EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{45}H_{54}O_5N_{24}Co_2$
Formula Weight	1128.95
Crystal Color, Habit	red, prismatic
Crystal Dimensions	0.21 X 0.25 X 0.26 mm
Crystal System	orthorhombic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	12 (45.0 - 50.0°)
Omega Scan Peak Width at Half-height	0.32°
Lattice Parameters	a = 13.90(3) $\AA$ b = 31.2(1) $\AA$ c = 12.71(1) $\AA$ V = 5516(19) $\AA^3$
Space Group	$P2_12_12_1$ (#19)
Z value	4
D_{calc}	1.359 g/cm^3
F_{000}	2344.00
μ(CuKα)	52.63 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC7R (rotating anode)
Radiation	CuKα (λ = 1.54178 $\AA$) graphite monochromated
Attenuator	Ni foil (factor = 9.30)

Temperature	-123.0 °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	8.0°/min (in ω) (up to 5 scans)
Scan Width	(1.15 + 0.30 tan θ)°
$2\theta_{max}$	120.7°
No. of Reflections Measured	Total: 4214
Corrections	Lorentz-polarization Absorption (trans. factors: 0.4759 - 0.9918) Decay (0.37% increase) Secondary Extinction (coefficient: 1.37467e-06)

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	0.0600
Anomalous Dispersion	All non-hydrogen atoms
No. of Observations (I>3.00σ(I), 2θ<120.66°)	3327
No. Variables	686
Reflection/Parameter Ratio	4.85
Residuals: R; Rw	0.049 ; 0.068
Residuals: R1	0.049

No. of Reflections to calc R1	3327
Goodness of Fit Indicator	1.76
Max Shift/Error in Final Cycle	0.051
Maximum peak in Final Diff. Map	0.55 $e^-/\mathring{A}^3$
Minimum peak in Final Diff. Map	-0.44 $e^-/\mathring{A}^3$

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

atom	x	y	z	B_{eq}
Co(1)	0.39980(8)	0.31065(4)	0.4975(1)	3.32(3)
Co(2)	0.65570(8)	0.44463(4)	0.11454(9)	2.99(3)
O(1)	0.2654(4)	0.4093(2)	0.8762(4)	4.3(1)
O(4)	0.1890(4)	0.4493(2)	1.0568(5)	5.3(2)
O(6)	0.2312(4)	0.6615(2)	0.5143(5)	5.3(2)
O(7)	0.3415(4)	0.5792(2)	0.7635(6)	5.5(2)
O(8)	0.4056(6)	0.6701(3)	0.6049(5)	8.1(2)
N(1)	0.4464(4)	0.4422(2)	-0.1001(5)	3.9(2)
N(2)	0.3715(4)	0.4374(2)	0.1441(5)	3.8(2)
N(3)	0.7428(4)	0.3232(2)	0.1420(5)	3.4(1)
N(4)	0.4090(4)	0.2495(2)	0.4852(5)	3.3(1)
N(5)	0.6406(4)	0.3625(2)	0.6086(5)	3.8(2)
N(6)	0.6760(4)	0.3850(2)	0.0879(4)	3.1(1)
N(7)	0.7129(4)	0.4304(2)	0.2483(5)	3.0(1)
N(8)	0.3929(4)	0.3708(2)	0.5205(5)	3.4(1)
N(9)	0.7761(5)	0.3817(2)	0.3527(5)	3.8(2)
N(10)	0.3736(4)	0.1850(2)	0.5548(5)	3.3(1)
N(11)	0.5876(4)	0.4512(2)	-0.0166(5)	3.3(1)
N(12)	0.5295(4)	0.3195(2)	0.5481(5)	3.4(1)
N(13)	0.2715(4)	0.3117(2)	0.4420(5)	3.7(2)
N(14)	0.7796(4)	0.4578(2)	0.0572(5)	3.0(1)
N(16)	0.1758(5)	0.3266(2)	0.3071(5)	4.0(2)
N(17)	0.7462(4)	0.5644(2)	0.1647(5)	3.2(1)
N(18)	0.4706(5)	0.4325(2)	0.5590(5)	3.4(1)

