SUPPORTING INFORMATION

A Flexible Interpenetrated Coordination Framework with a Bimodal Porous Functionality

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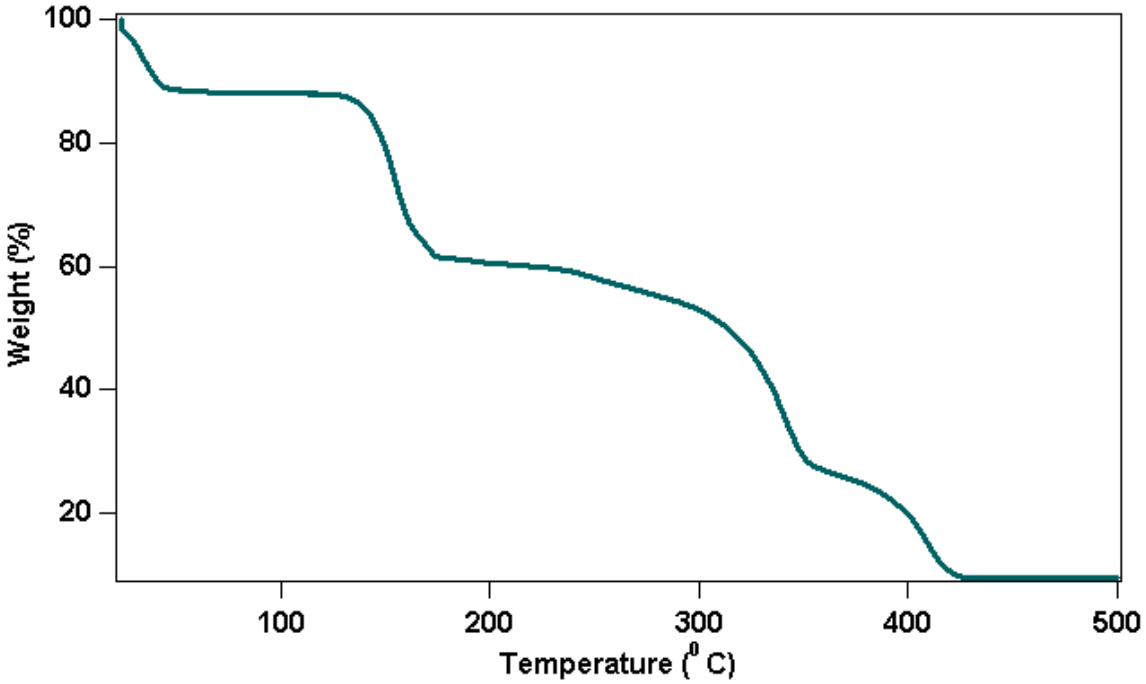

Figure SI(1): TG analysis of $\{[Ni(bpe)_2(N(CN)_2)](N(CN)_2)(5H_2O)\}_n$ (1) over the temperature range from 25-500°C at heating rate of 0.5°C/min under the N_2 environment and atmospheric pressure.

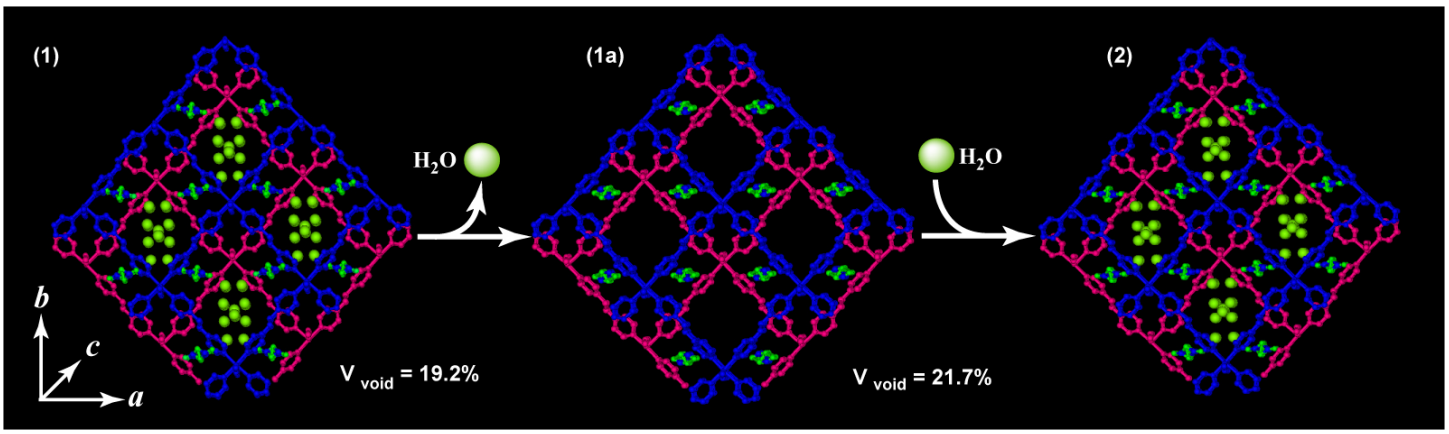

Figure SI(2): Views of the 3D interpentrated framework of (**1**) as-synthesized (**1a**) dehydrated and (**2**) rehydrated; showing that channel size slightly increases in the dehydrated state.

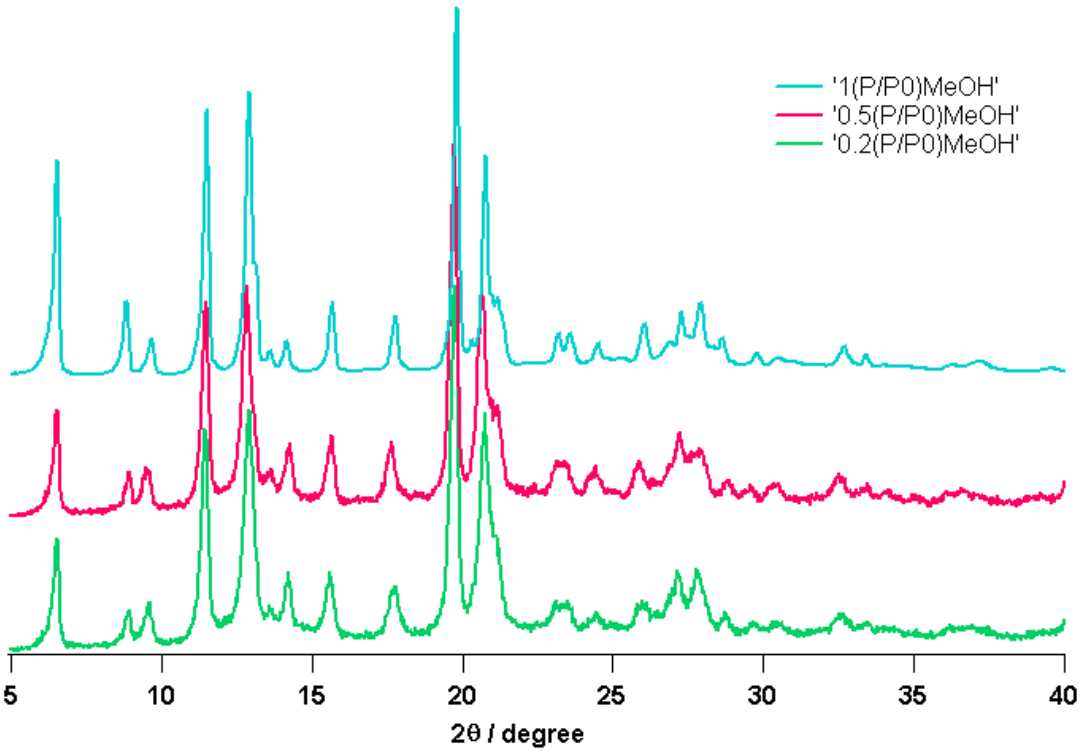

Figure SI(3): Powder XRD pattern of $\{[Ni(bpe)_2(N(CN)_2)](N(CN)_2)\}_n$ (**1a**) exposed to the different P/P_0 of MeOH.

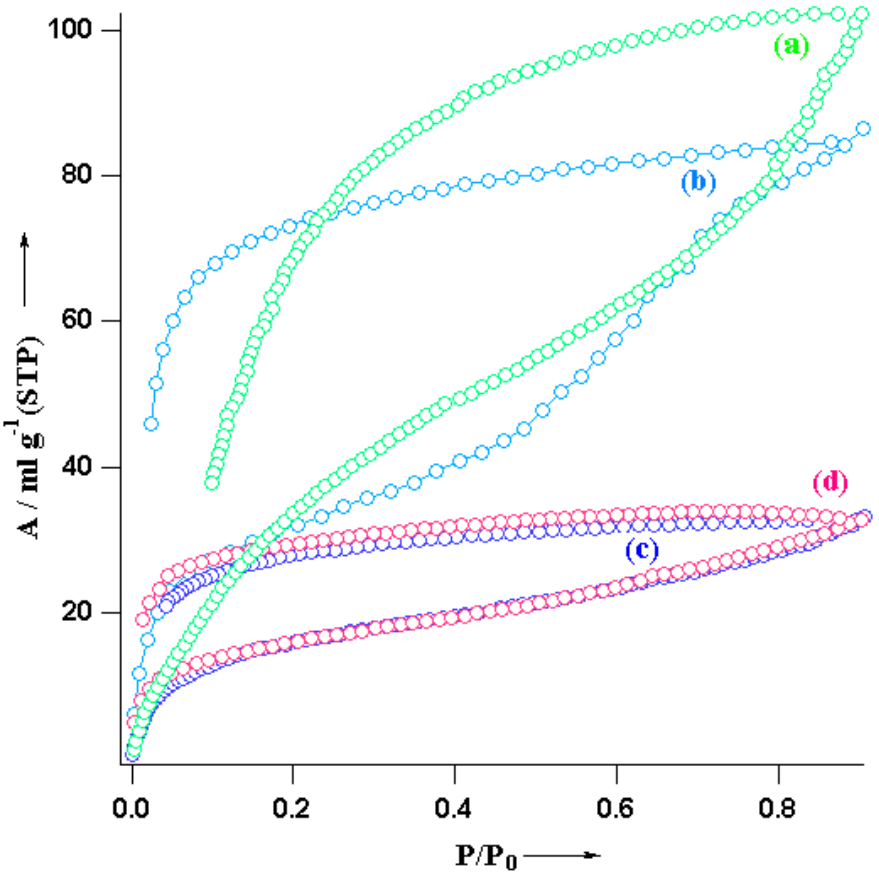

Figure SI(4): Hysteretic isotherm for (**a**) H_2O, (**b**) MeOH, (**c**) EtOH and (**d**) Me_2CO vapor adsorption-desorption, A, at 298 K. P_0 is the saturated vapor pressure at 298 K; 3.17 kPa (H_2O), 16.94 kPa (MeOH), 7.87 kPa (EtOH), 30.59 kPa (Me_2CO). STP is standard temperature and pressure.

