checkCIF/PLATON report

Structure factors have been supplied for datablock(s) NiL2_Cl

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: NiL2_Cl

Bond precision: C-C = 0.0098 A Wavelength=0.71073

Cell: a=13.555(2) b=15.389(3) c=17.007(3)
alpha=77.732(3) beta=70.231(3) gamma=81.830(3)
Temperature: 120 K

	Calculated	Reported
Volume	3252.8(10)	3253.0(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C59 H49 N10 Ni2 O2), 1.5(C4 H10 O), 4(C H4 O), 2(Cl) [+ solve	C59 H49 N10 Ni2 O2, Cl, 2(C H4 O), 0.75(C4 H10 O)
Sum formula	C128 H129 Cl2 N20 Ni4 O9.50 [+ solvent]	C64 H64.50 Cl N10 Ni2 O4.75
Mr	2405.18	1202.62
Dx,g cm-3	1.228	1.228
Z	1	2
Mu (mm-1)	0.673	0.673
F000	1259.0	1259.0
F000'	1261.04	
h,k,lmax	17,19,21	17,19,21
Nref	14191	14150
Tmin,Tmax	0.976,0.987	0.571,0.746
Tmin'	0.935	

Correction method= # Reported T Limits: Tmin=0.571 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 26.998

R(reflections)= 0.0794(6921)

wR2(reflections)= 0.2189(14150)

S = 0.955 Npar= 756

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 C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.159
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .....      0.159 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..     49% Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..  Please Check
PLAT213_ALERT_2_C Atom C20             has ADP max/min Ratio .....     3.4 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range     4.4 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range     5.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C52      --C53      .     0.18 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C10 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....     2.2 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O3S   0.113 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............  0.00982 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...  -7.535 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600      14 Report
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............       2 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......  Please Check
PLAT014_ALERT_1_G No       _shelx_fab_checksum Found in CIF ......  Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ  Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.500 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large    0.10 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.003 Degree
PLAT300_ALERT_4_G Atom Site Occupancy of O3S        Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3S        Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4S        Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5S        Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6S        Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3SA       Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3SB       Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SA       Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SB       Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SC       Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5SA       Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5SB       Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6SA       Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6SB       Constrained at    0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6SC       Constrained at    0.75 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )     100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )   11.25 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure     405 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      16 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       4 Note
```

```
             C H4 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
             Cl
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1       (II)      .       2.13 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni2       (II)      .       2.17 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         26 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          6 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...          9 Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       54.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  37 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
  24 ALERT type 4 Improvement, methodology, query or suggestion
   4 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* or *IUCrData*, 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 18/05/2022; check.def file version of 17/05/2022

Datablock NiL2_Cl - ellipsoid plot