EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{44}H_{36}N_{20}Ni_2$
Formula Weight	962.30
Crystal Color, Habit	orange, prismatic
Crystal Dimensions	0.21 X 0.18 X 0.27 mm
Crystal System	orthorhombic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	20 (20.1 - 27.9°)
Omega Scan Peak Width at Half-height	0.42°
Lattice Parameters	a = 33.248(6) $\AA$ b = 16.832(5) $\AA$ c = 16.279(4) $\AA$ V = 9110(6) $\AA^3$
Space Group	Pbca (#61)
Z value	8
D_{calc}	1.403 g/cm^3
F_{000}	3968.00
μ(MoKα)	8.84 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC7R (rotating anode)
Radiation	MoKα (λ = 0.71069 $\AA$) graphite monochromated
Attenuator	Zr foil (factor = 8.71)

Temperature	20.0 °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	400 mm
Scan Type	ω-2θ
Scan Rate	16.0°/min (in ω) (up to 3 scans)
Scan Width	(0.73 + 0.30 tan θ)°
$2\theta_{max}$	60.0°
No. of Reflections Measured	Total: 11611
Corrections	Lorentz-polarization Absorption (trans. factors: 0.3770 - 0.8529) Decay (0.37% increase)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXS-86)
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	0.0070
Anomalous Dispersion	All non-hydrogen atoms
No. of Observations (I>3.00σ(I), 2θ<0.00°)	3727
No. Variables	740
Reflection/Parameter Ratio	5.04
Residuals: R; Rw	0.041 ; 0.033
Residuals: R1	0.041
No. of Reflections to calc R1	3727

Goodness of Fit Indicator	1.51
Max Shift/Error in Final Cycle	5.452
Maximum peak in Final Diff. Map	0.22 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.17 $e^-/\AA^3$

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

atom	x	y	z	B_{eq}
Ni(1)	0.83690(2)	0.19531(4)	0.23093(4)	4.48(2)
Ni(2)	0.58512(2)	0.25019(5)	0.06842(5)	5.36(2)
N(1)	0.8681(1)	0.1388(3)	0.3266(3)	5.0(1)
N(2)	0.8961(1)	0.1965(3)	0.1876(3)	5.6(1)
N(3)	0.8354(1)	0.3026(3)	0.2968(3)	4.7(1)
N(4)	0.8058(2)	0.4200(3)	0.3036(3)	5.3(1)
N(5)	0.8123(1)	0.2693(3)	0.1430(3)	4.8(1)
N(6)	0.7781(1)	0.3850(3)	0.1245(3)	5.4(1)
N(7)	0.7810(1)	0.1613(3)	0.2768(3)	4.2(1)
N(8)	0.7351(1)	0.0625(3)	0.2830(3)	5.6(1)
N(9)	0.8280(1)	0.0883(3)	0.1650(3)	4.5(1)
N(10)	0.7853(1)	-0.0089(3)	0.1391(3)	4.8(1)
N(11)	0.6416(2)	0.1985(3)	0.0456(3)	6.3(2)
N(12)	0.6207(2)	0.2980(3)	0.1630(3)	5.8(2)
N(13)	0.5895(2)	0.3552(3)	0.0001(3)	5.3(1)
N(14)	0.5577(2)	0.4654(3)	-0.0413(3)	5.5(2)