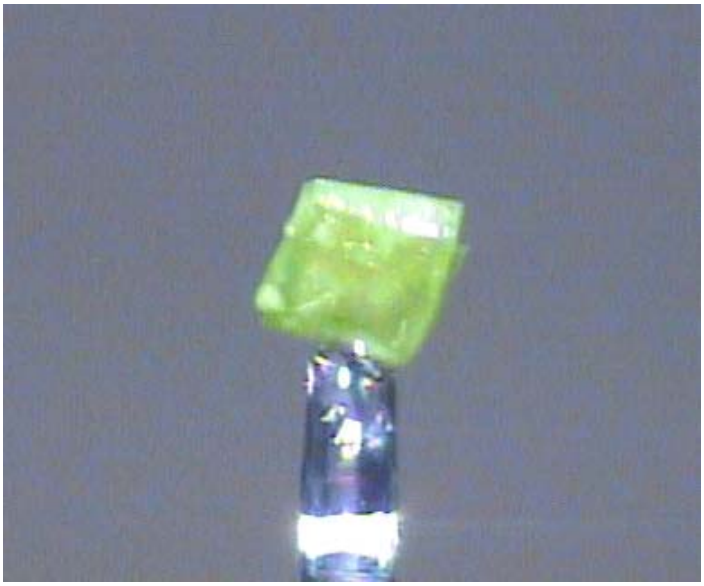

Figure SI(5): as-synthesized violet crystal $[Ni(bpe)_2(N(CN)_2)](N(CN)_2)(5H_2O)]\}_n$ **(1)** turns to green, $[Ni(bpe)_2(N(CN)_2)](N_3)(5H_2O)]\}_n$ after one day in the NaN_3 solution.

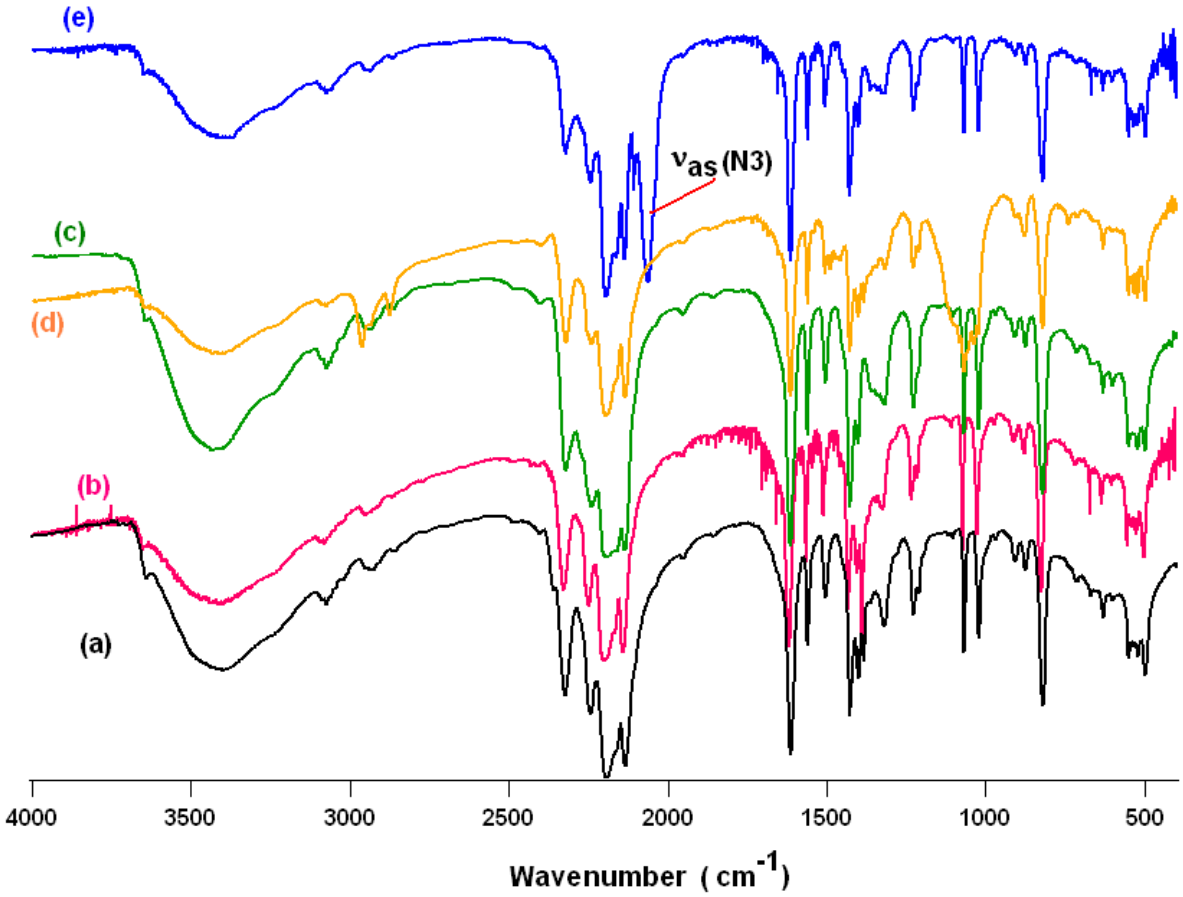

Figure SI(6): IR spectra of as-synthesized $[Ni(bpe)_2(N(CN)_2)](N(CN)_2)(5H_2O)]\}_n$ (**1**) and of solid obtained after treating with different anions solutions: (**a**) as-synthesized (**1**); (**b**) $NaNO_3$ solution (violet); (**c**) NaNCO solution (violet); (**d**) $NaBF_4$ solution (violet) and (**e**) NaN_3 solution (green).

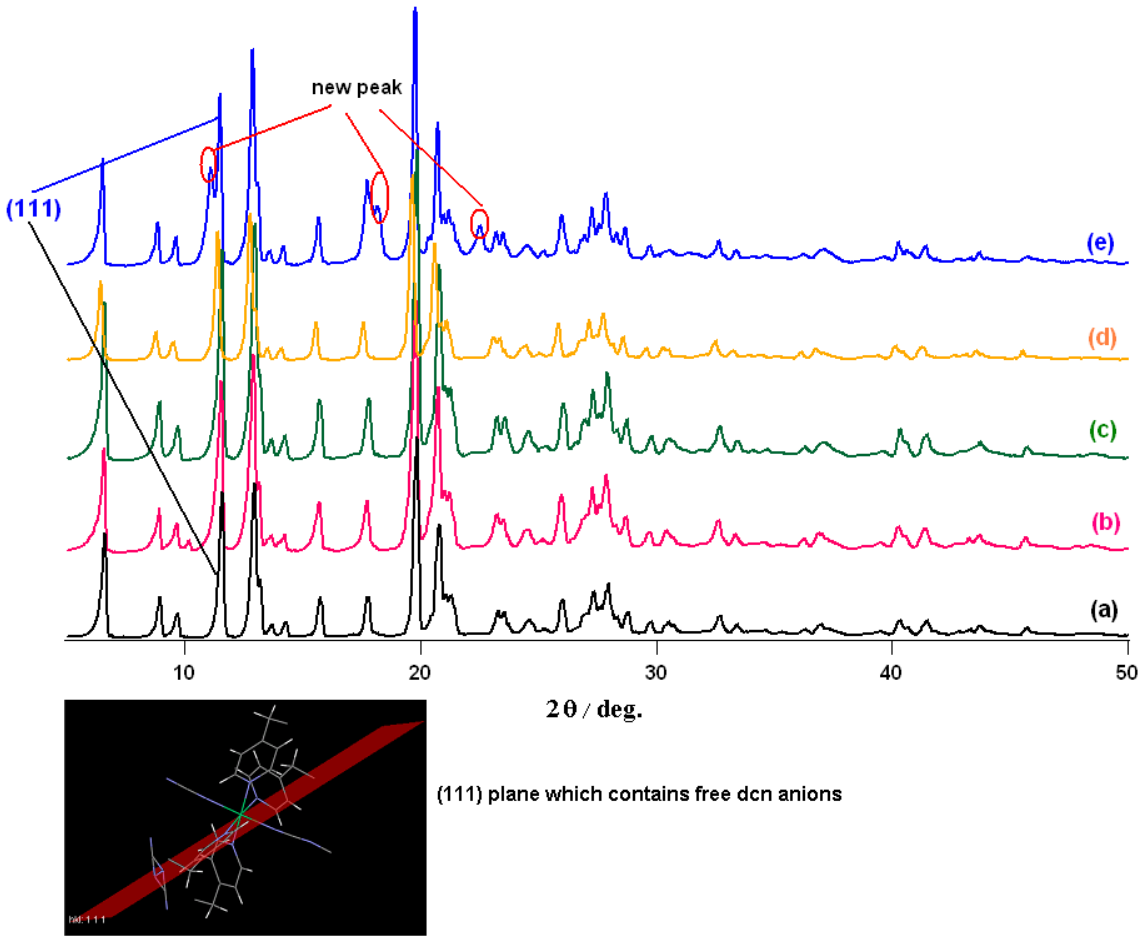

Figure SI(7): Comparison of the XRPD patterns of the as-synthesized compound (**a**) and with solid obtained after treating framework $[Ni(bpe)_2(N(CN)_2)](N(CN)_2)(5H_2O)]\}_n$ (**1**) in (**b**) aqueous $NaNO_3$ solution (violet); (**c**) NaNCO solution (violet); (**d**) $NaBF_4$ solution (violet); (**e**) NaN_3 solution (green).

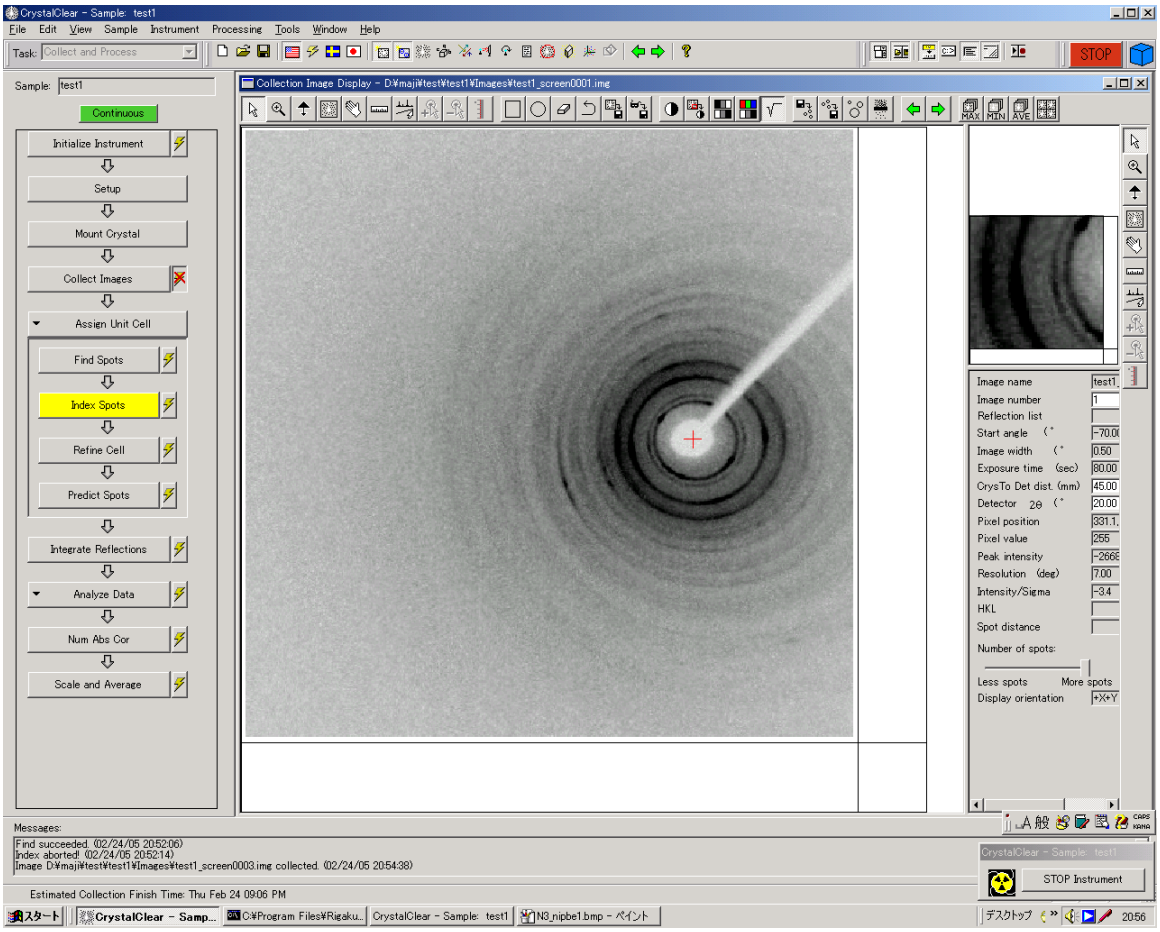

Figure SI(8): View of the diffraction image (CCD) of the N_3-exchanged green crystal showing that single crystallinity is lost after the exchange with the N_3^-.

