checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: ni

Bond precision: C-C = 0.0003 A Wavelength=0.71073

Cell: a=6.5784(3) b=7.3916(9) c=13.2645(7)
alpha=74.252(6) beta=88.589(5) gamma=77.892(6)
Temperature: 100 K

	Calculated	Reported
Volume	606.61(9)	606.61(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C7 H5 O6 S), H12 Ni O6, 2(H2 O)	2(C7 H5 O6 S), H12 Ni O6, 2(H2 O)
Sum formula	C14 H26 Ni O20 S2	C14 H26 Ni O20 S2
Mr	637.16	637.18
Dx,g cm-3	1.744	1.744
Z	1	1
Mu (mm-1)	1.065	1.065
F000	330.0	330.0
F000'	330.81	
h,k,lmax	15,17,31	15,17,31
Nref	17538	17461
Tmin,Tmax	0.734,0.791	0.643,0.743
Tmin'	0.719	

Correction method= # Reported T Limits: Tmin=0.643 Tmax=0.743
AbsCorr = GAUSSIAN

Data completeness= 0.996 Theta(max)= 58.497

R(reflections)= 0.0164(15967) wR2(reflections)= 0.0469(17059)

S = 0.993 Npar= 775

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

PLAT417_ALERT_2_B Short Inter D-H..H-D H9O ..H10B . 2.10 Ang.
x,y,1+z = 1_556 Check

Alert level C

PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H1WA 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H1WB 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H2WA 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H2WB 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H3WA 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H3WB 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H7O 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H9O 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H2C 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H3C 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H6C 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H10A 6 Check
PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for H10B 6 Check
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O7 - H7O . 1.02 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O9 - H9O . 1.05 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O1 - H1WA . 1.02 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O2 - H2WA . 1.02 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O2 - H2WB . 1.03 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O3 - H3WA . 1.02 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O10 - H10A . 1.03 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O10 - H10B . 1.01 Ang.
PLAT417_ALERT_2_C Short Inter D-H..H-D H3WA ..H10B . 2.13 Ang.
x,y,z = 1_555 Check

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 3 Note
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni1 --O1 . 24.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni1 --O2 . 21.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni1 --O3 . 23.4 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 6 Note
H(1WA) H(1WB) H(2WA) H(2WB) H(3WA) H(3WB)
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1 (II) . 2.07 Info
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ..... Please Do !
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !

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

  2 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
 21 ALERT type 3 Indicator that the structure quality may be low
  2 ALERT type 4 Improvement, methodology, query or suggestion
  2 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 04/06/2025; check.def file version of 17/09/2025

duplicate check

A reduced cell check using CCDC's cellCheckCSD service has found that one or more structures in this CIF are similar to those previously published in the CSD.

DATABLOCK: ni

- CSD Refcode: KEJVOO

  

  [Cell Parameters for KEJVOO: 6.5986,7.4183,13.2847(74.1712,88.6035,77.92)]

DATABLOCK: ni

- Bettinger, R. T., Squattrito, P. J., Aulakh, D. & Gianopoulos, C. G. (2022). *Acta Cryst.* E**78**, 961-965

  

  [Cell: 6.5986,7.4183,13.2847(74.1712,88.6035,77.9200)]

Datablock ni - ellipsoid plot

