EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{30}H_{36}N_{10}Ni$
Formula Weight	595.38
Crystal Color, Habit	violet, prismatic
Crystal Dimensions	0.25 X 0.47 X 0.15 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (24.0 - 31.0°)
Omega Scan Peak Width at Half-height	0.44°
Lattice Parameters	a = 10.395(8) $\AA$ b = 11.117(6) $\AA$ c = 8.425(4) $\AA$ α = 106.84(5)° β = 106.97(5)° γ = 104.33(6)° V = 830(1) $\AA^3$
Space Group	$P\bar{1}$ (#2)
Z value	1
D_{calc}	1.190 g/cm^3
F_{000}	314.00
μ(MoKα)	6.18 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC7R (rotating anode)
Radiation	MoKα (λ = 0.71069 $\AA$) graphite monochromated

Attenuator	Zr foil (factor = 8.66)
Temperature	23.0 °C
Collimator Size	1.0 mm
Take-off Angle	6.0°
Detector Aperture	9.0 mm horizontal 13.0 mm vertical
Crystal to Detector Distance	235 mm
Scan Type	ω-2θ
Scan Rate	16.0°/min (in ω) (up to 5 scans)
Scan Width	(1.84 + 0.30 tan θ)°
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 4102 Unique: 3827 (R_{int} = 0.037)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.7831 - 0.9972) Decay (0.99% decline)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF94 PATTY)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$
p-factor	0.1020
Anomalous Dispersion	All non-hydrogen atoms
No. of Observations (I>4.00σ(I), 2θ<55.03°)	1314
No. Variables	163
Reflection/Parameter Ratio	8.06
Residuals: R; Rw	0.089 ; 0.119

Residuals: R1	0.089
No. of Reflections to calc R1	1314
Goodness of Fit Indicator	1.76
Max Shift/Error in Final Cycle	0.371
Maximum peak in Final Diff. Map	1.13 $e^-/\mathring{A}^3$
Minimum peak in Final Diff. Map	-0.54 $e^-/\mathring{A}^3$

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Ni(1)	0.0000	0.0000	0.0000	1.84(6)	0.5000
N(1)	-0.169(1)	0.0522(10)	-0.132(1)	2.5(2)	1.0000
N(2)	-0.386(1)	0.0592(10)	-0.154(1)	3.1(3)	1.0000
N(3)	0.137(1)	0.0504(10)	-0.125(1)	2.6(2)	1.0000
N(4)	0.350(1)	0.059(1)	-0.144(1)	3.3(3)	1.0000
N(5)	0.099(1)	0.199(1)	0.203(1)	3.6(3)	1.0000
C(1)	-0.216(1)	0.103(1)	-0.259(2)	3.6(3)	1.0000
C(2)	-0.348(1)	0.105(1)	-0.274(2)	3.6(3)	1.0000
C(3)	-0.274(1)	0.028(1)	-0.072(1)	2.2(3)	1.0000
C(4)	0.153(1)	0.101(1)	-0.253(2)	3.1(3)	1.0000
C(5)	0.281(1)	0.107(1)	-0.264(2)	3.9(4)	1.0000
C(6)	0.258(1)	0.028(1)	-0.068(1)	1.9(3)	1.0000
C(7)	0.139(2)	0.218(2)	0.375(2)	5.6(5)	1.0000
C(8)	0.208(2)	0.346(2)	0.520(2)	8.0(6)	1.0000
C(9)	0.230(2)	0.457(2)	0.480(3)	6.9(6)	1.0000
C(10)	0.196(3)	0.442(2)	0.308(3)	8.6(7)	1.0000
C(11)	0.123(2)	0.309(2)	0.167(2)	6.7(6)	1.0000
C(12)	0.307(4)	0.593(3)	0.628(6)	16(1)	1.0000
C(13)	0.3340	0.5997	0.8104	36(2)	1.0000
C(14)	0.2175	0.6962	0.5974	19(1)	1.0000
C(15)	0.4587	0.6782	0.6242	25(1)	1.0000
H(1)	-0.1691	0.1343	-0.3300	4.7	1.0000
H(2)	-0.4142	0.1270	-0.3574	5.0	1.0000
H(3)	-0.4700	0.0529	-0.1282	5.0	0.5000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(4)	0.0840	0.1267	-0.3291	4.6	1.0000
H(5)	0.3237	0.1383	-0.3377	5.1	1.0000
H(6)	0.4418	0.0497	-0.1173	4.4	0.5000
H(7)	0.1190	0.1334	0.3997	7.6	1.0000
H(8)	0.2396	0.3547	0.6401	10.4	1.0000
H(9)	0.2181	0.5194	0.2757	13.3	1.0000
H(10)	0.0878	0.2929	0.0362	9.2	1.0000