Table SI (1): **Comparison of bond distances (Å) of $\{[Ni(bpe)_2(N(CN)_2)](N(CN)_2)(5H_2O)]\}_n$ (1), $\{[Ni(bpe)_2(N(CN)_2)](N(CN)_2)]\}_n$ (1a) and $\{[Ni(bpe)_2(N(CN)_2)](N(CN)_2)(5H_2O)]\}_n$ (2)**

(1)	**lengths (Å)**	**(1a)**	**lengths (Å)**	**(2)**	**lengths (Å)**
Ni1-N1	2.094(5)	Ni1-N1	2.11(3)	Ni1-N1	2.096(12)
Ni1-N2	2.137(5)	Ni1-N2	2.16(3)	Ni1-N2	2.137(12)
Ni1-N3	2.074(5)	Ni1-N3	2.05(3)	Ni1-N3	2.070(12)
Ni1-N1_a	2.094(5)	Ni1-N1_b	2.11(3)	Ni1-N1_a	2.096(12)
Ni1-N2_a	2.137(5)	Ni1-N2_b	2.16(3)	Ni1-N2_a	2.137(12)
Ni1-N3_a	2.074(5)	Ni1-N3_b	2.05(3)	Ni1-N3_a	2.070(12)

Symmetry code (**1**): a = 1-x, y, 1/2-z; (**1a**): b = 1-x, y, 1/2-z; (**2**): a = 1-x, y, 1/2-z

Table SI **(2): Comparison of bond angles (°) of 1, 1a and 2**

(1)	angles (°)	(1a)	angles (°)	(2)	(°)
N1-Ni1-N2	175.86(14)	N1-Ni1-N2	177.0(6)	N1-Ni1-N2	176.3(3)
N1-Ni1-N3	93.70(15)	N1-Ni1-N3	92.8(7)	N1-Ni1-N3	93.5(3)
N1-Ni1-N1_a	85.74(13)	N1-Ni1-N1_b	87.6(6)	N1-Ni1-N1_a	85.9(3)
N1-Ni1-N2_a	90.39(14)	N1-Ni1-N2_b	89.5(6)	N1-Ni1-N2_a	90.5(3)
N1-Ni1-N3_a	91.66(15)	N1-Ni1-N3_b	92.3(7)	N1-Ni1-N3_a	91.9(3)
N2-Ni1-N3	87.87(15)	N2-Ni1-N3	88.1(7)	N2-Ni1-N3	87.8(3)
N1_a-Ni1-N2	90.39(14)	N1_b-Ni1-N2	89.5(6)	N1_a-Ni1-N2	90.5(3)
N2-Ni1-N2_a	93.53(16)	N2-Ni1-N2_b	93.4(6)	N2-Ni1-N2_a	93.0(3)
N2-Ni1-N3_a	87.13(15)	N2-Ni1-N3_b	87.1(7)	N2-Ni1-N3_a	87.2(3)
N1_a-Ni1-N3	91.66(15)	N1_b-Ni1-N3	92.3(7)	N1_a-Ni1-N3	91.9(3)
N2_a-Ni1-N3	87.13(15)	N2_b-Ni1-N3	87.1(7)	N2_a-Ni1-N3	87.2(3)
N3-Ni1-N3_a	172.70(17)	N3-Ni1-N3_b	173.0(7)	N3-Ni1-N3_a	172.7(3)
N1_a-Ni1-N2_a	175.86(14)	N1_b-Ni1-N2_b	177.0(6)	N1_a-Ni1-N2_a	176.3(3)
N1_a-Ni1-N3_a	93.70(15)	N1_b-Ni1-N3_b	92.8(7)	N1_a-Ni1-N3_a	93.5(3)
N2_a-Ni1-N3_a	87.87(15)	N2_b-Ni1-Nb_a	88.1(7)	N2_a-Ni1-N3_a	87.8(3)

Symmetry code:(1) a = 1-x,y,1/2-z; (1a): b = 1-x,y,1/2-z; (2): a = 1-x, y, 1/2-z

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 C(4)    0.058(3)    0.040(3)    0.030(2)    -0.026(2)   0.003(2)    0.011(2)
 C(5)    0.032(2)    0.031(2)    0.024(2)    -0.011(2)   -0.001(2)   0.006(2)
 C(6)    0.090(5)    0.072(4)    0.053(4)    -0.063(4)   -0.016(3)   0.017(3)
 C(7)    0.045(3)    0.023(2)    0.037(3)    -0.008(2)   -0.007(2)   -0.005(2)
 C(8)    0.061(3)    0.031(3)    0.051(3)    -0.020(2)   -0.015(3)   0.005(2)
 C(9)    0.065(4)    0.050(3)    0.040(3)    -0.041(3)   -0.017(3)   0.019(2)
 C(10)   0.034(3)    0.072(4)    0.046(3)    -0.024(2)   0.005(2)    0.022(3)
 C(11)   0.031(2)    0.037(2)    0.033(2)    -0.009(2)   0.007(2)    0.008(2)
 C(12)   0.098(5)    0.094(5)    0.063(4)    -0.078(4)   -0.018(4)   0.023(4)
 C(13)   0.064(3)    0.023(2)    0.024(2)    0.000(2)    0.011(2)    -0.003(2)
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 Ni(1)     N(1)      2.096(3)   . 2_655 yes
 Ni(1)     N(2)      2.137(4)   . . yes
 Ni(1)     N(2)      2.137(4)   . 2_655 yes
 Ni(1)     N(3)      2.074(3)   . . yes
 Ni(1)     N(3)      2.074(3)   . 2_655 yes
 N(1)      C(1)      1.342(5)   . . yes
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 N(2)      C(7)      1.344(5)   . . yes
 N(2)      C(11)     1.334(6)   . . yes
 N(3)      C(13)     1.132(5)   . . yes
 N(4)      C(13)     1.297(5)   . . yes
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 N(4)      C(13)     1.297(5)   . 2_656 yes
 N(5)      C(14)     1.19(2)    . . yes
 N(6)      N(6)      1.36(3)    . 7_655 yes
 N(6)      C(14)     1.15(2)    . . yes
 N(6)      C(14)     1.35(2)    . 7_655 yes
 C(1)      C(2)      1.375(6)   . . yes
 C(2)      C(3)      1.376(6)   . . yes
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 C(3)      C(6)      1.517(6)   . . yes
 C(4)      C(5)      1.383(6)   . . yes
 C(6)      C(12)     1.428(8)   . 5_555 yes
 C(7)      C(8)      1.391(6)   . . yes
 C(8)      C(9)      1.363(8)   . . yes
 C(9)      C(10)     1.388(8)   . . yes
 C(9)      C(12)     1.507(7)   . . yes
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   N(1)      Ni(1)     N(2)      90.4(2)    . . 2_655 yes
   N(1)      Ni(1)     N(3)      93.7(1)    . . . yes
   N(1)      Ni(1)     N(3)      91.6(1)    . . 2_655 yes
   N(1)      Ni(1)     N(2)      90.4(2)    2_655 . . yes
   N(1)      Ni(1)     N(2)      175.8(1)   2_655 . 2_655 yes
   N(1)      Ni(1)     N(3)      91.6(1)    2_655 . . yes
   N(1)      Ni(1)     N(3)      93.7(1)    2_655 . 2_655 yes
   N(2)      Ni(1)     N(2)      93.5(2)    . . 2_655 yes
   N(2)      Ni(1)     N(3)      87.9(1)    . . . yes
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   N(2)      Ni(1)     N(3)      87.2(1)    2_655 . . yes
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   Ni(1)     N(1)      C(5)      118.4(2)   . . . yes
   C(1)      N(1)      C(5)      117.5(3)   . . . yes
   Ni(1)     N(2)      C(7)      122.0(3)   . . . yes
   Ni(1)     N(2)      C(11)     120.8(3)   . . . yes
   C(7)      N(2)      C(11)     117.2(4)   . . . yes
   Ni(1)     N(3)      C(13)     166.7(3)   . . . yes
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   C(2)      C(3)      C(4)      117.0(4)   . . . yes
```

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   C(4)      C(3)      C(6)      122.3(4)   . . . yes
   C(3)      C(4)      C(5)      119.7(4)   . . . yes
   N(1)      C(5)      C(4)      122.7(4)   . . . yes
   C(3)      C(6)      C(12)     117.2(4)   . . 5_555 yes
   N(2)      C(7)      C(8)      123.1(5)   . . . yes
   C(7)      C(8)      C(9)      120.2(5)   . . . yes
   C(8)      C(9)      C(10)     116.9(4)   . . . yes
   C(8)      C(9)      C(12)     121.5(6)   . . . yes
   C(10)     C(9)      C(12)     121.6(6)   . . . yes
   C(9)      C(10)     C(11)     120.4(5)   . . . yes
   N(2)      C(11)     C(10)     122.2(4)   . . . yes
   C(6)      C(12)     C(9)      114.4(5)   5_445 . . yes
   N(3)      C(13)     N(4)      170.7(5)   . . . yes
   N(5)      C(14)     N(6)      132(1)     . . . yes
   N(5)      C(14)     N(6)      153(1)     . . 7_655 yes
   N(6)      C(14)     N(6)      65(1)      . . 7_655 yes
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 Ni(1)     N(1)      C(1)      H(1)      0.9        . . . . no
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 Ni(1)     N(1)      C(5)      H(4)      -0.1       . . . . no
 Ni(1)     N(1)      C(1)      C(2)      179.9(3)   . 2_655 2_655 2_655 yes
 Ni(1)     N(1)      C(1)      H(1)      0.9        . 2_655 2_655 2_655 no
 Ni(1)     N(1)      C(5)      C(4)      179.3(4)   . 2_655 2_655 2_655 yes
 Ni(1)     N(1)      C(5)      H(4)      -0.1       . 2_655 2_655 2_655 no
 Ni(1)     N(2)      C(7)      C(8)      175.7(3)   . . . . yes
 Ni(1)     N(2)      C(7)      H(10)     -3.9       . . . . no
 Ni(1)     N(2)      C(11)     C(10)     -178.5(3)  . . . . yes
 Ni(1)     N(2)      C(11)     H(7)      1.6        . . . . no
 Ni(1)     N(2)      C(7)      C(8)      175.7(3)   . 2_655 2_655 2_655 yes
 Ni(1)     N(2)      C(7)      H(10)     -3.9       . 2_655 2_655 2_655 no
 Ni(1)     N(2)      C(11)     C(10)     -178.5(3)  . 2_655 2_655 2_655 yes
 Ni(1)     N(2)      C(11)     H(7)      1.6        . 2_655 2_655 2_655 no
 Ni(1)     N(3)      C(13)     N(4)      1(4)       . . . . yes
 Ni(1)     N(3)      C(13)     N(4)      1(4)       . 2_655 2_655 2_655 yes
 N(1)      Ni(1)     N(1)      C(1)      117.6(3)   . . 2_655 2_655 yes
 N(1)      Ni(1)     N(1)      C(5)      -60.2(3)   . . 2_655 2_655 yes
 N(1)      Ni(1)     N(2)      C(7)      126(1)     . . . . yes
 N(1)      Ni(1)     N(2)      C(11)     -55(1)     . . . . yes
 N(1)      Ni(1)     N(2)      C(7)      146.8(3)   . . 2_655 2_655 yes
 N(1)      Ni(1)     N(2)      C(11)     -35.0(3)   . . 2_655 2_655 yes
 N(1)      Ni(1)     N(3)      C(13)     -140(1)    . . . . yes
 N(1)      Ni(1)     N(3)      C(13)     133(1)     . . 2_655 2_655 yes
```

