checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: char342a

Bond precision: C-C = 0.0035 A Wavelength=0.71073

Cell: a=8.924(3) b=8.624(3) c=8.937(3)
alpha=90 beta=115.063(4) gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	623.0(4)	623.0(4)
Space group	P 21	P2(1)
Hall group	P 2yb	?
Moiety formula	C10 H13 N Ni O3 S2	?
Sum formula	C10 H13 N Ni O3 S2	C10 H13 N Ni O3 S2
Mr	318.04	318.04
Dx,g cm-3	1.695	1.695
Z	2	2
Mu (mm-1)	1.886	1.886
F000	328.0	328.0
F000'	329.27	
h,k,lmax	11,11,11	11,11,11
Nref	1650[3102]	3098
Tmin,Tmax	0.561,0.876	0.552,0.881
Tmin'	0.502	

Correction method= MULTI-SCAN

Data completeness= 1.88/1.00 **Theta(max)= 28.280**

R(reflections)= 0.0258(3070) **wR2(reflections)= 0.0711(3098)**

S = 1.065 **Npar= 156**

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for O2 -- N1 .. 7.14 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Ni -- O1 .. 10.88 su

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Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.98

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PLAT153_ALERT_1_C The su's on the Cell Axes   are Equal (x 100000)        300 Ang.
PLAT195_ALERT_1_C Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_C Missing _cell_measurement_theta_min   datum ....          ?
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Ni     --  S1      ..       6.50 su
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         N1
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Alert level G

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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           28.28
          From the CIF: _reflns_number_total               3098
          Count of symmetry unique reflns         1650
          Completeness (_total/calc)            187.76%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured      1448
          Fraction of Friedel pairs measured     0.878
          Are heavy atom types Z>Si present        yes
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          3
           S2  -NI  -S1  -C7   -152.68  0.18   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          6
           S2  -NI  -S1  -C8    -45.85  0.18   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          9
           S1  -NI  -S2  -C9     95.80  0.19   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         12
           S1  -NI  -S2  -C10    -6.70  0.19   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         13
           C1  -NI  -O1  -N1   -168.70  0.80   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         18
           O1  -NI  -C1  -C6    -89.90  0.90   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         21
           O1  -NI  -C1  -C2     87.60  0.90   1.555   1.555   1.555   1.555
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

3 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
0 ALERT type 3 Indicator that the structure quality may be low
8 ALERT type 4 Improvement, methodology, query or suggestion
0 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*, 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 16/02/2011; check.def file version of 16/02/2011

Datablock char342a - ellipsoid plot