N(15)	0.5329(1)	0.3080(3)	0.1037(3)	5.1(1)
N(16)	0.4916(2)	0.4113(3)	0.0837(3)	5.5(1)
N(17)	0.5570(1)	0.1955(3)	-0.0306(3)	4.9(1)
N(18)	0.5180(1)	0.0959(3)	-0.0726(3)	5.2(1)
N(19)	0.5665(1)	0.1449(3)	0.1250(3)	5.1(1)
N(20)	0.5308(1)	0.0314(3)	0.1068(3)	5.0(1)
C(1)	0.8528(2)	0.1195(4)	0.3992(4)	6.0(2)
C(2)	0.8753(3)	0.0896(5)	0.4630(5)	7.7(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(3)	0.9153(3)	0.0793(6)	0.4491(6)	9.5(3)
C(4)	0.9320(2)	0.0975(5)	0.3751(6)	8.1(3)
C(5)	0.9077(2)	0.1281(4)	0.3122(4)	5.6(2)
C(6)	0.9216(2)	0.1524(4)	0.2312(5)	6.0(2)
C(7)	0.9593(2)	0.1303(5)	0.2011(6)	8.6(3)
C(8)	0.9691(3)	0.1571(7)	0.1229(7)	10.4(4)
C(9)	0.9442(3)	0.2019(6)	0.0805(6)	9.4(3)
C(10)	0.9074(2)	0.2212(4)	0.1141(5)	7.1(2)
C(11)	0.8138(2)	0.3561(4)	0.2570(3)	4.5(2)
C(12)	0.8012(2)	0.3393(4)	0.1737(4)	4.7(2)
C(13)	0.8415(2)	0.3340(4)	0.3744(4)	5.6(2)
C(14)	0.8237(2)	0.4048(4)	0.3781(4)	5.9(2)
C(15)	0.7959(2)	0.2702(4)	0.0660(4)	5.7(2)
C(16)	0.7751(2)	0.3387(5)	0.0555(4)	6.4(2)
C(17)	0.7688(2)	0.0907(3)	0.2480(3)	4.2(1)
C(18)	0.7931(2)	0.0552(3)	0.1850(3)	4.1(1)
C(19)	0.7530(2)	0.1808(4)	0.3346(4)	5.1(2)
C(20)	0.7259(2)	0.1212(5)	0.3378(4)	6.1(2)
C(21)	0.8431(2)	0.0414(4)	0.1032(4)	5.0(2)
C(22)	0.8179(2)	-0.0178(4)	0.0874(4)	5.5(2)
C(23)	0.6487(2)	0.1441(6)	-0.0101(5)	7.8(3)
C(24)	0.6840(3)	0.1005(6)	-0.0139(6)	9.3(3)
C(25)	0.7126(3)	0.1154(8)	0.0443(7)	11.3(4)
C(26)	0.7053(3)	0.1722(7)	0.1024(6)	10.5(4)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(27)	0.6696(2)	0.2142(5)	0.1041(5)	6.7(2)
C(28)	0.6586(3)	0.2746(5)	0.1630(4)	6.7(2)
C(29)	0.6868(3)	0.3102(7)	0.2164(6)	8.9(3)
C(30)	0.6749(4)	0.3680(8)	0.2663(6)	10.8(4)
C(31)	0.6361(3)	0.3934(5)	0.2672(5)	8.7(3)
C(32)	0.6100(2)	0.3564(5)	0.2133(5)	7.2(2)
C(33)	0.5572(2)	0.4022(4)	0.0095(4)	5.0(2)
C(34)	0.5267(2)	0.3767(4)	0.0659(4)	4.9(2)
C(35)	0.6117(2)	0.3915(5)	-0.0604(5)	6.0(2)
C(36)	0.5926(2)	0.4578(5)	-0.0866(4)	6.2(2)
C(37)	0.4992(2)	0.2963(4)	0.1498(4)	5.7(2)
C(38)	0.4741(2)	0.3578(5)	0.1372(4)	6.1(2)
C(39)	0.5389(2)	0.1281(4)	-0.0095(4)	4.4(2)
C(40)	0.5443(2)	0.0997(4)	0.0744(4)	4.3(2)
C(41)	0.5471(2)	0.2060(4)	-0.1118(4)	5.7(2)
C(42)	0.5239(2)	0.1463(5)	-0.1374(4)	6.1(2)
C(43)	0.5671(2)	0.1012(5)	0.1956(4)	5.9(2)
C(44)	0.5461(2)	0.0338(4)	0.1854(4)	6.0(2)
H(1)	0.824(1)	0.130(3)	0.405(3)	4(1)
H(2)	0.864(3)	0.075(5)	0.527(5)	19.7(6)