N(1)	C(1)	C(2)	C(3)	1.2(7)	. . . . yes
N(1)	C(1)	C(2)	H(2)	-179.6	. . . . no
N(1)	C(5)	C(4)	C(3)	0.8(8)	. . . . yes
N(1)	C(5)	C(4)	H(3)	-179.8	. . . . no
N(2)	Ni(1)	N(1)	C(1)	138(1)	. . . . yes
N(2)	Ni(1)	N(1)	C(5)	-39(1)	. . . . yes
N(2)	Ni(1)	N(1)	C(1)	-60.9(3)	. . 2_655 2_655 yes
N(2)	Ni(1)	N(1)	C(5)	121.3(3)	. . 2_655 2_655 yes
N(2)	Ni(1)	N(2)	C(7)	-34.6(3)	. . 2_655 2_655 yes
N(2)	Ni(1)	N(2)	C(11)	143.6(3)	. . 2_655 2_655 yes
N(2)	Ni(1)	N(3)	C(13)	43(1)	. . . . yes
N(2)	Ni(1)	N(3)	C(13)	-50(1)	. . 2_655 2_655 yes
N(2)	C(7)	C(8)	C(9)	3.6(7)	. . . . yes
N(2)	C(7)	C(8)	H(9)	-178.5	. . . . no
N(2)	C(11)	C(10)	C(9)	2.1(7)	. . . . yes
N(2)	C(11)	C(10)	H(8)	-177.3	. . . . no
N(3)	Ni(1)	N(1)	C(1)	26.2(3)	. . . . yes
N(3)	Ni(1)	N(1)	C(5)	-151.6(3)	. . . . yes
N(3)	Ni(1)	N(1)	C(1)	-148.8(3)	. . 2_655 2_655 yes
N(3)	Ni(1)	N(1)	C(5)	33.4(3)	. . 2_655 2_655 yes
N(3)	Ni(1)	N(2)	C(7)	-121.6(3)	. . . . yes
N(3)	Ni(1)	N(2)	C(11)	56.6(3)	. . . . yes
N(3)	Ni(1)	N(2)	C(7)	53.1(3)	. . 2_655 2_655 yes
N(3)	Ni(1)	N(2)	C(11)	-128.7(3)	. . 2_655 2_655 yes
N(3)	Ni(1)	N(3)	C(13)	-3(1)	. . 2_655 2_655 yes
N(3)	C(13)	N(4)	C(13)	-178(3)	. . . 2_656 yes
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C(1)	N(1)	C(5)	C(4)	1.3(7)	. . . . yes
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C(1)	C(2)	C(3)	C(4)	1.0(8)	. . . . yes
C(1)	C(2)	C(3)	C(6)	-178.4(5)	. . . . yes
C(2)	C(1)	N(1)	C(5)	-2.3(6)	. . . . yes
C(2)	C(3)	C(4)	C(5)	-1.9(8)	. . . . yes
C(2)	C(3)	C(4)	H(3)	178.7	. . . . no
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C(2)	C(3)	C(6)	H(6)	52.7	. . . . no
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C(3)	C(4)	C(5)	H(4)	-179.9	. . . . no
C(4)	C(3)	C(2)	H(2)	-178.3	. . . . no
C(4)	C(3)	C(6)	C(12)	-6(1)	. . . 5_555 yes
C(4)	C(3)	C(6)	H(5)	118.1	. . . . no
C(4)	C(3)	C(6)	H(6)	-126.7	. . . . no
C(5)	N(1)	C(1)	H(1)	178.7	. . . . no
C(5)	C(4)	C(3)	C(6)	177.5(5)	. . . . yes
C(6)	C(3)	C(2)	H(2)	2.3	. . . . no
C(6)	C(3)	C(4)	H(3)	-1.9	. . . . no
C(7)	N(2)	C(11)	C(10)	-0.3(6)	. . . . yes
C(7)	N(2)	C(11)	H(7)	179.9	. . . . no
C(7)	C(8)	C(9)	C(10)	-1.6(7)	. . . . yes

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C(7)      C(8)      C(9)      C(12)     178.1(4)   . . . . yes
C(8)      C(7)      N(2)      C(11)     -2.5(6)    . . . . yes
C(8)      C(9)      C(10)     C(11)     -1.1(7)    . . . . yes
C(8)      C(9)      C(10)     H(8)      178.4      . . . . no
C(8)      C(9)      C(12)     H(11)     -137.1     . . . . no
C(8)      C(9)      C(12)     H(12)     -21.6      . . . . no
C(9)      C(8)      C(7)      H(10)     -176.8     . . . . no
C(9)      C(10)     C(11)     H(7)      -178.1     . . . . no
C(10)     C(9)      C(8)      H(9)      -179.5     . . . . no
C(10)     C(9)      C(12)     H(11)     42.6       . . . . no
C(10)     C(9)      C(12)     H(12)     158.1      . . . . no
C(11)     N(2)      C(7)      H(10)     177.9      . . . . no
C(11)     C(10)     C(9)      C(12)     179.2(4)   . . . . yes
C(12)     C(9)      C(8)      H(9)      0.2        . . . . no
C(12)     C(9)      C(10)     H(8)      -1.4       . . . . no
C(14)     N(6)      N(6)      C(14)     180.0      . . 7_655 7_655 yes
C(14)     N(6)      C(14)     N(6)      0.0000(1)  . . 7_655 7_655 yes
C(14)     N(6)      N(6)      C(14)     180.0      . 7_655 . 7_655 yes
C(14)     N(6)      C(14)     N(6)      0.0000(1)  . 7_655 7_655 . yes
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H(3)      C(4)      C(5)      H(4)      -0.4       . . . . no
H(7)      C(11)     C(10)     H(8)      2.5        . . . . no
H(9)      C(8)      C(7)      H(10)     1.1        . . . . no
H(9)      C(8)      C(7)      H(10)     1.1        . . . . no
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Single Crystal Structure Analysis Software. Version 1.11.
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Rigaku, 3-9-12 Akishima, Tokyo, Japan.
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#-----------------------------------------------------------------------------
# EXPERIMENTAL DATA
_diffrn_radiation_type                 'Mo K¥a'
_diffrn_radiation_wavelength            0.7107
_diffrn_measurement_device_type        'Rigaku/MSC Mercury CCD'
_diffrn_measurement_method              ¥w
_diffrn_detector_area_resol_mean        14.71
_diffrn_reflns_number                   13863
_diffrn_reflns_av_R_equivalents         0.083
_diffrn_reflns_theta_max                27.47
_diffrn_measured_fraction_theta_max     0.9444
_diffrn_reflns_theta_full               27.47
_diffrn_measured_fraction_theta_full    0.9444
_diffrn_reflns_limit_h_min              -23
_diffrn_reflns_limit_h_max              23
_diffrn_reflns_limit_k_min              -25
_diffrn_reflns_limit_k_max              21
_diffrn_reflns_limit_l_min              -11
_diffrn_reflns_limit_l_max              10
```

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#------------------------------------------------------------------------------
# REFINEMENT DATA
_refine_special_details
;
Refinement using reflections with F^2^ > 1.0 sigma(F^2^). The weighted R-factor
(wR), goodness of fit (S) and R-factor (gt) are based on F, with F set to zero
for negative F. The threshold expression of F^2^ > 2.0 sigma(F^2^) is used only
for calculating R-factor (gt).
;
_reflns_number_total                    3366
_reflns_number_gt                       637
_reflns_threshold_expression            F^2^>2.0¥s(F^2^)
_refine_ls_structure_factor_coef        F
_refine_ls_R_factor_gt                  0.1148
_refine_ls_wR_factor_ref                0.1867
_refine_ls_hydrogen_treatment           noref
_refine_ls_number_reflns                1753
_refine_ls_number_parameters            162
_refine_ls_goodness_of_fit_ref          1.692
_refine_ls_weighting_scheme             calc
_refine_ls_weighting_details
   'w = 1/[¥s^2^(Fo) + 0.00063|Fo|^2^]'
_refine_ls_shift/su_max                 0.0032
_refine_diff_density_max                1.52
_refine_diff_density_min                -0.73
_refine_ls_extinction_method            none
_refine_ls_extinction_coef              ?
_refine_ls_abs_structure_details        ?
_refine_ls_abs_structure_Flack          ?
loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
  'Ni' 'Ni'  0.339 1.112
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
  'C' 'C'  0.003 0.002
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
  'N' 'N'  0.006 0.003
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
  'H' 'H'  0.000 0.000
;International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.2)
;
#------------------------------------------------------------------------------
# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS
loop_
_atom_site_label
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_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
 Ni(1)  Ni 0.5000      0.1771(2)   0.2500      0.057(1)    Uani 1.00 d S . .
 N(1)   N  0.5799(7)   0.2544(7)   0.280(2)    0.050(4)    Uani 1.00 d . . .
 N(2)   N  0.4141(8)   0.1021(7)   0.221(2)    0.059(5)    Uani 1.00 d . . .
 N(3)   N  0.4989(8)   0.1707(8)   0.012(2)    0.058(5)    Uani 1.00 d . . .
 N(4)   N  0.5000      0.124(2)    -0.2500     0.17(2)     Uani 1.00 d S . .
 N(5)   N  0.729(4)    0.222(3)    -0.006(9)   0.16(2)     Uiso 0.50 d P . .
 N(6)   N  0.817(2)    0.250(2)    0.164(4)    0.23(1)     Uiso 1.00 d . . .
 C(1)   C  0.582(1)    0.295(1)    0.162(2)    0.078(8)    Uani 1.00 d . . .
 C(2)   C  0.637(1)    0.3481(10)  0.168(3)    0.092(9)    Uani 1.00 d . . .
 C(3)   C  0.686(1)    0.355(1)    0.304(3)    0.090(8)    Uani 1.00 d . . .
 C(4)   C  0.684(1)    0.312(1)    0.426(2)    0.081(8)    Uani 1.00 d . . .
 C(5)   C  0.629(1)    0.2651(10)  0.412(2)    0.072(7)    Uani 1.00 d . . .
 C(6)   C  0.744(2)    0.406(2)    0.312(3)    0.19(2)     Uani 1.00 d . . .
 C(7)   C  0.353(1)    0.117(1)    0.274(3)    0.084(8)    Uani 1.00 d . . .
 C(8)   C  0.295(1)    0.066(1)    0.259(3)    0.100(10)   Uani 1.00 d . . .
 C(9)   C  0.307(2)    0.004(1)    0.190(3)    0.101(10)   Uani 1.00 d . . .
 C(10)  C  0.370(2)    -0.006(1)   0.135(4)    0.12(1)     Uani 1.00 d . . .
 C(11)  C  0.422(1)    0.042(1)    0.148(2)    0.080(6)    Uiso 1.00 d . . .
 C(12)  C  0.240(2)    -0.046(1)   0.184(3)    0.15(1)     Uani 1.00 d . . .
 C(13)  C  0.499(1)    0.1551(10)  -0.109(3)   0.069(7)    Uani 1.00 d . . .
 C(14)  C  0.770(3)    0.227(3)    0.088(7)    0.10(1)     Uiso 0.50 d P . .
 H(1)   H  0.5470      0.2926      0.0557      0.0670      Uiso 1.00 calc . . .
 H(2)   H  0.6422      0.3772      0.0757      0.1065      Uiso 1.00 calc . . .
 H(3)   H  0.7184      0.3201      0.5325      0.0953      Uiso 1.00 calc . . .
 H(4)   H  0.6267      0.2326      0.4954      0.0805      Uiso 1.00 calc . . .
 H(5)   H  0.7412      0.4370      0.4036      0.1886      Uiso 1.00 calc . . .
 H(6)   H  0.7909      0.3867      0.3332      0.1886      Uiso 1.00 calc . . .
 H(7)   H  0.3477      0.1623      0.3265      0.1126      Uiso 1.00 calc . . .
 H(8)   H  0.2491      0.0783      0.2986      0.1141      Uiso 1.00 calc . . .
 H(9)   H  0.3807      -0.0468     0.0783      0.1282      Uiso 1.00 calc . . .
 H(10)  H  0.4721      0.0308      0.1155      0.1213      Uiso 1.00 calc . . .
 H(11)  H  0.1928      -0.0273     0.1670      0.1423      Uiso 1.00 calc . . .
 H(12)  H  0.2378      -0.0803     0.0916      0.1423      Uiso 1.00 calc . . .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
 Ni(1)  0.063(2)    0.042(2)    0.071(2)    0.0000      0.023(2)    0.0000
 N(1)   0.056(9)    0.035(9)    0.058(9)    -0.002(7)   0.004(8)    0.008(7)
```