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

atom	x	y	z	B_{eq}
N(20)	0.4318(5)	0.3182(2)	0.3515(5)	3.7(2)
N(21)	0.3053(5)	0.2470(2)	0.7474(5)	3.7(2)
N(22)	0.3851(5)	0.3265(2)	0.1856(5)	4.2(2)
N(24)	0.3553(5)	0.2968(2)	0.6365(5)	3.6(1)
N(25)	0.9021(4)	0.5030(2)	0.0458(5)	3.6(1)
N(26)	0.6576(4)	0.5037(2)	0.1498(5)	3.4(1)
N(27)	0.5282(4)	0.4373(2)	0.1699(5)	3.2(1)
C(1)	0.6051(6)	0.4520(2)	-0.1216(6)	3.4(2)
C(2)	0.7430(5)	0.5242(2)	0.1340(6)	2.9(2)
C(3)	0.4893(5)	0.4444(3)	-0.0066(7)	3.6(2)
C(4)	0.6089(6)	0.2949(3)	0.5756(7)	3.8(2)
C(5)	0.4750(5)	0.3903(2)	0.5498(6)	3.2(2)
C(6)	0.7394(5)	0.3896(2)	0.2565(5)	2.9(2)
C(7)	0.8111(5)	0.4966(3)	0.0795(5)	3.1(2)
C(8)	0.8530(5)	0.4369(2)	0.0059(6)	3.4(2)
C(9)	0.3725(5)	0.2277(3)	0.5664(6)	3.1(2)
C(10)	0.3863(6)	0.4332(3)	0.2496(7)	3.9(2)
C(11)	0.4607(5)	0.4392(3)	0.0978(6)	3.3(2)
C(12)	0.6017(5)	0.5350(3)	0.1974(6)	3.5(2)
C(13)	0.1792(6)	0.3132(3)	0.4789(6)	4.0(2)
C(14)	0.7323(5)	0.4496(3)	0.3426(6)	3.4(2)
C(15)	0.3590(6)	0.3233(3)	0.2876(6)	3.6(2)
C(16)	0.3418(5)	0.2548(2)	0.6512(6)	3.3(2)
C(17)	0.6699(5)	0.3560(3)	0.0074(6)	3.6(2)

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

atom	x	y	z	B_{eq}
C(18)	0.6559(6)	0.5717(3)	0.2059(6)	3.6(2)
C(19)	0.4845(6)	0.4331(3)	0.2662(6)	3.4(2)
C(20)	0.5190(6)	0.4469(3)	-0.1722(6)	4.2(2)
C(21)	0.2657(5)	0.3199(3)	0.3396(6)	3.6(2)
C(23)	0.5509(6)	0.3599(3)	0.5700(7)	3.8(2)
C(24)	0.2187(7)	0.4198(3)	0.7790(7)	4.7(2)
C(25)	0.9291(5)	0.4643(3)	-0.0010(7)	3.8(2)
C(26)	0.4135(6)	0.1798(3)	0.4558(7)	4.1(2)
C(27)	0.7723(6)	0.4202(3)	0.4055(6)	3.7(2)
C(28)	0.3284(5)	0.4034(3)	0.5069(6)	3.8(2)
C(29)	0.4881(6)	0.3252(3)	0.1892(6)	4.1(2)
C(30)	0.6773(6)	0.3220(3)	0.6137(8)	4.4(2)
C(31)	0.1217(6)	0.3219(3)	0.3958(7)	4.2(2)
C(32)	0.5142(6)	0.3198(3)	0.2889(7)	4.1(2)
C(33)	0.3757(5)	0.4419(3)	0.5322(6)	3.5(2)
C(34)	0.3261(6)	0.3167(3)	0.7257(6)	4.2(2)
C(35)	0.7115(6)	0.3188(3)	0.0416(6)	3.8(2)
C(36)	0.4362(5)	0.2190(3)	0.4130(6)	3.6(2)
C(37)	0.2951(6)	0.2872(3)	0.7950(7)	4.4(2)
C(38)	0.4272(6)	0.5573(3)	0.7992(9)	5.5(2)
C(39)	0.1262(7)	0.3945(4)	0.7752(9)	6.3(3)
C(40)	0.2012(7)	0.4663(3)	0.7705(8)	5.9(3)
C(41)	0.4292(8)	0.5545(3)	0.9178(9)	6.3(3)
C(42)	0.5142(7)	0.5787(4)	0.7571(10)	6.4(3)

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

atom	x	y	z	B_{eq}
C(43)	0.4867(8)	0.6985(5)	0.592(1)	9.0(4)
C(44)	0.510(1)	0.6963(10)	0.477(1)	19.8(9)
C(45)	0.465(1)	0.7422(6)	0.628(2)	13.8(7)
C(46)	0.7209(5)	0.3642(3)	0.1653(6)	3.3(2)
H(1)	0.3786	0.4372	-0.1153	4.1
H(2)	0.7700	0.3016	0.1856	3.7
H(3)	0.6749	0.3904	0.6285	4.3
H(4)	0.3544	0.1621	0.6041	3.6
H(5)	0.1528	0.3326	0.2347	4.8
H(6)	0.7975	0.5854	0.1569	3.3
H(7)	0.6678	0.4553	-0.1574	3.6
H(8)	0.6142	0.2635	0.5726	4.5
H(9)	0.8535	0.4069	-0.0233	4.6
H(10)	0.3361	0.4290	0.3038	3.7
H(11)	0.5345	0.5305	0.2248	3.6
H(12)	0.1555	0.3105	0.5565	5.2
H(13)	0.7215	0.4805	0.3610	3.5
H(14)	0.6427	0.3612	-0.0640	3.7
H(15)	0.6329	0.5996	0.2371	4.1
H(16)	0.5170	0.4317	0.3386	3.4
H(17)	0.5080	0.4481	-0.2508	5.0
H(18)	0.9915	0.4594	-0.0346	4.1
H(19)	0.4241	0.1517	0.4206	4.3
H(20)	0.7901	0.4243	0.4786	4.0

