

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 6

Bond precision: C-C = 0.0126 Å

Wavelength=0.71073

Cell: a=10.4540(2)
 alpha=90

 b=15.6610(1)
 beta=90

 c=20.8026(3)
 gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	3405.80(8)	3405.80(8)
Space group	P 21 21 21	P2(1)2(1)2(1)
Hall group	P 2ac 2ab	?
Moiety formula	C21 H13 B F21 N7 Ni O3	?
Sum formula	C21 H13 B F21 N7 Ni O3	C21 H13 B F21 N7 Ni O3
Mr	879.88	879.90
Dx, g cm-3	1.716	1.716
Z	4	4
Mu (mm-1)	0.721	0.721
F000	1736.0	1736.0
F000'	1739.04	
h, k, lmax	11, 17, 22	11, 17, 22
Nref	2668[4693]	4448
Tmin, Tmax	0.841, 0.897	0.786, 0.900
Tmin'	0.777	

Correction method= MULTI-SCAN

Data completeness= 1.67/0.95

Theta(max)= 22.890

R(reflections)= 0.0646(3925)

wR2(reflections)= 0.1749(4448)

S = 1.069

Npar= 491

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 A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550

Calculated sin(theta_max)/wavelength = 0.5473

PLAT220_ALERT_2_A Large Non-Solvent F Ueq(max)/Ueq(min) ... 4.64 Ratio

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C21

🟡 Alert level B

PLAT234_ALERT_4_B Large Hirshfeld Difference F19 -- C21 .. 0.23 Ang.

🟢 Alert level C

REFNR01_ALERT_3_C Ratio of reflections to parameters is < 10 for a
non-centrosymmetric structure, where ZMAX > 18
sine(theta)/lambda 0.5473
Proportion of unique data used 1.0000
Ratio reflections to parameters 9.0591

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.97
PLAT083_ALERT_2_C SHELXL Second Parameter in WGHT unusually Large. 12.00
PLAT213_ALERT_2_C Atom F21 has ADP max/min Ratio 3.30 prola
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 2.60 Ratio
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for 02
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for N7
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C6
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C20
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ... 13
PLAT142_ALERT_4_C su on b - Axis Small or Missing (x 100000) 10 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ni -- 01 .. 0.12 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ni -- 02 .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ni -- N3 .. 0.12 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ni -- N5 .. 0.14 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F4 -- C6 .. 0.15 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F6 -- C7 .. 0.14 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F10 -- C13 .. 0.11 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F11 -- C13 .. 0.11 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F12 -- C14 .. 0.15 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference 02 -- N7 .. 0.13 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference 03 -- N7 .. 0.14 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5 -- N6 .. 0.12 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5 -- C17 .. 0.11 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1 -- C2 .. 0.14 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C6 -- C7 .. 0.13 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C8 -- C9 .. 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C9 -- C10 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C15 -- C18 .. 0.13 Ang.

🟡 Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
correct. If it is not, please give the correct count in the
_publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflns_theta_max 22.89
From the CIF: _reflns_number_total 4448
Count of symmetry unique reflns 2668
Completeness (_total/calc) 166.72%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 1780
Fraction of Friedel pairs measured 0.667
Are heavy atom types Z>Si present yes

3 ALERT level A = In general: serious problem

1 ALERT level B = Potentially serious problem

29 ALERT level C = Check and explain

1 ALERT level G = General alerts; check

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

9 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
21 ALERT type 4 Improvement, methodology, query or suggestion
0 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 12/11/2008; check.def file version of 12/11/2008

Datablock 6 - ellipsoid plot