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 N(2)   0.068(10)   0.041(10)   0.07(1)     -0.007(8)   0.017(8)    -0.002(8)
 N(3)   0.09(1)     0.06(1)     0.036(8)    -0.005(9)   0.028(8)    -0.002(8)
 N(4)   0.38(6)     0.09(2)     0.05(2)     0.0000      0.07(3)     0.0000
 C(1)   0.12(2)     0.07(2)     0.04(1)     0.01(1)     0.01(1)     0.00(1)
 C(2)   0.14(2)     0.05(1)     0.09(2)     -0.05(1)    0.04(2)     0.01(1)
 C(3)   0.08(1)     0.10(2)     0.09(2)     -0.05(1)    0.00(1)     -0.03(1)
 C(4)   0.11(2)     0.08(2)     0.05(1)     -0.05(1)    0.02(1)     0.01(1)
 C(5)   0.09(2)     0.06(1)     0.07(1)     -0.01(1)    0.02(1)     -0.01(1)
 C(6)   0.21(3)     0.22(4)     0.12(2)     -0.18(3)    0.01(2)     0.04(2)
 C(7)   0.07(1)     0.08(2)     0.12(2)     0.00(1)     0.04(1)     0.01(1)
 C(8)   0.07(1)     0.13(2)     0.11(2)     -0.02(2)    0.04(1)     0.01(2)
 C(9)   0.16(3)     0.07(2)     0.06(2)     -0.05(2)    -0.01(2)    0.02(1)
 C(10)  0.10(2)     0.08(2)     0.17(3)     -0.01(2)    0.00(2)     -0.03(2)
 C(12)  0.17(3)     0.15(3)     0.13(2)     -0.13(2)    -0.01(2)    0.01(2)
 C(13)  0.08(1)     0.05(1)     0.08(2)     0.00(1)     0.01(1)     0.02(1)
#------------------------------------------------------------------------------
_computing_data_collection            'CRYSTALCLEAR'
_computing_cell_refinement            'CRYSTALCLEAR'
_computing_data_reduction             'teXsan Ver. 1.11'
_computing_structure_solution          SIR97
_computing_structure_refinement       'teXsan Ver. 1.10'
_computing_publication_material       'teXsan Ver. 1.11'
_computing_molecular_graphics          ?
#------------------------------------------------------------------------------
_geom_special_details
;
 ?
;
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 Ni(1)     N(1)      2.11(1)    . . yes
 Ni(1)     N(1)      2.11(1)    . 2_655 yes
 Ni(1)     N(2)      2.16(2)    . . yes
 Ni(1)     N(2)      2.16(2)    . 2_655 yes
 Ni(1)     N(3)      2.05(1)    . . yes
 Ni(1)     N(3)      2.05(1)    . 2_655 yes
 N(1)      C(1)      1.31(2)    . . yes
 N(1)      C(5)      1.34(2)    . . yes
 N(2)      C(7)      1.34(2)    . . yes
 N(2)      C(11)     1.36(2)    . . yes
 N(3)      C(13)     1.09(2)    . . yes
 N(4)      C(13)     1.36(2)    . . yes
 N(4)      C(13)     1.36(2)    . 2_654 yes
 N(5)      N(5)      1.3(1)     . 7_655 yes
 N(5)      N(6)      1.57(9)    . 7_655 yes
 N(5)      C(14)     1.02(6)    . . yes
 N(5)      C(14)     1.22(6)    . 7_655 yes
 N(6)      C(14)     1.09(7)    . . yes
 C(1)      C(2)      1.45(3)    . . yes
 C(2)      C(3)      1.36(3)    . . yes
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 C(3)      C(4)      1.36(3)    . . yes
 C(3)      C(6)      1.47(3)    . . yes
 C(4)      C(5)      1.37(2)    . . yes
 C(6)      C(12)     1.44(3)    . 5_555 yes
 C(7)      C(8)      1.45(3)    . . yes
 C(8)      C(9)      1.39(3)    . . yes
 C(9)      C(10)     1.36(3)    . . yes
 C(9)      C(12)     1.58(3)    . . yes
 C(10)     C(11)     1.34(3)    . . yes
 C(14)     C(14)     1.8(1)     . 7_655 yes
#------------------------------------------------------------------------------
loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
   N(1)      Ni(1)     N(1)      87.6(8)    . . 2_655 yes
   N(1)      Ni(1)     N(2)      176.9(6)   . . . yes
   N(1)      Ni(1)     N(2)      89.5(6)    . . 2_655 yes
   N(1)      Ni(1)     N(3)      92.9(6)    . . . yes
   N(1)      Ni(1)     N(3)      92.2(6)    . . 2_655 yes
   N(1)      Ni(1)     N(2)      89.5(6)    2_655 . . yes
   N(1)      Ni(1)     N(2)      176.9(6)   2_655 . 2_655 yes
   N(1)      Ni(1)     N(3)      92.2(6)    2_655 . . yes
   N(1)      Ni(1)     N(3)      92.9(6)    2_655 . 2_655 yes
   N(2)      Ni(1)     N(2)      93.5(9)    . . 2_655 yes
   N(2)      Ni(1)     N(3)      88.1(6)    . . . yes
   N(2)      Ni(1)     N(3)      87.1(6)    . . 2_655 yes
   N(2)      Ni(1)     N(3)      87.1(6)    2_655 . . yes
   N(2)      Ni(1)     N(3)      88.1(6)    2_655 . 2_655 yes
   N(3)      Ni(1)     N(3)      173.0(9)   . . 2_655 yes
   Ni(1)     N(1)      C(1)      117(1)     . . . yes
   Ni(1)     N(1)      C(5)      125(1)     . . . yes
   C(1)      N(1)      C(5)      116(1)     . . . yes
   Ni(1)     N(2)      C(7)      118(1)     . . . yes
   Ni(1)     N(2)      C(11)     120(1)     . . . yes
   C(7)      N(2)      C(11)     121(1)     . . . yes
   Ni(1)     N(3)      C(13)     167(1)     . . . yes
   C(13)     N(4)      C(13)     127(2)     . . 2_654 yes
   N(5)      N(5)      N(6)      90(7)      7_655 . 7_655 yes
   N(5)      N(5)      C(14)     60(5)      7_655 . . yes
   N(5)      N(5)      C(14)     46(4)      7_655 . 7_655 yes
   N(6)      N(5)      C(14)     150(8)     7_655 . . yes
   N(6)      N(5)      C(14)     43(5)      7_655 . 7_655 yes
   C(14)     N(5)      C(14)     106(6)     . . 7_655 yes
   N(5)      N(6)      C(14)     50(3)      7_655 . . yes
   N(1)      C(1)      C(2)      122(1)     . . . yes
   C(1)      C(2)      C(3)      117(1)     . . . yes
   C(2)      C(3)      C(4)      120(1)     . . . yes
   C(2)      C(3)      C(6)      118(2)     . . . yes
   C(4)      C(3)      C(6)      120(2)     . . . yes
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```
   C(3)      C(4)      C(5)      118(1)     . . . yes
   N(1)      C(5)      C(4)      124(1)     . . . yes
   C(3)      C(6)      C(12)     118(2)     . . 5_555 yes
   N(2)      C(7)      C(8)      119(2)     . . . yes
   C(7)      C(8)      C(9)      117(2)     . . . yes
   C(8)      C(9)      C(10)     119(2)     . . . yes
   C(8)      C(9)      C(12)     112(2)     . . . yes
   C(10)     C(9)      C(12)     128(2)     . . . yes
   C(9)      C(10)     C(11)     121(2)     . . . yes
   N(2)      C(11)     C(10)     120(2)     . . . yes
   C(6)      C(12)     C(9)      117(2)     5_445 . . yes
   N(3)      C(13)     N(4)      170(2)     . . . yes
   N(5)      C(14)     N(5)      73(6)      . . 7_655 yes
   N(5)      C(14)     N(6)      158(9)     . . . yes
   N(5)      C(14)     C(14)     40(4)      . . 7_655 yes
   N(5)      C(14)     N(6)      85(7)      7_655 . . yes
   N(5)      C(14)     C(14)     32(3)      7_655 . 7_655 yes
   N(6)      C(14)     C(14)     118(7)     . . 7_655 yes
#-------------------------------------------------------------------------------
loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 Ni(1)     N(1)      C(1)      C(2)      -177(1)    . . . . yes
 Ni(1)     N(1)      C(1)      H(1)      1.5        . . . . no
 Ni(1)     N(1)      C(5)      C(4)      174(1)     . . . . yes
 Ni(1)     N(1)      C(5)      H(4)      2.1        . . . . no
 Ni(1)     N(1)      C(1)      C(2)      -177(1)    . 2_655 2_655 2_655 yes
 Ni(1)     N(1)      C(1)      H(1)      1.5        . 2_655 2_655 2_655 no
 Ni(1)     N(1)      C(5)      C(4)      174(1)     . 2_655 2_655 2_655 yes
 Ni(1)     N(1)      C(5)      H(4)      2.1        . 2_655 2_655 2_655 no
 Ni(1)     N(2)      C(7)      C(8)      -178(1)    . . . . yes
 Ni(1)     N(2)      C(7)      H(7)      0.1        . . . . no
 Ni(1)     N(2)      C(11)     C(10)     177(1)     . . . . yes
 Ni(1)     N(2)      C(11)     H(10)     5.2        . . . . no
 Ni(1)     N(2)      C(7)      C(8)      -178(1)    . 2_655 2_655 2_655 yes
 Ni(1)     N(2)      C(7)      H(7)      0.1        . 2_655 2_655 2_655 no
 Ni(1)     N(2)      C(11)     C(10)     177(1)     . 2_655 2_655 2_655 yes
 Ni(1)     N(2)      C(11)     H(10)     5.2        . 2_655 2_655 2_655 no
 Ni(1)     N(3)      C(13)     N(4)      -4(19)     . . . . yes
 Ni(1)     N(3)      C(13)     N(4)      -4(19)     . 2_655 2_655 2_655 yes
 N(1)      Ni(1)     N(1)      C(1)      -63(1)     . . 2_655 2_655 yes
 N(1)      Ni(1)     N(1)      C(5)      117(1)     . . 2_655 2_655 yes
 N(1)      Ni(1)     N(2)      C(7)      -17(11)    . . . . yes
 N(1)      Ni(1)     N(2)      C(11)     161(9)     . . . . yes
 N(1)      Ni(1)     N(2)      C(7)      -33(1)     . . 2_655 2_655 yes
 N(1)      Ni(1)     N(2)      C(11)     145(1)     . . 2_655 2_655 yes
 N(1)      Ni(1)     N(3)      C(13)     134(7)     . . . . yes
```

N(1)	Ni(1)	N(3)	C(13)	-137(7)	. . 2_655 2_655 yes
N(1)	C(1)	C(2)	C(3)	-1(3)	. . . . yes
N(1)	C(1)	C(2)	H(2)	175.3	. . . . no
N(1)	C(5)	C(4)	C(3)	6(3)	. . . . yes
N(1)	C(5)	C(4)	H(3)	175.6	. . . . no
N(2)	Ni(1)	N(1)	C(1)	-79(10)	. . . . yes
N(2)	Ni(1)	N(1)	C(5)	101(10)	. . . . yes
N(2)	Ni(1)	N(1)	C(1)	115(1)	. . 2_655 2_655 yes
N(2)	Ni(1)	N(1)	C(5)	-63(1)	. . 2_655 2_655 yes
N(2)	Ni(1)	N(2)	C(7)	147(1)	. . 2_655 2_655 yes
N(2)	Ni(1)	N(2)	C(11)	-33(1)	. . 2_655 2_655 yes
N(2)	Ni(1)	N(3)	C(13)	-48(7)	. . . . yes
N(2)	Ni(1)	N(3)	C(13)	44(7)	. . 2_655 2_655 yes
N(2)	C(7)	C(8)	C(9)	0(3)	. . . . yes
N(2)	C(7)	C(8)	H(8)	-179.3	. . . . no
N(2)	C(11)	C(10)	C(9)	1(4)	. . . . yes
N(2)	C(11)	C(10)	H(9)	178.3	. . . . no
N(3)	Ni(1)	N(1)	C(1)	28(1)	. . . . yes
N(3)	Ni(1)	N(1)	C(5)	-150(1)	. . . . yes
N(3)	Ni(1)	N(1)	C(1)	-155(1)	. . 2_655 2_655 yes
N(3)	Ni(1)	N(1)	C(5)	24(1)	. . 2_655 2_655 yes
N(3)	Ni(1)	N(2)	C(7)	-125(1)	. . . . yes
N(3)	Ni(1)	N(2)	C(11)	53(1)	. . . . yes
N(3)	Ni(1)	N(2)	C(7)	59(1)	. . 2_655 2_655 yes
N(3)	Ni(1)	N(2)	C(11)	-121(1)	. . 2_655 2_655 yes
N(3)	Ni(1)	N(3)	C(13)	-1(7)	. . 2_655 2_655 yes
N(3)	C(13)	N(4)	C(13)	-172(12)	. . . 2_654 yes
N(5)	N(5)	N(6)	C(14)	0(5)	. 7_655 . . yes
N(5)	N(5)	C(14)	N(6)	179(7)	. 7_655 . . yes
N(5)	N(5)	C(14)	C(14)	0.0	. 7_655 . 7_655 yes
N(5)	N(5)	C(14)	N(6)	1(21)	. 7_655 7_655 7_655 yes
N(5)	N(5)	C(14)	C(14)	0.0000(1)	. 7_655 7_655 . yes
N(5)	N(6)	C(14)	C(14)	0(4)	. 7_655 7_655 . yes
N(5)	C(14)	N(5)	N(6)	-179(7)	. . 7_655 . yes
N(5)	C(14)	N(5)	C(14)	0.0	. . 7_655 7_655 yes
N(5)	C(14)	C(14)	N(5)	180.0	. . 7_655 7_655 yes
N(5)	C(14)	C(14)	N(6)	0(8)	. . 7_655 7_655 yes
N(5)	C(14)	N(5)	N(6)	0(10)	. 7_655 7_655 . yes
N(5)	C(14)	N(5)	C(14)	0.0	. 7_655 7_655 . yes
N(5)	C(14)	C(14)	N(5)	180.0	. 7_655 . 7_655 yes
N(5)	C(14)	C(14)	N(6)	179(8)	. 7_655 . . yes
N(6)	N(5)	N(5)	N(6)	-180.0	. 7_655 . 7_655 yes
N(6)	N(5)	N(5)	C(14)	0(5)	. 7_655 . . yes
N(6)	N(5)	N(5)	C(14)	-179(5)	. 7_655 . 7_655 yes
N(6)	N(5)	C(14)	C(14)	-179(7)	. 7_655 . 7_655 yes
N(6)	N(5)	C(14)	C(14)	0(10)	. 7_655 7_655 . yes
N(6)	C(14)	N(5)	C(14)	-1(21)	. . . 7_655 yes
N(6)	C(14)	N(5)	C(14)	179(7)	. . 7_655 7_655 yes
N(6)	C(14)	C(14)	N(6)	-180.0	. . 7_655 7_655 yes
C(1)	N(1)	C(5)	C(4)	-5(3)	. . . . yes
C(1)	N(1)	C(5)	H(4)	-177.6	. . . . no
C(1)	C(2)	C(3)	C(4)	2(3)	. . . . yes
C(1)	C(2)	C(3)	C(6)	177(2)	. . . . yes
C(2)	C(1)	N(1)	C(5)	2(3)	. . . . yes
C(2)	C(3)	C(4)	C(5)	-5(3)	. . . . yes

