checkCIF/PLATON report

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

Datablock: chgr90

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=25.3512(13) b=9.4487(4) c=23.5171(13)
alpha=90 beta=108.730(2) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	5334.9(5)	5334.9(5)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C24 H37 B N2 Ni O2 S2	?
Sum formula	C24 H37 B N2 Ni O2 S2	C24 H37 B N2 Ni O2 S2
Mr	519.20	519.20
Dx,g cm-3	1.293	1.293
Z	8	8
Mu (mm-1)	0.906	0.906
F000	2208.0	2208.0
F000’	2213.27	
h,k,lmax	33,12,31	33,11,31
Nref	6632	5700
Tmin,Tmax	0.654,0.762	0.660,0.773
Tmin’	0.629	

Correction method= MULTI-SCAN

Data completeness= 0.859 Theta(max)= 28.290

R(reflections)= 0.0304(4759) wR2(reflections)= 0.0782(5700)

S = 1.017 Npar= 297

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
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low 0.92

Author Response: Crystals consistently weak diffracters. The data herein represent the best of several trials.

Alert level C

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PLAT194_ALERT_1_C Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_C Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_C Missing _cell_measurement_theta_min   datum ....          ?
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   1 ALERT level A = In general: serious problem
   0 ALERT level B = Potentially serious problem
   3 ALERT level C = Check and explain
   0 ALERT level G = General alerts; check

   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
   1 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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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 13/08/2009; check.def file version of 12/08/2009

Datablock chgr90 - ellipsoid plot