = Potentially serious problem
9 **ALERT level C** = Check and explain
9 **ALERT level G** = General alerts; check

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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*, 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 22/10/2010; check.def file version of 11/10/2010

Datablock shelxs - ellipsoid plot