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni(1)	0.014(1)	0.020(1)	0.024(2)	0.005(1)	0.005(1)	-0.003(1)
N(1)	0.037(6)	0.036(6)	0.030(6)	0.016(5)	0.018(5)	0.015(5)
N(2)	0.031(7)	0.050(7)	0.049(7)	0.021(5)	0.019(6)	0.026(6)
N(3)	0.042(6)	0.036(6)	0.025(5)	0.015(5)	0.017(5)	0.014(5)
N(4)	0.049(7)	0.047(7)	0.051(7)	0.020(6)	0.037(6)	0.028(6)
N(5)	0.062(8)	0.034(7)	0.043(7)	0.021(6)	0.025(6)	0.012(6)
C(1)	0.045(8)	0.053(9)	0.043(8)	0.014(7)	0.024(7)	0.020(7)
C(2)	0.055(9)	0.061(9)	0.039(8)	0.027(7)	0.021(7)	0.035(7)
C(3)	0.033(7)	0.028(7)	0.026(7)	0.017(6)	0.014(6)	0.009(6)
C(4)	0.028(7)	0.058(9)	0.044(8)	0.025(6)	0.018(6)	0.025(7)
C(5)	0.050(9)	0.062(10)	0.051(9)	0.024(8)	0.024(7)	0.037(8)
C(6)	0.021(6)	0.026(6)	0.022(6)	0.008(5)	0.006(5)	0.008(6)
C(7)	0.09(1)	0.07(1)	0.06(1)	0.041(10)	0.026(10)	0.04(1)
C(8)	0.14(2)	0.08(2)	0.05(1)	0.03(1)	0.01(1)	0.00(1)
C(9)	0.12(2)	0.06(1)	0.06(1)	0.02(1)	0.02(1)	0.01(1)
C(10)	0.15(2)	0.03(1)	0.11(2)	0.02(1)	0.03(2)	0.01(1)
C(11)	0.11(2)	0.09(2)	0.08(1)	0.05(1)	0.05(1)	0.05(1)
C(12)	0.29(4)	0.14(3)	0.33(5)	0.10(3)	0.20(4)	0.16(3)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Ni(1)	N(1)	2.09(1)	Ni(1)	N(1)[1)]	2.09(1)
Ni(1)	N(3)	2.066(9)	Ni(1)	N(3)[1)]	2.066(9)
Ni(1)	N(5)	2.13(1)	Ni(1)	N(5)[1)]	2.13(1)
N(1)	C(1)	1.38(2)	N(1)	C(3)	1.33(1)
N(2)	C(2)	1.36(2)	N(2)	C(3)	1.35(1)
N(2)	H(3)	0.95	N(3)	C(4)	1.38(1)
N(3)	C(6)	1.33(1)	N(4)	C(5)	1.38(2)
N(4)	C(6)	1.33(1)	N(4)	H(6)	0.95
N(5)	C(7)	1.32(2)	N(5)	C(11)	1.33(2)
C(1)	C(2)	1.34(2)	C(1)	H(1)	0.96
C(2)	H(2)	0.97	C(3)	C(6)[1)]	1.47(2)
C(4)	C(5)	1.35(2)	C(4)	H(4)	0.97
C(5)	H(5)	0.95	C(7)	C(8)	1.42(2)
C(7)	H(7)	1.00	C(8)	C(9)	1.36(2)
C(8)	H(8)	0.93	C(9)	C(10)	1.34(3)
C(9)	C(12)	1.48(4)	C(10)	C(11)	1.44(2)
C(10)	H(9)	0.97	C(11)	H(10)	1.00
C(12)	C(13)	1.45(4)	C(12)	C(14)	1.68(3)
C(12)	C(15)	1.64(3)			