H(3)	0.930(2)	0.062(4)	0.489(4)	8.9(9)
H(4)	0.960(2)	0.097(4)	0.361(4)	9.4(9)
H(5)	0.974(2)	0.092(4)	0.233(4)	10.0(8)
H(6)	0.991(2)	0.138(4)	0.100(4)	11.7(7)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(7)	0.946(2)	0.228(3)	0.028(3)	6(1)
H(8)	0.889(1)	0.257(2)	0.089(2)	2.6(10)
H(9)	0.856(1)	0.305(3)	0.412(3)	4(1)
H(10)	0.825(1)	0.443(3)	0.416(3)	4(1)
H(11)	0.798(1)	0.224(3)	0.035(3)	4(1)
H(12)	0.764(2)	0.361(3)	0.009(3)	8(1)
H(13)	0.793(1)	0.470(3)	0.289(3)	4(1)
H(14)	0.755(1)	0.230(2)	0.357(2)	3(1)
H(15)	0.703(1)	0.119(3)	0.362(3)	5(1)
H(16)	0.868(1)	0.053(2)	0.081(3)	3.5(10)
H(17)	0.818(1)	-0.057(3)	0.055(3)	3(1)
H(18)	0.766(2)	-0.039(3)	0.140(4)	7.4(9)
H(19)	0.630(2)	0.140(3)	-0.055(3)	7(1)
H(20)	0.687(2)	0.058(3)	-0.056(4)	7.7(9)
H(21)	0.738(2)	0.089(4)	0.039(4)	10.7(8)
H(22)	0.721(2)	0.185(5)	0.148(4)	11.2(8)
H(23)	0.708(2)	0.282(4)	0.212(4)	8.2(8)
H(24)	0.692(2)	0.396(5)	0.300(5)	14.4(6)
H(25)	0.624(3)	0.449(5)	0.297(5)	19.1(6)
H(26)	0.582(2)	0.376(3)	0.204(4)	7.9(10)
H(27)	0.635(1)	0.360(3)	-0.076(3)	4(1)
H(28)	0.598(2)	0.502(3)	-0.125(3)	6(1)
H(29)	0.496(1)	0.246(3)	0.177(3)	4(1)
H(30)	0.451(1)	0.365(3)	0.159(3)	3(1)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(31)	0.531(3)	0.517(6)	-0.053(5)	20.4(6)
H(32)	0.560(1)	0.248(3)	-0.139(3)	6(1)
H(33)	0.511(2)	0.134(3)	-0.189(3)	7(1)
H(34)	0.580(2)	0.123(3)	0.235(3)	5(1)
H(35)	0.544(2)	-0.008(3)	0.220(3)	6(1)
H(36)	0.506(2)	0.045(4)	-0.083(4)	10.2(9)

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni(1)	0.0476(4)	0.0707(5)	0.0518(4)	0.0012(4)	0.0012(4)	-0.0007(4)
Ni(2)	0.0582(4)	0.0809(5)	0.0647(5)	-0.0069(5)	-0.0088(4)	0.0062(5)
N(1)	0.058(3)	0.074(4)	0.059(3)	0.004(3)	-0.006(3)	0.006(3)
N(2)	0.052(3)	0.097(4)	0.061(3)	-0.013(3)	0.012(3)	-0.002(3)
N(3)	0.058(3)	0.069(3)	0.052(3)	0.004(3)	-0.010(2)	0.003(3)
N(4)	0.079(4)	0.066(4)	0.055(3)	0.014(3)	-0.017(3)	-0.006(3)
N(5)	0.064(3)	0.073(4)	0.045(3)	0.009(3)	-0.002(3)	-0.001(3)
N(6)	0.078(4)	0.082(4)	0.046(3)	0.015(3)	-0.003(3)	-0.005(3)
N(7)	0.050(3)	0.066(3)	0.042(3)	0.002(2)	0.003(2)	-0.002(3)
N(8)	0.062(3)	0.087(4)	0.062(3)	-0.013(3)	0.015(3)	-0.014(3)
N(9)	0.046(3)	0.064(3)	0.061(3)	0.003(3)	0.009(2)	-0.003(3)
N(10)	0.056(4)	0.070(4)	0.057(3)	-0.004(3)	0.006(3)	-0.007(3)
N(11)	0.063(4)	0.100(5)	0.075(4)	0.007(4)	-0.002(3)	0.009(3)