```
C(2)      C(3)      C(4)      H(3)      -174.3    . . . . no
C(2)      C(3)      C(6)      C(12)     9(4)      . . . 5_555 yes
C(2)      C(3)      C(6)      H(5)      124.4     . . . . no
C(2)      C(3)      C(6)      H(6)      -119.5    . . . . no
C(3)      C(2)      C(1)      H(1)      179.9     . . . . no
C(3)      C(4)      C(5)      H(4)      178.4     . . . . no
C(4)      C(3)      C(2)      H(2)      -174.2    . . . . no
C(4)      C(3)      C(6)      C(12)     -175(2)   . . . 5_555 yes
C(4)      C(3)      C(6)      H(5)      -60.6     . . . . no
C(4)      C(3)      C(6)      H(6)      55.5      . . . . no
C(5)      N(1)      C(1)      H(1)      -178.8    . . . . no
C(5)      C(4)      C(3)      C(6)      180.0     . . . . yes
C(6)      C(3)      C(2)      H(2)      0.8       . . . . no
C(6)      C(3)      C(4)      H(3)      10.9      . . . . no
C(7)      N(2)      C(11)     C(10)     -3(3)     . . . . yes
C(7)      N(2)      C(11)     H(10)     -175.7    . . . . no
C(7)      C(8)      C(9)      C(10)     -2(3)     . . . . yes
C(7)      C(8)      C(9)      C(12)     178(2)    . . . . yes
C(8)      C(7)      N(2)      C(11)     2(3)      . . . . yes
C(8)      C(9)      C(10)     C(11)     1(4)      . . . . yes
C(8)      C(9)      C(10)     H(9)      -175.3    . . . . no
C(8)      C(9)      C(12)     H(11)     35.3      . . . . no
C(8)      C(9)      C(12)     H(12)     152.9     . . . . no
C(9)      C(8)      C(7)      H(7)      -178.1    . . . . no
C(9)      C(10)     C(11)     H(10)     173.8     . . . . no
C(10)     C(9)      C(8)      H(8)      177.4     . . . . no
C(10)     C(9)      C(12)     H(11)     -143.4    . . . . no
C(10)     C(9)      C(12)     H(12)     -25.8     . . . . no
C(11)     N(2)      C(7)      H(7)      -179.1    . . . . no
C(11)     C(10)     C(9)      C(12)     -179(2)   . . . . yes
C(12)     C(9)      C(8)      H(8)      -1.4      . . . . no
C(12)     C(9)      C(10)     H(9)      3.4       . . . . no
C(14)     N(5)      N(5)      C(14)     180.0     . . 7_655 7_655 yes
C(14)     N(5)      C(14)     N(5)      0.0       . . 7_655 7_655 yes
C(14)     N(5)      N(5)      C(14)     -180.0    . 7_655 . 7_655 yes
C(14)     N(5)      C(14)     N(5)      0.0       . 7_655 7_655 . yes
H(1)      C(1)      C(2)      H(2)      -3.4      . . . . no
H(3)      C(4)      C(5)      H(4)      -12.6     . . . . no
H(7)      C(7)      C(8)      H(8)      2.1       . . . . no
H(9)      C(10)     C(11)     H(10)     -9.3      . . . . no
H(9)      C(10)     C(11)     H(10)     -9.3      . . . . no
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Complex2.cif