Symmetry operations

(1) -X,-Y,-Z

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Ni(1)	N(1)$^{1)}$	180.0	N(1)	Ni(1)	N(3)	99.0(4)
N(1)	Ni(1)	N(3)$^{1)}$	81.0(4)	N(1)	Ni(1)	N(5)	89.7(4)
N(1)	Ni(1)	N(5)$^{1)}$	90.3(4)	N(1)$^{1)}$	Ni(1)	N(3)	81.0(4)
N(1)$^{1)}$	Ni(1)	N(3)$^{1)}$	99.0(4)	N(1)$^{1)}$	Ni(1)	N(5)	90.3(4)
N(1)$^{1)}$	Ni(1)	N(5)$^{1)}$	89.7(4)	N(3)	Ni(1)	N(3)$^{1)}$	180.0
N(3)	Ni(1)	N(5)	90.2(4)	N(3)	Ni(1)	N(5)$^{1)}$	89.8(4)
N(3)$^{1)}$	Ni(1)	N(5)	89.8(4)	N(3)$^{1)}$	Ni(1)	N(5)$^{1)}$	90.2(4)
N(5)	Ni(1)	N(5)$^{1)}$	180.0	Ni(1)	N(1)	C(1)	144.8(8)
Ni(1)	N(1)	C(3)	110.5(8)	C(1)	N(1)	C(3)	104(1)
C(2)	N(2)	C(3)	104.7(10)	C(2)	N(2)	H(3)	129.1
C(3)	N(2)	H(3)	126.2	Ni(1)	N(3)	C(4)	144.2(9)
Ni(1)	N(3)	C(6)	113.4(8)	C(4)	N(3)	C(6)	102.4(10)
C(5)	N(4)	C(6)	103.5(10)	C(5)	N(4)	H(6)	130.3
C(6)	N(4)	H(6)	126.2	Ni(1)	N(5)	C(7)	120(1)
Ni(1)	N(5)	C(11)	123(1)	C(7)	N(5)	C(11)	116(1)
N(1)	C(1)	C(2)	108(1)	N(1)	C(1)	H(1)	129.4
C(2)	C(1)	H(1)	121.9	N(2)	C(2)	C(1)	109(1)
N(2)	C(2)	H(2)	121.1	C(1)	C(2)	H(2)	129.6
N(1)	C(3)	N(2)	112.6(10)	N(1)	C(3)	C(6)$^{1)}$	119(1)
N(2)	C(3)	C(6)$^{1)}$	128(1)	N(3)	C(4)	C(5)	110(1)
N(3)	C(4)	H(4)	127.2	C(5)	C(4)	H(4)	122.6
N(4)	C(5)	C(4)	108(1)	N(4)	C(5)	H(5)	121.7
C(4)	C(5)	H(5)	130.2	N(3)	C(6)	N(4)	115(1)
N(3)	C(6)	C(3)$^{1)}$	115.8(10)	N(4)	C(6)	C(3)$^{1)}$	128(1)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(5)	C(7)	C(8)	124(1)	N(5)	C(7)	H(7)	115.4
C(8)	C(7)	H(7)	120.1	C(7)	C(8)	C(9)	117(1)
C(7)	C(8)	H(8)	121.4	C(9)	C(8)	H(8)	120.6
C(8)	C(9)	C(10)	118(1)	C(8)	C(9)	C(12)	119(2)
C(10)	C(9)	C(12)	121(2)	C(9)	C(10)	C(11)	120(1)
C(9)	C(10)	H(9)	120.8	C(11)	C(10)	H(9)	119.2
N(5)	C(11)	C(10)	121(1)	N(5)	C(11)	H(10)	115.5
C(10)	C(11)	H(10)	122.8	C(9)	C(12)	C(13)	117(1)
C(9)	C(12)	C(14)	110(2)	C(9)	C(12)	C(15)	113(2)
C(13)	C(12)	C(14)	106(2)	C(13)	C(12)	C(15)	108(2)
C(14)	C(12)	C(15)	98(1)				

Symmetry operations

(1)	-X,-Y,-Z