N(12)	0.067(4)	0.090(4)	0.064(4)	-0.016(3)	-0.015(3)	0.012(3)
N(13)	0.052(3)	0.085(4)	0.065(3)	-0.018(3)	-0.001(3)	0.013(3)
N(14)	0.062(4)	0.080(4)	0.068(4)	-0.012(3)	-0.003(3)	0.013(3)
N(15)	0.060(3)	0.075(4)	0.061(3)	-0.008(3)	0.001(3)	0.002(3)
N(16)	0.068(4)	0.082(4)	0.058(3)	-0.002(3)	0.005(3)	0.003(3)
N(17)	0.054(3)	0.078(4)	0.056(3)	-0.004(3)	-0.008(3)	0.006(3)
N(18)	0.060(3)	0.076(4)	0.060(3)	-0.001(3)	-0.009(3)	-0.001(3)
N(19)	0.061(3)	0.074(4)	0.058(3)	-0.007(3)	-0.013(3)	0.001(3)
N(20)	0.056(3)	0.077(4)	0.057(3)	0.001(3)	-0.004(3)	0.003(3)
C(1)	0.073(5)	0.084(5)	0.072(5)	0.009(4)	-0.015(4)	0.011(4)
C(2)	0.104(6)	0.103(6)	0.087(6)	0.015(5)	-0.026(5)	0.024(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(3)	0.131(9)	0.123(7)	0.108(8)	0.028(7)	-0.051(7)	0.028(6)
C(4)	0.070(5)	0.118(7)	0.120(7)	0.022(5)	-0.024(6)	-0.002(6)
C(5)	0.056(4)	0.076(4)	0.083(5)	0.008(4)	-0.005(4)	-0.013(4)
C(6)	0.048(4)	0.093(5)	0.087(5)	0.001(4)	-0.003(4)	-0.028(5)
C(7)	0.068(6)	0.138(8)	0.122(8)	0.019(5)	0.013(5)	-0.030(6)
C(8)	0.070(7)	0.19(1)	0.14(1)	-0.014(7)	0.033(7)	-0.061(9)
C(9)	0.091(7)	0.17(1)	0.098(8)	-0.014(7)	0.030(6)	-0.013(7)
C(10)	0.062(5)	0.105(7)	0.102(7)	-0.001(4)	0.014(5)	-0.010(5)
C(11)	0.060(4)	0.064(4)	0.046(4)	0.000(3)	-0.003(3)	-0.008(3)
C(12)	0.060(4)	0.067(4)	0.050(4)	0.002(3)	0.005(3)	0.000(4)
C(13)	0.072(5)	0.083(6)	0.057(4)	0.005(4)	-0.015(4)	0.005(4)
C(14)	0.089(5)	0.081(6)	0.056(5)	-0.001(5)	-0.016(4)	-0.012(4)
C(15)	0.076(5)	0.082(6)	0.057(4)	0.011(4)	0.003(4)	-0.023(4)
C(16)	0.090(5)	0.106(6)	0.046(4)	0.022(5)	-0.005(4)	-0.010(4)
C(17)	0.047(4)	0.066(4)	0.045(3)	0.002(3)	-0.003(3)	-0.005(3)
C(18)	0.053(4)	0.059(4)	0.042(3)	0.005(3)	-0.002(3)	0.000(3)
C(19)	0.066(4)	0.069(5)	0.058(4)	0.006(4)	0.004(3)	-0.017(4)
C(20)	0.058(5)	0.103(6)	0.072(5)	-0.009(5)	0.019(4)	-0.016(4)
C(21)	0.054(4)	0.080(5)	0.058(4)	0.006(4)	0.022(3)	-0.004(4)
C(22)	0.082(5)	0.074(5)	0.054(4)	-0.001(4)	0.013(4)	-0.006(4)
C(23)	0.063(5)	0.143(8)	0.091(6)	0.022(5)	-0.007(4)	0.011(6)
C(24)	0.097(7)	0.138(9)	0.118(8)	0.038(7)	-0.005(6)	0.005(6)
C(25)	0.083(7)	0.20(1)	0.14(1)	0.054(8)	-0.002(7)	0.043(9)
C(26)	0.090(8)	0.19(1)	0.118(9)	0.028(7)	-0.035(6)	0.029(8)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(27)	0.048(5)	0.122(7)	0.084(5)	-0.013(4)	-0.019(4)	0.041(5)