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

atom	x	y	z	B_{eq}
H(21)	0.2584	0.4017	0.4861	3.7
H(22)	0.5312	0.3278	0.1271	4.7
H(23)	0.7419	0.3170	0.6398	5.2
H(24)	0.0520	0.3264	0.3969	4.5
H(25)	0.5797	0.3204	0.3125	4.4
H(26)	0.3449	0.4712	0.5294	4.1
H(27)	0.3266	0.3492	0.7409	4.7
H(28)	0.7175	0.2935	-0.0038	4.2
H(29)	0.4685	0.2241	0.3420	4.1
H(30)	0.2706	0.2930	0.8684	5.1
H(31)	0.2578	0.4105	0.7178	4.7
H(32)	0.4234	0.5258	0.7735	6.9
H(33)	0.0858	0.4017	0.8354	6.5
H(34)	0.0889	0.3975	0.7138	6.5
H(35)	0.1389	0.3634	0.7838	6.5
H(36)	0.2609	0.4833	0.7768	6.0
H(37)	0.1720	0.4763	0.7051	6.0
H(38)	0.1599	0.4771	0.8264	6.0
H(39)	0.4797	0.5384	0.9478	6.6
H(40)	0.4312	0.5832	0.9476	6.6
H(41)	0.3685	0.5421	0.9485	6.6
H(42)	0.5690	0.5632	0.7798	7.3
H(43)	0.5092	0.5795	0.6849	7.3
H(44)	0.5130	0.6061	0.7878	7.3

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

atom	x	y	z	B_{eq}
H(45)	0.5434	0.6886	0.6270	10.7
H(46)	0.5271	0.6679	0.4536	18.3
H(47)	0.4565	0.7055	0.4331	18.3
H(48)	0.5641	0.7148	0.4558	18.3
H(49)	0.5235	0.7602	0.6114	12.9
H(50)	0.4159	0.7536	0.5832	12.9
H(51)	0.4527	0.7426	0.6953	12.9
H(52)	0.3948	0.6649	0.6777	6.7
H(53)	0.2807	0.6685	0.5216	6.7
H(54)	0.1885	0.6782	0.5227	6.7
H(55)	0.3384	0.6158	0.7673	6.7
H(56)	0.2298	0.3947	0.9273	6.7
H(57)	0.1696	0.4169	1.0766	6.7
H(58)	0.2115	0.4283	0.9791	6.7