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Molecular Structure Corporation, Rigaku Corporation. (2000). teXsan.
Single Crystal Structure Analysis Software. Version 1.11.
MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Rigaku, 3-9-12 Akishima, Tokyo, Japan.
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-x,-y,-z
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1/2+x,1/2+y,z
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1/2+x,1/2-y,1/2+z
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_cell_length_c                          8.63(4)
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_cell_volume                            3092(1)
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_refine_special_details
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Refinement using reflections with F^2^ > 3.0 sigma(F^2^). The weighted R-factor
(wR), goodness of fit (S) and R-factor (gt) are based on F, with F set to zero
for negative F. The threshold expression of F^2^ > 3.0 sigma(F^2^) is used only
for calculating R-factor (gt).
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_reflns_number_total                    3530
_reflns_number_gt                       1454
_reflns_threshold_expression            F^2^>3.0¥s(F^2^)
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_refine_ls_wR_factor_ref                0.1130
_refine_ls_hydrogen_treatment           noref
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_refine_ls_number_parameters            177
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_refine_ls_weighting_scheme             calc
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(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
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(1992, Vol. C, Table 6.1.1.2)
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(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
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_atom_site_disorder_group
 Ni(1)  Ni 0.5000      0.17556(8)  0.2500      0.0332(5)   Uani 1.00 d S . .
 O(1)   O  1.0000      0.009(3)    0.7500      0.54(2)     Uiso 1.00 d S . .
 O(2)   O  0.946(2)    -0.045(2)   0.957(4)    0.47(2)     Uiso 1.00 d . . .
 O(3)   O  0.062(2)    0.168(1)    0.222(4)    0.38(1)     Uiso 1.00 d . . .
 N(1)   N  0.5794(4)   0.2526(3)   0.2756(8)   0.034(2)    Uani 1.00 d . . .
 N(2)   N  0.4138(4)   0.1017(3)   0.2170(8)   0.036(2)    Uani 1.00 d . . .
 N(3)   N  0.5005(4)   0.1689(3)   0.4895(9)   0.037(2)    Uani 1.00 d . . .
 N(4)   N  0.5000      0.1243(7)   0.7500      0.113(7)    Uani 1.00 d S . .
 N(5)   N  0.843(2)    0.248(2)    0.188(4)    0.28(1)     Uiso 1.00 d . . .
 N(6)   N  0.743(2)    0.215(1)    0.040(4)    0.125(9)    Uiso 0.50 d P . .
 C(1)   C  0.6293(5)   0.2634(5)   0.408(1)    0.043(3)    Uani 1.00 d . . .
 C(2)   C  0.6821(5)   0.3137(4)   0.421(1)    0.046(3)    Uani 1.00 d . . .
 C(3)   C  0.6839(6)   0.3562(5)   0.296(1)    0.049(3)    Uani 1.00 d . . .
 C(4)   C  0.6316(6)   0.3456(5)   0.159(1)    0.056(3)    Uani 1.00 d . . .
 C(5)   C  0.5806(6)   0.2946(5)   0.156(1)    0.044(3)    Uani 1.00 d . . .
 C(6)   C  0.7426(7)   0.4104(6)   0.306(1)    0.075(4)    Uani 1.00 d . . .
 C(7)   C  0.4204(6)   0.0436(4)   0.145(1)    0.047(3)    Uani 1.00 d . . .
 C(8)   C  0.3674(7)   -0.0061(5)  0.132(1)    0.060(4)    Uani 1.00 d . . .
 C(9)   C  0.3020(7)   0.0047(6)   0.185(1)    0.062(4)    Uani 1.00 d . . .
 C(10)  C  0.2935(6)   0.0646(6)   0.254(1)    0.059(4)    Uani 1.00 d . . .
 C(11)  C  0.3506(5)   0.1115(5)   0.269(1)    0.047(3)    Uani 1.00 d . . .
 C(12)  C  0.2423(8)   -0.0488(7)  0.167(2)    0.090(5)    Uani 1.00 d . . .
 C(13)  C  0.5001(6)   0.1528(5)   0.617(1)    0.048(3)    Uani 1.00 d . . .
 C(14)  C  0.794(2)    0.246(1)    0.106(3)    0.174(9)    Uiso 1.00 d . . .
 H(1)   H  0.6290      0.2342      0.4968      0.0538      Uiso 1.00 calc . . .
 H(2)   H  0.7182      0.3186      0.5150      0.0580      Uiso 1.00 calc . . .
 H(3)   H  0.6299      0.3753      0.0701      0.0690      Uiso 1.00 calc . . .
 H(4)   H  0.5426      0.2887      0.0614      0.0568      Uiso 1.00 calc . . .
 H(5)   H  0.7909      0.3894      0.3285      0.0947      Uiso 1.00 calc . . .
 H(6)   H  0.7375      0.4398      0.3883      0.0947      Uiso 1.00 calc . . .
 H(7)   H  0.4645      0.0367      0.0979      0.0568      Uiso 1.00 calc . . .
 H(8)   H  0.3775      -0.0498     0.0826      0.0751      Uiso 1.00 calc . . .
 H(9)   H  0.2487      0.0748      0.2950      0.0771      Uiso 1.00 calc . . .
 H(10)  H  0.3449      0.1538      0.3226      0.0575      Uiso 1.00 calc . . .
 H(11)  H  0.2471      -0.0785     0.0774      0.1105      Uiso 1.00 calc . . .
 H(12)  H  0.1942      -0.0278     0.1378      0.1105      Uiso 1.00 calc . . .