C(28)	0.081(6)	0.112(7)	0.064(5)	-0.026(5)	-0.017(4)	0.019(4)
C(29)	0.096(7)	0.16(1)	0.085(6)	-0.023(8)	-0.024(6)	0.034(7)
C(30)	0.14(1)	0.19(1)	0.082(7)	-0.077(9)	-0.026(8)	0.009(7)
C(31)	0.136(8)	0.128(8)	0.067(5)	-0.049(7)	-0.016(6)	0.004(5)
C(32)	0.100(6)	0.103(7)	0.070(5)	-0.019(6)	-0.016(5)	0.007(5)
C(33)	0.060(4)	0.068(5)	0.061(4)	-0.016(4)	-0.014(4)	0.003(4)
C(34)	0.062(4)	0.070(5)	0.053(4)	-0.010(4)	-0.004(4)	0.011(4)
C(35)	0.055(5)	0.089(6)	0.085(5)	-0.005(4)	-0.011(4)	0.003(5)
C(36)	0.064(5)	0.095(6)	0.079(5)	-0.022(4)	-0.004(4)	0.022(4)
C(37)	0.081(5)	0.075(5)	0.061(4)	-0.009(5)	-0.004(4)	0.002(4)
C(38)	0.068(5)	0.103(6)	0.062(5)	-0.006(5)	0.014(4)	0.000(4)
C(39)	0.037(3)	0.072(5)	0.059(4)	0.009(3)	0.001(3)	0.006(4)
C(40)	0.044(4)	0.064(4)	0.056(4)	0.009(3)	0.000(3)	0.006(4)
C(41)	0.064(4)	0.087(6)	0.066(5)	-0.012(4)	-0.004(4)	0.018(4)
C(42)	0.072(5)	0.097(6)	0.061(5)	-0.009(4)	-0.012(4)	0.013(5)
C(43)	0.080(5)	0.087(6)	0.055(5)	-0.003(4)	-0.013(4)	0.003(4)
C(44)	0.078(5)	0.078(5)	0.073(5)	0.004(4)	-0.009(4)	0.013(5)

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)	2.100(5)	Ni(1)	N(2)	2.090(4)
Ni(1)	N(3)	2.100(4)	Ni(1)	N(5)	2.066(4)
Ni(1)	N(7)	2.083(4)	Ni(1)	N(9)	2.117(4)
Ni(2)	N(11)	2.102(5)	Ni(2)	N(12)	2.102(5)
Ni(2)	N(13)	2.093(5)	Ni(2)	N(15)	2.071(5)
Ni(2)	N(17)	2.079(5)	Ni(2)	N(19)	2.090(5)
N(1)	C(1)	1.327(7)	N(1)	C(5)	1.347(7)
N(2)	C(6)	1.334(7)	N(2)	C(10)	1.321(8)
N(3)	C(11)	1.322(6)	N(3)	C(13)	1.384(7)
N(4)	C(11)	1.343(6)	N(4)	C(14)	1.375(7)
N(4)	H(13)	0.96(4)	N(5)	C(12)	1.333(6)
N(5)	C(15)	1.366(7)	N(6)	C(12)	1.349(6)
N(6)	C(16)	1.372(7)	N(7)	C(17)	1.340(6)
N(7)	C(19)	1.363(6)	N(8)	C(17)	1.344(6)
N(8)	C(20)	1.366(7)	N(9)	C(18)	1.327(6)
N(9)	C(21)	1.374(6)	N(10)	C(18)	1.338(6)
N(10)	C(22)	1.380(7)	N(10)	H(18)	0.81(5)
N(11)	C(23)	1.311(9)	N(11)	C(27)	1.357(7)
N(12)	C(28)	1.320(8)	N(12)	C(32)	1.328(8)
N(13)	C(33)	1.343(7)	N(13)	C(35)	1.374(8)
N(14)	C(33)	1.348(7)	N(14)	C(36)	1.380(7)
N(14)	H(31)	1.3(1)	N(15)	C(34)	1.326(6)
N(15)	C(37)	1.363(7)	N(16)	C(34)	1.338(7)
N(16)	C(38)	1.381(8)	N(17)	C(39)	1.330(6)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
N(17)	C(41)	1.374(7)	N(18)	C(39)	1.352(7)
N(18)	C(42)	1.367(7)	N(18)	H(36)	0.96(6)
N(19)	C(40)	1.344(6)	N(19)	C(43)	1.364(7)
N(20)	C(40)	1.343(6)	N(20)	C(44)	1.378(7)
C(1)	C(2)	1.374(9)	C(1)	H(1)	0.97(4)
