checkCIF/PLATON report (publication check)

No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: 1

Bond precision: C-C = 0.0104 A Wavelength=0.71073
Cell: a=8.180(3) b=18.411(3) c=14.435(3)
alpha=90 beta=92.79(2) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	2171.4(10)	2171.3(10)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C8 H20 N, C8 N4 Ni S4	C16 H20 N5 NI1 S4
Sum formula	C16 H20 N5 Ni S4	C16 H20 N5 Ni1 S4
Mr	469.34	469.34
Dx,g cm-3	1.436	1.436
Z	4	4
Mu (mm-1)	1.288	1.288
F000	972.0	972.0
F000'	975.49	
h,k,lmax	10,23,18	9,23,18
Nref	4987	4092
Tmin,Tmax	0.655,0.824	0.650,0.820
Tmin'	0.591	

Correction method= PSI-SCAN
Data completeness= 0.821 Theta(max)= 27.504
R(reflections)= 0.0476(2011) wR2(reflections)= 0.1176(2011)
S = 1.024 Npar= 235

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

PLAT022_ALERT_3_A Ratio Unique / Expected Reflections too Low 0.82

Author Response: This is an old dataset collected on four-circle diffractometer with pin-point detector. Several missing hkl indexes were not collected because beam stopper interference.

PLAT940_ALERT_3_A F**2 Refinement with I .GT. n * Sigma(I) only .. ?

Author Response: This is an old dataset collected on four-circle diffractometer with pin-point detector. Following suggestions for non-CCD datasets, refinement was conducted using I > 2sigma conditions.

Alert level C

REFNR01_ALERT_3_C Ratio of reflections to parameters is < 10 for a centrosymmetric structure
sine(theta)/lambda 0.6498
Proportion of unique data used 0.4914
Ratio reflections to parameters 8.5574

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low .... 49 Perc.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.98
PLAT088_ALERT_3_C Poor Data / Parameter Ratio 8.56
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 10
PLAT371_ALERT_2_C Long C(sp2)-C(sp1) Bond C1 - C3 ... 1.43 Ang.
PLAT371_ALERT_2_C Long C(sp2)-C(sp1) Bond C2 - C4 ... 1.45 Ang.
PLAT371_ALERT_2_C Long C(sp2)-C(sp1) Bond C5 - C7 ... 1.44 Ang.

```
PLAT371_ALERT_2_C Long   C(sp2)-C(sp1) Bond  C6     -   C8     ...       1.44 Ang.
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ         ?
PLAT153_ALERT_1_C The su's on the Cell Axes   are Equal (x 100000)        300 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5     --  C11     ..       0.15 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13    --  C14     ..       0.18 Ang.
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of         C13
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of          N5
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1
             C8 H20 N
```

Alert level G

```
PLAT128_ALERT_4_G Non-standard setting of Space-group P21/c   ....      P21/n
PLAT808_ALERT_5_G No Parsable SHELXL style Weighting Scheme Found          !
```

```
  2 ALERT level A = In general: serious problem
  0 ALERT level B = Potentially serious problem
 16 ALERT level C = Check and explain
  2 ALERT level G = General alerts; check

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  4 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
  6 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
```

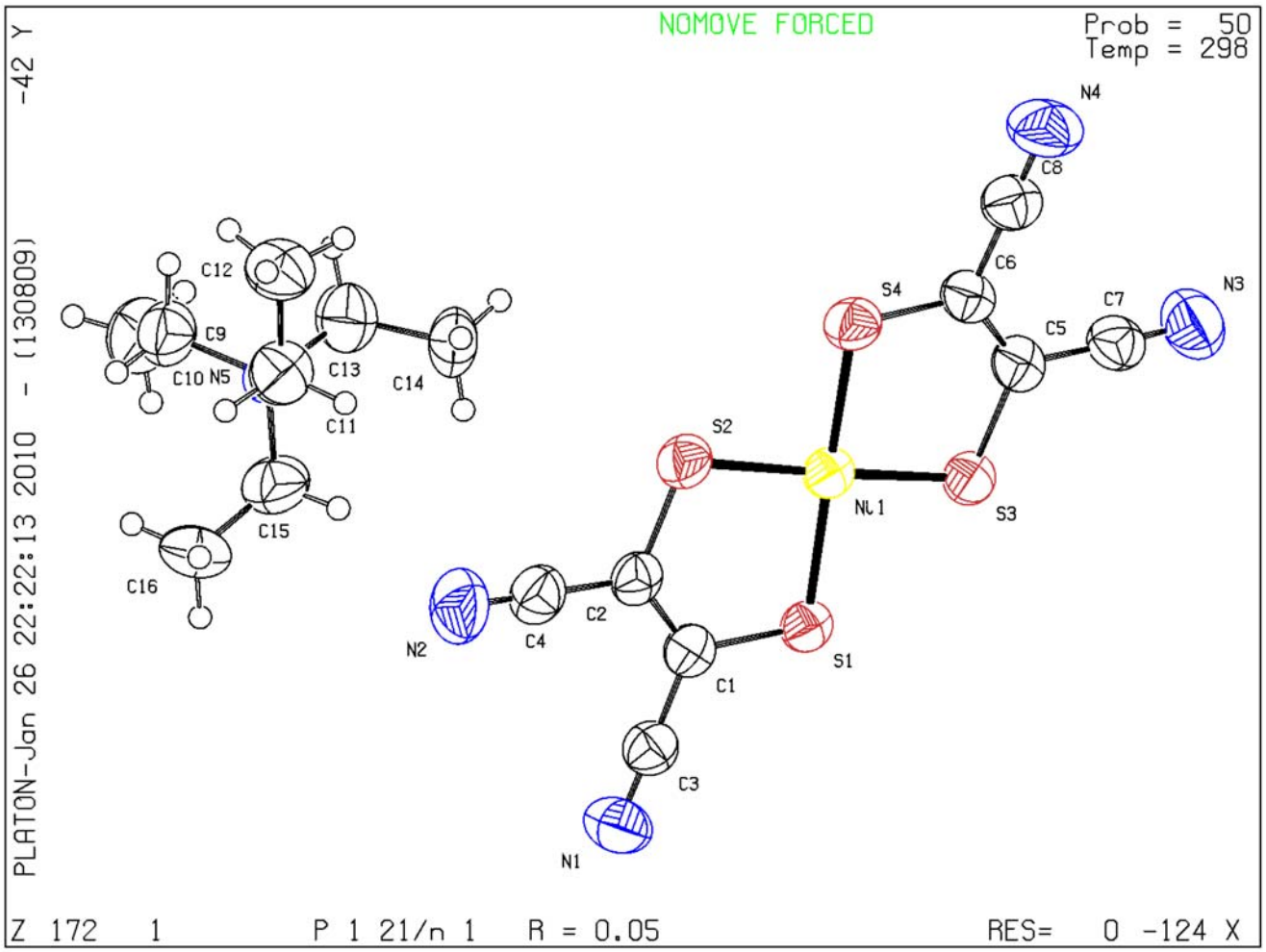
Publication of your CIF

You should always 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 nature of your study may justify the reported deviations from the submission requirements of the journal and these should be commented upon in the discussion or experimental section of a paper - after all, they might represent an interesting feature.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 13/08/2009; check.def file version of 12/08/2009

Datablock 1 - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry