checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cs6-100k

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: cs6-100k

Bond precision: C-C = 0.0110 A Wavelength=0.82641

Cell: a=25.3086(13) b=14.9637(7) c=39.809(2)
alpha=90 beta=94.401(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	15031.6(13)	15031.6(13)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C82 N U), 2(C36 H44 N4 Ni), 3.652(C6 H6), C0.70 S0.70	C36 H44 N4 Ni, C82 N U1, 3.65(C3 H3), 0.35(C S)
Sum formula	C258.61 H109.91 N10 Ni2 S0.70 U2	C129.30 H54.96 N5 Ni S0.35 U
Mr	3972.48	1986.26
Dx,g cm-3	1.755	1.755
Z	4	8
Mu (mm-1)	1.837	1.871
F000	7930.7	7931.0
F000'	7888.07	
h,k,lmax	31,18,49	31,18,48
Nref	14824	14570
Tmin,Tmax		0.764,0.829
Tmin'		

Correction method= # Reported T Limits: Tmin=0.764 Tmax=0.829
AbsCorr = MULTI-SCAN

Data completeness= 0.983 Theta(max)= 30.672

R(reflections)= 0.0764(13753)

wR2(reflections)= 0.1961(14570)

S = 1.025 Npar= 1288

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

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT213_ALERT_2_C Atom C2 has ADP max/min Ratio ..... 3.5 oblate
PLAT213_ALERT_2_C Atom C3 has ADP max/min Ratio ..... 3.3 oblate
PLAT213_ALERT_2_C Atom C20 has ADP max/min Ratio ..... 3.6 prolat
PLAT213_ALERT_2_C Atom C21 has ADP max/min Ratio ..... 3.3 oblate
PLAT213_ALERT_2_C Atom C39 has ADP max/min Ratio ..... 3.2 oblate
PLAT213_ALERT_2_C Atom C44 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C50 has ADP max/min Ratio ..... 3.1 oblate
PLAT213_ALERT_2_C Atom C53 has ADP max/min Ratio ..... 3.6 oblate
PLAT213_ALERT_2_C Atom C74 has ADP max/min Ratio ..... 3.7 oblate
PLAT213_ALERT_2_C Atom C75 has ADP max/min Ratio ..... 3.5 oblate
PLAT214_ALERT_2_C Atom C12P (Anion/Solvent) ADP max/min Ratio 4.4 oblate
PLAT214_ALERT_2_C Atom C13P (Anion/Solvent) ADP max/min Ratio 4.1 prolat
PLAT214_ALERT_2_C Atom C18P (Anion/Solvent) ADP max/min Ratio 4.7 oblate
PLAT214_ALERT_2_C Atom C26P (Anion/Solvent) ADP max/min Ratio 4.2 prolat
PLAT221_ALERT_2_C Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range 7.2 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range 8.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference U4 --C43 . 0.16 Ang.
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C6S Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.1 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C2S 0.102 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including S1S 0.104 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01102 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C38 - C62 . 1.53 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C63 - C64 . 1.53 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C81 - C82 . 1.53 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.172 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 63 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 17 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.33A From Ni1P 1.95 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.30A From C73 1.72 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.30A From Ni1P 1.65 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.95A From C78 1.61 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.89A From C43 1.51 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.86A From U1 -1.67 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.66A From U3 -1.58 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2S -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H13S -0.38 eA-3

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is

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           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C129.3 H54.96 N5 Ni1 S0.35 U1
           Atom count from _chemical_formula_moiety:C129.3 H54.95 N5 Ni1 S0.35 U1
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
          From the CIF: _cell_formula_units_Z    8
          From the CIF: _chemical_formula_sum  C129.30 H54.96 N5 Ni S0.35 U
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C       1034.40   1034.45   -0.05
          H        439.68    439.65    0.03
          N         40.00     40.00    0.00
          Ni         8.00      8.00    0.00
          S          2.80      2.78    0.02
          U          8.00      8.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         2 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       128 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ    Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    331.62 Why ?
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka   0.82641 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        2 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U1       --N1       .       7.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U1       --C2       .       5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U2       --C20      .       7.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U2       --C41      .       7.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U2       --C44      .      11.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U3       --N1       .       5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U3       --C22      .       6.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U3       --C28      .       8.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U4       --C19      .       6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U4       --C20      .       7.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U4       --C41      .       6.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U4       --C42      .       8.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U4       --C62      .       7.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U4       --C63      .      10.2 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        1% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )      100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )      7.82 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  6  )      1.40 Check
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing).       C1S Check
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C3       -C15      .      1.42 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C11      -C29      .      1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C12      -C32      .      1.42 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C14      -C34      .      1.44 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C20      -C43      .      1.45 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C19      -C40           0.20 Ang.
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C47 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C6       - C7       .      1.51 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...     29.70 Deg.
              U2   -N1   -U4      1_555   1_555   1_555 ......     #  346 Check
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PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      28.49 Deg.
              U3   -N1   -U1      1_555   1_555   1_555 ......     #  347 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      14.85 Deg.
              U1   -C1   -U3      1_555   1_555   1_555 ......     #  349 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      16.74 Deg.
              U1   -C6   -U3      1_555   1_555   1_555 ......     #  380 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      18.64 Deg.
              U3   -C7   -U1      1_555   1_555   1_555 ......     #  390 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      16.15 Deg.
              U3   -C8   -U1      1_555   1_555   1_555 ......     #  400 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      17.62 Deg.
              U3   -C9   -U1      1_555   1_555   1_555 ......     #  410 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      17.84 Deg.
              U1   -C10  -U3      1_555   1_555   1_555 ......     #  420 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      18.68 Deg.
              U4   -C20  -U2      1_555   1_555   1_555 ......     #  463 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      16.95 Deg.
              U3   -C22  -U1      1_555   1_555   1_555 ......     #  479 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      18.30 Deg.
              U4   -C41  -U2      1_555   1_555   1_555 ......     #  564 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      20.54 Deg.
              U2   -C42  -U4      1_555   1_555   1_555 ......     #  574 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      18.94 Deg.
              U2   -C43  -U4      1_555   1_555   1_555 ......     #  584 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      16.67 Deg.
              U4   -C63  -U2      1_555   1_555   1_555 ......     #  660 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      18.06 Deg.
              U2   -C64  -U4      1_555   1_555   1_555 ......     #  670 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      17.61 Deg.
              U2   -C65  -U4      1_555   1_555   1_555 ......     #  680 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1P      (II)      .       1.98 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1082 Note
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        186 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
PLAT984_ALERT_1_G The Ni-f'=    0.3120 Deviates from the B&C-Value     0.2982 Check
PLAT984_ALERT_1_G The  S-f'=    0.1246 Deviates from the B&C-Value     0.1576 Check
PLAT984_ALERT_1_G The  U-f'=   -6.3260 Deviates from the B&C-Value    -6.1890 Check
PLAT985_ALERT_1_G The Ni-f"=    1.4720 Deviates from the B&C-Value     1.4582 Check
PLAT985_ALERT_1_G The  S-f"=    0.1234 Deviates from the B&C-Value     0.1682 Check
PLAT985_ALERT_1_G The  U-f"=    5.5940 Deviates from the B&C-Value     5.0831 Check
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
 40 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 69 ALERT level G = General information/check it is not something unexpected

 13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 58 ALERT type 2 Indicator that the structure model may be wrong or deficient
  8 ALERT type 3 Indicator that the structure quality may be low
 29 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
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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 13/07/2021; check.def file version of 13/07/2021

Datablock cs6-100k - ellipsoid plot