C(2)	C(3)	1.36(1)	C(2)	H(2)	1.13(8)
C(3)	C(4)	1.36(1)	C(3)	H(3)	0.87(6)
C(4)	C(5)	1.403(9)	C(4)	H(4)	0.95(6)
C(5)	C(6)	1.457(8)	C(6)	C(7)	1.395(9)
C(7)	C(8)	1.39(1)	C(7)	H(5)	0.97(6)
C(8)	C(9)	1.32(1)	C(8)	H(6)	0.87(7)
C(9)	C(10)	1.38(1)	C(9)	H(7)	0.96(5)
C(10)	H(8)	0.96(4)	C(11)	C(12)	1.449(7)
C(13)	C(14)	1.332(8)	C(13)	H(9)	0.91(4)
C(14)	H(10)	0.90(4)	C(15)	C(16)	1.356(8)
C(15)	H(11)	0.93(4)	C(16)	H(12)	0.92(5)
C(17)	C(18)	1.436(7)	C(19)	C(20)	1.351(8)
C(19)	H(14)	0.91(4)	C(20)	H(15)	0.87(4)
C(21)	C(22)	1.328(8)	C(21)	H(16)	0.92(4)
C(22)	H(17)	0.85(4)	C(23)	C(24)	1.39(1)
C(23)	H(19)	0.97(5)	C(24)	C(25)	1.37(1)
C(24)	H(20)	1.00(5)	C(25)	C(26)	1.37(1)
C(25)	H(21)	0.97(6)	C(26)	C(27)	1.38(1)
C(26)	H(22)	0.93(6)	C(27)	C(28)	1.444(9)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(28)	C(29)	1.41(1)	C(29)	C(30)	1.33(1)
C(29)	H(23)	0.86(6)	C(30)	C(31)	1.36(1)
C(30)	H(24)	0.91(7)	C(31)	C(32)	1.383(10)
C(31)	H(25)	1.13(8)	C(32)	H(26)	0.99(5)
C(33)	C(34)	1.434(8)	C(35)	C(36)	1.352(8)
C(35)	H(27)	0.97(4)	C(36)	H(28)	1.00(5)
C(37)	C(38)	1.345(9)	C(37)	H(29)	0.96(4)
C(38)	H(30)	0.86(4)	C(39)	C(40)	1.457(7)
C(41)	C(42)	1.333(8)	C(41)	H(32)	0.93(5)
C(42)	H(33)	0.96(5)	C(43)	C(44)	1.342(8)
C(43)	H(34)	0.86(4)	C(44)	H(35)	0.91(5)

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Ni(1)	N(2)	77.9(2)	N(1)	Ni(1)	N(3)	91.3(2)
N(1)	Ni(1)	N(5)	169.3(2)	N(1)	Ni(1)	N(7)	92.9(2)
N(1)	Ni(1)	N(9)	93.4(2)	N(2)	Ni(1)	N(3)	100.7(2)
N(2)	Ni(1)	N(5)	97.6(2)	N(2)	Ni(1)	N(7)	164.5(2)
N(2)	Ni(1)	N(9)	88.2(2)	N(3)	Ni(1)	N(5)	80.0(2)
N(3)	Ni(1)	N(7)	91.9(2)	N(3)	Ni(1)	N(9)	170.6(2)
N(5)	Ni(1)	N(7)	93.5(2)	N(5)	Ni(1)	N(9)	96.1(2)
N(7)	Ni(1)	N(9)	79.8(2)	N(11)	Ni(2)	N(12)	77.6(2)
N(11)	Ni(2)	N(13)	101.1(2)	N(11)	Ni(2)	N(15)	172.7(2)
N(11)	Ni(2)	N(17)	94.7(2)	N(11)	Ni(2)	N(19)	89.5(2)
N(12)	Ni(2)	N(13)	91.5(2)	N(12)	Ni(2)	N(15)	95.1(2)
N(12)	Ni(2)	N(17)	172.3(2)	N(12)	Ni(2)	N(19)	99.7(2)
N(13)	Ni(2)	N(15)	79.0(2)	N(13)	Ni(2)	N(17)	89.6(2)
N(13)	Ni(2)	N(19)	166.1(2)	N(15)	Ni(2)	N(17)	92.7(2)
N(15)	Ni(2)	N(19)	91.6(2)	N(17)	Ni(2)	N(19)	80.4(2)
Ni(1)	N(1)	C(1)	125.6(4)	Ni(1)	N(1)	C(5)	114.4(4)
C(1)	N(1)	C(5)	119.7(6)	Ni(1)	N(2)	C(6)	114.5(4)
Ni(1)	N(2)	C(10)	125.3(5)	C(6)	N(2)	C(10)	118.4(6)
Ni(1)	N(3)	C(11)	110.4(4)	Ni(1)	N(3)	C(13)	142.2(4)
C(11)	N(3)	C(13)	105.4(5)	C(11)	N(4)	C(14)	105.2(5)