loop_
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_atom_site_aniso_U_11
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 N(1)    0.039(5)    0.032(4)    0.028(5)    0.002(4)    0.003(4)    0.004(4)
 N(2)    0.042(5)    0.032(4)    0.034(5)    -0.006(4)   0.006(4)    0.000(4)
 N(3)    0.053(5)    0.031(4)    0.028(4)    0.001(4)    0.010(3)    -0.002(4)
 N(4)    0.26(2)     0.065(10)   0.017(7)    0.0000      0.04(1)     0.0000
 C(1)    0.049(6)    0.039(6)    0.040(6)    -0.005(5)   0.002(5)    0.001(5)
 C(2)    0.051(6)    0.042(6)    0.043(6)    -0.017(5)   0.002(5)    -0.002(5)
 C(3)    0.064(7)    0.039(6)    0.046(7)    -0.019(5)   0.016(5)    0.001(5)
 C(4)    0.069(8)    0.052(6)    0.041(6)    -0.027(6)   -0.003(6)   0.010(5)
 C(5)    0.062(7)    0.033(5)    0.035(6)    -0.014(5)   0.003(5)    0.006(5)
 C(6)    0.092(10)   0.066(8)    0.061(8)    -0.058(7)   0.000(7)    0.013(6)
 C(7)    0.057(7)    0.028(5)    0.052(7)    -0.004(5)   -0.002(5)   -0.004(5)
 C(8)    0.073(8)    0.034(6)    0.069(8)    -0.016(6)   -0.004(6)   0.001(5)
 C(9)    0.068(8)    0.048(7)    0.062(8)    -0.035(6)   -0.012(6)   0.008(6)
 C(10)   0.049(7)    0.068(8)    0.060(7)    -0.028(6)   0.012(5)    0.015(6)
 C(11)   0.043(6)    0.049(6)    0.051(6)    -0.008(5)   0.012(5)    0.001(5)
 C(12)   0.09(1)     0.088(9)    0.084(10)   -0.064(8)   0.003(8)    0.016(8)
 C(13)   0.075(8)    0.035(5)    0.033(7)    0.002(5)    0.009(6)    -0.011(5)
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 Ni(1)     N(1)      2.098(8)   . 2_655 yes
 Ni(1)     N(2)      2.138(8)   . . yes
 Ni(1)     N(2)      2.138(8)   . 2_655 yes
 Ni(1)     N(3)      2.070(7)   . . yes
 Ni(1)     N(3)      2.070(7)   . 2_655 yes
 N(1)      C(1)      1.35(1)    . . yes
 N(1)      C(5)      1.33(1)    . . yes
 N(2)      C(7)      1.33(1)    . . yes
 N(2)      C(11)     1.33(1)    . . yes
 N(3)      C(13)     1.15(1)    . . yes
 N(4)      C(13)     1.28(1)    . . yes
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 N(4)      C(13)     1.28(1)    . 2_656 yes
 N(5)      C(14)     1.04(3)    . . yes
 N(6)      N(6)      1.60(6)    . 7_655 yes
 N(6)      C(14)     1.17(3)    . . yes
 N(6)      C(14)     1.53(3)    . 7_655 yes
 C(1)      C(2)      1.38(1)    . . yes
 C(2)      C(3)      1.37(1)    . . yes
 C(3)      C(4)      1.40(1)    . . yes
 C(3)      C(6)      1.51(1)    . . yes
 C(4)      C(5)      1.38(1)    . . yes
 C(6)      C(12)     1.45(2)    . 5_555 yes
 C(7)      C(8)      1.38(1)    . . yes
 C(8)      C(9)      1.37(2)    . . yes
 C(9)      C(10)     1.35(2)    . . yes
 C(9)      C(12)     1.51(1)    . . yes
 C(10)     C(11)     1.39(1)    . . yes
#-------------------------------------------------------------------------------
loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
   N(1)      Ni(1)     N(1)      86.0(4)    . . 2_655 yes
   N(1)      Ni(1)     N(2)      176.3(3)   . . . yes
   N(1)      Ni(1)     N(2)      90.5(3)    . . 2_655 yes
   N(1)      Ni(1)     N(3)      93.5(3)    . . . yes
   N(1)      Ni(1)     N(3)      91.9(3)    . . 2_655 yes
   N(1)      Ni(1)     N(2)      90.5(3)    2_655 . . yes
   N(1)      Ni(1)     N(2)      176.3(3)   2_655 . 2_655 yes
   N(1)      Ni(1)     N(3)      91.9(3)    2_655 . . yes
   N(1)      Ni(1)     N(3)      93.5(3)    2_655 . 2_655 yes
   N(2)      Ni(1)     N(2)      93.1(4)    . . 2_655 yes
   N(2)      Ni(1)     N(3)      87.8(3)    . . . yes
   N(2)      Ni(1)     N(3)      87.1(3)    . . 2_655 yes
   N(2)      Ni(1)     N(3)      87.1(3)    2_655 . . yes
   N(2)      Ni(1)     N(3)      87.8(3)    2_655 . 2_655 yes
   N(3)      Ni(1)     N(3)      172.7(4)   . . 2_655 yes
   Ni(1)     N(1)      C(1)      124.0(6)   . . . yes
   Ni(1)     N(1)      C(5)      118.9(6)   . . . yes
   C(1)      N(1)      C(5)      117.1(8)   . . . yes
   Ni(1)     N(2)      C(7)      122.4(6)   . . . yes
   Ni(1)     N(2)      C(11)     121.3(6)   . . . yes
   C(7)      N(2)      C(11)     116.3(8)   . . . yes
   Ni(1)     N(3)      C(13)     167.4(7)   . . . yes
   C(13)     N(4)      C(13)     127(1)     . . 2_656 yes
   N(6)      N(6)      C(14)     64(2)      7_655 . . yes
   N(6)      N(6)      C(14)     43(1)      7_655 . 7_655 yes
   C(14)     N(6)      C(14)     108(3)     . . 7_655 yes
   N(1)      C(1)      C(2)      122.8(8)   . . . yes
   C(1)      C(2)      C(3)      119.8(9)   . . . yes
   C(2)      C(3)      C(4)      117.4(9)   . . . yes
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   C(2)      C(3)      C(6)      120.6(9)   . . . yes
   C(4)      C(3)      C(6)      122.0(9)   . . . yes
   C(3)      C(4)      C(5)      119.2(9)   . . . yes
   N(1)      C(5)      C(4)      123.5(9)   . . . yes
   C(3)      C(6)      C(12)     116.9(9)   . . 5_555 yes
   N(2)      C(7)      C(8)      123.2(10)  . . . yes
   C(7)      C(8)      C(9)      119(1)     . . . yes
   C(8)      C(9)      C(10)     117.4(9)   . . . yes
   C(8)      C(9)      C(12)     120(1)     . . . yes
   C(10)     C(9)      C(12)     121(1)     . . . yes
   C(9)      C(10)     C(11)     119(1)     . . . yes
   N(2)      C(11)     C(10)     123.6(10)  . . . yes
   C(6)      C(12)     C(9)      114(1)     5_445 . . yes
   N(3)      C(13)     N(4)      169(1)     . . . yes
   N(5)      C(14)     N(6)      149(4)     . . . yes
   N(5)      C(14)     N(6)      137(4)     . . 7_655 yes
   N(6)      C(14)     N(6)      71(3)      . . 7_655 yes
#-------------------------------------------------------------------------------
loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 Ni(1)     N(1)      C(1)      C(2)      178.6(7)   . . . . yes
 Ni(1)     N(1)      C(1)      H(1)      -0.1       . . . . no
 Ni(1)     N(1)      C(5)      C(4)      -178.2(8)  . . . . yes
 Ni(1)     N(1)      C(5)      H(4)      2.3        . . . . no
 Ni(1)     N(1)      C(1)      C(2)      178.6(7)   . 2_655 2_655 2_655 yes
 Ni(1)     N(1)      C(1)      H(1)      -0.1       . 2_655 2_655 2_655 no
 Ni(1)     N(1)      C(5)      C(4)      -178.2(8)  . 2_655 2_655 2_655 yes
 Ni(1)     N(1)      C(5)      H(4)      2.3        . 2_655 2_655 2_655 no
 Ni(1)     N(2)      C(7)      C(8)      175.9(7)   . . . . yes
 Ni(1)     N(2)      C(7)      H(7)      -5.8       . . . . no
 Ni(1)     N(2)      C(11)     C(10)     -178.7(8)  . . . . yes
 Ni(1)     N(2)      C(11)     H(10)     0.4        . . . . no
 Ni(1)     N(2)      C(7)      C(8)      175.9(7)   . 2_655 2_655 2_655 yes
 Ni(1)     N(2)      C(7)      H(7)      -5.8       . 2_655 2_655 2_655 no
 Ni(1)     N(2)      C(11)     C(10)     -178.7(8)  . 2_655 2_655 2_655 yes
 Ni(1)     N(2)      C(11)     H(10)     0.4        . 2_655 2_655 2_655 no
 Ni(1)     N(3)      C(13)     N(4)      4(9)       . . . . yes
 Ni(1)     N(3)      C(13)     N(4)      4(9)       . 2_655 2_655 2_655 yes
 N(1)      Ni(1)     N(1)      C(1)      116.2(8)   . . 2_655 2_655 yes
 N(1)      Ni(1)     N(1)      C(5)      -62.7(6)   . . 2_655 2_655 yes
 N(1)      Ni(1)     N(2)      C(7)      127(4)     . . . . yes
 N(1)      Ni(1)     N(2)      C(11)     -53(4)     . . . . yes
 N(1)      Ni(1)     N(2)      C(7)      146.3(7)   . . 2_655 2_655 yes
 N(1)      Ni(1)     N(2)      C(11)     -34.4(7)   . . 2_655 2_655 yes
 N(1)      Ni(1)     N(3)      C(13)     -139(3)    . . . . yes
 N(1)      Ni(1)     N(3)      C(13)     134(3)     . . 2_655 2_655 yes
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N(1)	C(1)	C(2)	C(3)	1(1)	.	.	.	.	yes
N(1)	C(1)	C(2)	H(2)	-177.1	.	.	.	.	no
N(1)	C(5)	C(4)	C(3)	-2(1)	.	.	.	.	yes
N(1)	C(5)	C(4)	H(3)	-179.0	.	.	.	.	no
N(2)	Ni(1)	N(1)	C(1)	135(4)	.	.	.	.	yes
N(2)	Ni(1)	N(1)	C(5)	-43(4)	.	.	.	.	yes
N(2)	Ni(1)	N(1)	C(1)	-62.6(7)	.	.	2_655	2_655	yes
N(2)	Ni(1)	N(1)	C(5)	118.5(7)	.	.	2_655	2_655	yes
N(2)	Ni(1)	N(2)	C(7)	-34.8(6)	.	.	2_655	2_655	yes
N(2)	Ni(1)	N(2)	C(11)	144.4(8)	.	.	2_655	2_655	yes
N(2)	Ni(1)	N(3)	C(13)	43(3)	.	.	.	.	yes
N(2)	Ni(1)	N(3)	C(13)	-49(3)	.	.	2_655	2_655	yes
N(2)	C(7)	C(8)	C(9)	3(1)	.	.	.	.	yes
N(2)	C(7)	C(8)	H(8)	-175.9	.	.	.	.	no
N(2)	C(11)	C(10)	C(9)	1(1)	.	.	.	.	yes
N(2)	C(11)	C(10)	H(9)	179.7	.	.	.	.	no
N(3)	Ni(1)	N(1)	C(1)	24.6(7)	.	.	.	.	yes
N(3)	Ni(1)	N(1)	C(5)	-154.3(7)	.	.	.	.	yes
N(3)	Ni(1)	N(1)	C(1)	-150.4(7)	.	.	2_655	2_655	yes
N(3)	Ni(1)	N(1)	C(5)	30.7(7)	.	.	2_655	2_655	yes
N(3)	Ni(1)	N(2)	C(7)	-121.9(7)	.	.	.	.	yes
N(3)	Ni(1)	N(2)	C(11)	57.4(7)	.	.	.	.	yes
N(3)	Ni(1)	N(2)	C(7)	52.8(7)	.	.	2_655	2_655	yes
N(3)	Ni(1)	N(2)	C(11)	-127.9(7)	.	.	2_655	2_655	yes
N(3)	Ni(1)	N(3)	C(13)	-2(3)	.	.	2_655	2_655	yes
N(3)	C(13)	N(4)	C(13)	178(6)	.	.	.	2_656	yes
N(5)	C(14)	N(6)	N(6)	-162(7)	.	.	.	7_655	yes
N(5)	C(14)	N(6)	C(14)	-162(7)	.	.	.	7_655	yes
N(5)	C(14)	N(6)	N(6)	166(5)	.	.	7_655	.	yes
N(5)	C(14)	N(6)	C(14)	166(5)	.	.	7_655	7_655	yes
N(6)	C(14)	N(6)	C(14)	0.0	.	.	7_655	7_655	yes
N(6)	C(14)	N(6)	C(14)	0.0	.	7_655	7_655	.	yes
C(1)	N(1)	C(5)	C(4)	2(1)	.	.	.	.	yes
C(1)	N(1)	C(5)	H(4)	-176.6	.	.	.	.	no
C(1)	C(2)	C(3)	C(4)	0(1)	.	.	.	.	yes
C(1)	C(2)	C(3)	C(6)	-178.3(10)	.	.	.	.	yes
C(2)	C(1)	N(1)	C(5)	-2(1)	.	.	.	.	yes
C(2)	C(3)	C(4)	C(5)	1(1)	.	.	.	.	yes
C(2)	C(3)	C(4)	H(3)	177.8	.	.	.	.	no
C(2)	C(3)	C(6)	C(12)	177(1)	.	.	.	5_555	yes
C(2)	C(3)	C(6)	H(5)	57.5	.	.	.	.	no
C(2)	C(3)	C(6)	H(6)	-61.1	.	.	.	.	no
C(3)	C(2)	C(1)	H(1)	-179.8	.	.	.	.	no
C(3)	C(4)	C(5)	H(4)	177.2	.	.	.	.	no
C(4)	C(3)	C(2)	H(2)	177.9	.	.	.	.	no
C(4)	C(3)	C(6)	C(12)	0(1)	.	.	.	5_555	yes
C(4)	C(3)	C(6)	H(5)	-120.0	.	.	.	.	no
C(4)	C(3)	C(6)	H(6)	121.4	.	.	.	.	no
C(5)	N(1)	C(1)	H(1)	178.8	.	.	.	.	no
C(5)	C(4)	C(3)	C(6)	178.6(10)	.	.	.	.	yes
C(6)	C(3)	C(2)	H(2)	0.3	.	.	.	.	no
C(6)	C(3)	C(4)	H(3)	-4.6	.	.	.	.	no
C(7)	N(2)	C(11)	C(10)	0(1)	.	.	.	.	yes
C(7)	N(2)	C(11)	H(10)	179.7	.	.	.	.	no
C(7)	C(8)	C(9)	C(10)	-1(1)	.	.	.	.	yes

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 C(7)      C(8)      C(9)      C(12)     178.3(10)  . . . . yes
 C(8)      C(7)      N(2)      C(11)     -3(1)      . . . . yes
 C(8)      C(9)      C(10)     C(11)     -1(1)      . . . . yes
 C(8)      C(9)      C(10)     H(9)      -179.2     . . . . no
 C(8)      C(9)      C(12)     H(11)     -24.9      . . . . no
 C(8)      C(9)      C(12)     H(12)     -139.8     . . . . no
 C(9)      C(8)      C(7)      H(7)      -174.4     . . . . no
 C(9)      C(10)     C(11)     H(10)     -177.5     . . . . no
 C(10)     C(9)      C(8)      H(8)      178.3      . . . . no
 C(10)     C(9)      C(12)     H(11)     154.9      . . . . no
 C(10)     C(9)      C(12)     H(12)     40.0       . . . . no
 C(11)     N(2)      C(7)      H(7)      174.9      . . . . no
 C(11)     C(10)     C(9)      C(12)     179(1)     . . . . yes
 C(12)     C(9)      C(8)      H(8)      -2.0       . . . . no
 C(12)     C(9)      C(10)     H(9)      1.1        . . . . no
 C(14)     N(6)      N(6)      C(14)     -180.0     . . 7_655 7_655 yes
 C(14)     N(6)      C(14)     N(6)      0.0        . . 7_655 7_655 yes
 C(14)     N(6)      N(6)      C(14)     180.0      . 7_655 . 7_655 yes
 C(14)     N(6)      C(14)     N(6)      0.0        . 7_655 7_655 . yes
 H(1)      C(1)      C(2)      H(2)      1.6        . . . . no
 H(3)      C(4)      C(5)      H(4)      0.5        . . . . no
 H(7)      C(7)      C(8)      H(8)      5.9        . . . . no
 H(9)      C(10)     C(11)     H(10)     0.6        . . . . no
 H(9)      C(10)     C(11)     H(10)     0.6        . . . . no
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