C(11)	N(4)	H(13)	129(2)	C(14)	N(4)	H(13)	124(2)
Ni(1)	N(5)	C(12)	112.5(4)	Ni(1)	N(5)	C(15)	143.2(5)
C(12)	N(5)	C(15)	102.8(5)	C(12)	N(6)	C(16)	101.8(5)
Ni(1)	N(7)	C(17)	112.9(4)	Ni(1)	N(7)	C(19)	142.2(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(17)	N(7)	C(19)	104.4(5)	C(17)	N(8)	C(20)	102.0(5)
Ni(1)	N(9)	C(18)	110.8(4)	Ni(1)	N(9)	C(21)	144.0(4)
C(18)	N(9)	C(21)	104.9(5)	C(18)	N(10)	C(22)	106.1(5)
C(18)	N(10)	H(18)	130(4)	C(22)	N(10)	H(18)	123(4)
Ni(2)	N(11)	C(23)	124.9(5)	Ni(2)	N(11)	C(27)	114.1(5)
C(23)	N(11)	C(27)	119.9(7)	Ni(2)	N(12)	C(28)	115.0(5)
Ni(2)	N(12)	C(32)	125.7(5)	C(28)	N(12)	C(32)	118.5(7)
Ni(2)	N(13)	C(33)	112.4(4)	Ni(2)	N(13)	C(35)	142.6(5)
C(33)	N(13)	C(35)	104.4(6)	C(33)	N(14)	C(36)	105.3(6)
C(33)	N(14)	H(31)	129(3)	C(36)	N(14)	H(31)	125(3)
Ni(2)	N(15)	C(34)	114.3(4)	Ni(2)	N(15)	C(37)	140.7(5)
C(34)	N(15)	C(37)	104.7(6)	C(34)	N(16)	C(38)	102.7(6)
Ni(2)	N(17)	C(39)	112.4(4)	Ni(2)	N(17)	C(41)	142.8(5)
C(39)	N(17)	C(41)	104.5(5)	C(39)	N(18)	C(42)	105.4(5)
C(39)	N(18)	H(36)	134(3)	C(42)	N(18)	H(36)	118(3)
Ni(2)	N(19)	C(40)	111.9(4)	Ni(2)	N(19)	C(43)	145.4(5)
C(40)	N(19)	C(43)	102.7(5)	C(40)	N(20)	C(44)	102.4(5)
N(1)	C(1)	C(2)	123.7(7)	N(1)	C(1)	H(1)	114(2)
C(2)	C(1)	H(1)	122(3)	C(1)	C(2)	C(3)	116.8(8)
C(1)	C(2)	H(2)	126(4)	C(3)	C(2)	H(2)	116(4)
C(2)	C(3)	C(4)	121.1(8)	C(2)	C(3)	H(3)	118(4)
C(4)	C(3)	H(3)	120(4)	C(3)	C(4)	C(5)	119.5(8)
C(3)	C(4)	H(4)	127(4)	C(5)	C(4)	H(4)	112(4)
N(1)	C(5)	C(4)	119.0(7)	N(1)	C(5)	C(6)	115.6(6)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(4)	C(5)	C(6)	125.4(7)	N(2)	C(6)	C(5)	115.8(6)
N(2)	C(6)	C(7)	122.2(7)	C(5)	C(6)	C(7)	122.0(8)
C(6)	C(7)	C(8)	116.6(9)	C(6)	C(7)	H(5)	116(4)
C(8)	C(7)	H(5)	126(4)	C(7)	C(8)	C(9)	121.2(10)
C(7)	C(8)	H(6)	117(5)	C(9)	C(8)	H(6)	120(5)
C(8)	C(9)	C(10)	119.1(10)	C(8)	C(9)	H(7)	133(3)
C(10)	C(9)	H(7)	107(3)	N(2)	C(10)	C(9)	122.6(8)
N(2)	C(10)	H(8)	113(2)	C(9)	C(10)	H(8)	123(2)
N(3)	C(11)	N(4)	112.2(5)	N(3)	C(11)	C(12)	118.9(6)
N(4)	C(11)	C(12)	128.9(6)	N(5)	C(12)	N(6)	116.1(5)
N(5)	C(12)	C(11)	116.3(6)	N(6)	C(12)	C(11)	127.5(6)
N(3)	C(13)	C(14)	108.6(6)	N(3)	C(13)	H(9)	118(3)
C(14)	C(13)	H(9)	132(3)	N(4)	C(14)	C(13)	108.6(6)
N(4)	C(14)	H(10)	119(3)	C(13)	C(14)	H(10)	131(3)
N(5)	C(15)	C(16)	109.3(6)	N(5)	C(15)	H(11)	116(2)
C(16)	C(15)	H(11)	133(3)	N(6)	C(16)	C(15)	110.0(6)
N(6)	C(16)	H(12)	118(3)	C(15)	C(16)	H(12)	130(3)
N(7)	C(17)	N(8)	114.7(5)	N(7)	C(17)	C(18)	116.6(5)
N(8)	C(17)	C(18)	128.7(6)	N(9)	C(18)	N(10)	111.8(5)
N(9)	C(18)	C(17)	119.5(5)	N(10)	C(18)	C(17)	128.7(6)
N(7)	C(19)	C(20)	107.7(6)	N(7)	C(19)	H(14)	116(2)
C(20)	C(19)	H(14)	134(2)	N(8)	C(20)	C(19)	111.2(6)
N(8)	C(20)	H(15)	117(3)	C(19)	C(20)	H(15)	130(3)
N(9)	C(21)	C(22)	110.1(6)	N(9)	C(21)	H(16)	119(2)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(22)	C(21)	H(16)	130(2)	N(10)	C(22)	C(21)	107.1(6)
N(10)	C(22)	H(17)	117(3)	C(21)	C(22)	H(17)	135(3)
N(11)	C(23)	C(24)	123.5(8)	N(11)	C(23)	H(19)	116(3)
C(24)	C(23)	H(19)	118(3)	C(23)	C(24)	C(25)	117.6(9)
C(23)	C(24)	H(20)	119(3)	C(25)	C(24)	H(20)	123(3)
C(24)	C(25)	C(26)	119.0(10)	C(24)	C(25)	H(21)	118(4)
C(26)	C(25)	H(21)	122(4)	C(25)	C(26)	C(27)	121.6(10)
C(25)	C(26)	H(22)	127(5)	C(27)	C(26)	H(22)	111(4)
N(11)	C(27)	C(26)	118.4(8)	N(11)	C(27)	C(28)	115.5(7)
C(26)	C(27)	C(28)	126.1(8)	N(12)	C(28)	C(27)	116.8(7)
N(12)	C(28)	C(29)	120.4(8)	C(27)	C(28)	C(29)	122.7(9)
C(28)	C(29)	C(30)	119.4(10)	C(28)	C(29)	H(23)	104(5)
C(30)	C(29)	H(23)	135(5)	C(29)	C(30)	C(31)	121(1)
C(29)	C(30)	H(24)	123(6)	C(31)	C(30)	H(24)	114(5)
C(30)	C(31)	C(32)	116.6(10)	C(30)	C(31)	H(25)	126(4)
C(32)	C(31)	H(25)	115(4)	N(12)	C(32)	C(31)	123.8(8)
N(12)	C(32)	H(26)	113(3)	C(31)	C(32)	H(26)	122(3)
N(13)	C(33)	N(14)	112.7(6)	N(13)	C(33)	C(34)	117.5(6)
N(14)	C(33)	C(34)	129.7(7)	N(15)	C(34)	N(16)	114.5(6)
N(15)	C(34)	C(33)	116.7(7)	N(16)	C(34)	C(33)	128.7(6)
N(13)	C(35)	C(36)	110.0(6)	N(13)	C(35)	H(27)	111(3)
C(36)	C(35)	H(27)	137(3)	N(14)	C(36)	C(35)	107.7(6)
N(14)	C(36)	H(28)	115(3)	C(35)	C(36)	H(28)	136(3)
N(15)	C(37)	C(38)	108.4(6)	N(15)	C(37)	H(29)	117(3)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(38)	C(37)	H(29)	132(3)	N(16)	C(38)	C(37)	109.7(6)
N(16)	C(38)	H(30)	123(3)	C(37)	C(38)	H(30)	127(3)
N(17)	C(39)	N(18)	112.1(5)	N(17)	C(39)	C(40)	117.7(6)
N(18)	C(39)	C(40)	130.1(6)	N(19)	C(40)	N(20)	115.4(5)
N(19)	C(40)	C(39)	117.2(6)	N(20)	C(40)	C(39)	127.4(6)
N(17)	C(41)	C(42)	110.1(6)	N(17)	C(41)	H(32)	116(3)
C(42)	C(41)	H(32)	132(3)	N(18)	C(42)	C(41)	107.9(6)
N(18)	C(42)	H(33)	117(3)	C(41)	C(42)	H(33)	134(3)
N(19)	C(43)	C(44)	110.1(6)	N(19)	C(43)	H(34)	114(3)
C(44)	C(43)	H(34)	135(3)	N(20)	C(44)	C(43)	109.4(6)
N(20)	C(44)	H(35)	121(3)	C(43)	C(44)	H(35)	128(3)