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co(1)	0.0204(6)	0.0582(7)	0.0475(7)	-0.0033(6)	0.0032(6)	0.0011(7)
Co(2)	0.0158(6)	0.0599(7)	0.0378(7)	-0.0017(6)	-0.0002(5)	0.0027(6)
O(1)	0.033(3)	0.081(4)	0.049(3)	-0.004(3)	-0.001(3)	0.010(3)
O(4)	0.028(3)	0.093(4)	0.080(4)	0.008(3)	0.004(3)	-0.004(4)
O(6)	0.043(3)	0.100(5)	0.060(4)	0.001(3)	-0.001(3)	0.002(4)
O(7)	0.035(3)	0.079(4)	0.096(5)	0.010(3)	-0.006(4)	-0.007(4)
O(8)	0.064(5)	0.193(9)	0.052(4)	-0.007(5)	-0.004(4)	0.006(5)
N(1)	0.020(3)	0.080(5)	0.048(4)	-0.005(3)	-0.002(3)	0.003(4)
N(2)	0.027(4)	0.078(5)	0.038(4)	0.000(3)	0.003(3)	0.006(3)
N(3)	0.029(4)	0.061(4)	0.040(4)	0.007(3)	-0.002(3)	0.000(3)
N(4)	0.019(3)	0.070(4)	0.038(4)	0.000(3)	0.005(3)	-0.006(3)
N(5)	0.017(3)	0.067(4)	0.060(4)	-0.004(3)	-0.001(3)	-0.004(4)
N(6)	0.021(3)	0.066(4)	0.030(3)	-0.004(3)	-0.001(3)	0.002(3)
N(7)	0.023(3)	0.054(4)	0.035(3)	0.001(3)	0.000(3)	-0.001(3)
N(8)	0.016(3)	0.060(4)	0.051(4)	-0.003(3)	0.003(3)	0.000(3)
N(9)	0.032(3)	0.073(4)	0.038(4)	-0.001(3)	0.007(3)	-0.008(3)
N(10)	0.026(4)	0.058(4)	0.042(4)	-0.003(3)	0.001(3)	0.006(3)
N(11)	0.020(3)	0.064(4)	0.042(4)	-0.003(3)	-0.005(3)	0.004(3)
N(12)	0.019(3)	0.059(4)	0.051(4)	-0.002(3)	0.003(3)	0.000(3)
N(13)	0.016(3)	0.078(5)	0.045(4)	-0.013(3)	0.006(3)	-0.002(4)
N(14)	0.017(3)	0.051(4)	0.045(4)	-0.010(3)	-0.001(3)	0.004(3)
N(16)	0.027(4)	0.079(5)	0.045(4)	0.003(3)	-0.010(3)	0.000(4)
N(17)	0.021(3)	0.059(4)	0.040(3)	-0.002(3)	0.001(3)	0.003(3)
N(18)	0.025(3)	0.065(4)	0.040(4)	0.004(3)	-0.004(3)	0.003(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(20)	0.035(4)	0.059(4)	0.047(4)	0.002(3)	-0.002(3)	0.001(3)
N(21)	0.038(4)	0.054(4)	0.048(4)	0.003(3)	0.005(3)	-0.009(3)
N(22)	0.033(4)	0.076(5)	0.050(4)	-0.005(3)	0.005(4)	0.002(4)
N(24)	0.028(3)	0.059(4)	0.051(4)	0.006(3)	-0.001(3)	0.003(3)
N(25)	0.017(3)	0.072(4)	0.046(4)	0.005(3)	0.003(3)	-0.002(3)
N(26)	0.016(3)	0.065(4)	0.048(4)	0.006(3)	0.000(3)	0.012(3)
N(27)	0.026(3)	0.065(4)	0.032(3)	0.000(3)	-0.002(3)	0.005(3)
C(1)	0.032(4)	0.065(5)	0.031(4)	-0.013(4)	0.003(4)	-0.003(4)
C(2)	0.022(4)	0.049(4)	0.038(4)	-0.001(3)	-0.004(3)	0.003(4)
C(3)	0.020(4)	0.069(5)	0.047(5)	0.002(4)	0.001(4)	0.003(5)
C(4)	0.027(4)	0.057(5)	0.063(5)	0.006(4)	0.009(4)	0.002(4)
C(5)	0.020(4)	0.053(5)	0.048(5)	0.002(4)	0.007(4)	0.001(4)
C(6)	0.017(4)	0.063(5)	0.030(4)	0.002(4)	0.001(3)	0.002(3)
C(7)	0.015(4)	0.069(5)	0.032(4)	-0.001(4)	0.000(3)	0.010(4)
C(8)	0.014(4)	0.062(4)	0.052(5)	0.008(4)	-0.001(4)	-0.003(4)
C(9)	0.019(4)	0.060(5)	0.039(4)	0.000(3)	0.002(4)	0.000(4)
C(10)	0.023(4)	0.070(5)	0.056(5)	0.001(4)	0.002(4)	-0.004(4)
C(11)	0.018(4)	0.061(5)	0.047(5)	0.002(4)	0.000(4)	0.003(4)
C(12)	0.025(4)	0.072(5)	0.035(4)	0.003(4)	0.003(4)	0.004(4)
C(13)	0.023(4)	0.079(6)	0.050(5)	-0.005(4)	0.001(4)	-0.007(4)
C(14)	0.025(4)	0.073(5)	0.032(4)	0.017(4)	-0.002(4)	-0.004(4)
C(15)	0.024(4)	0.066(5)	0.046(5)	-0.005(4)	0.002(4)	0.000(4)
C(16)	0.022(4)	0.065(5)	0.038(4)	0.006(4)	-0.002(4)	0.006(4)
C(17)	0.024(4)	0.080(5)	0.033(4)	0.001(4)	0.002(4)	-0.006(4)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(18)	0.030(4)	0.066(5)	0.041(4)	0.007(4)	0.005(4)	-0.002(4)
C(19)	0.027(4)	0.067(5)	0.037(4)	-0.004(4)	0.002(4)	0.003(4)
C(20)	0.040(5)	0.079(6)	0.040(5)	0.004(5)	-0.004(4)	-0.001(4)
C(21)	0.017(4)	0.078(6)	0.044(5)	-0.001(4)	0.002(4)	0.006(4)
C(23)	0.024(4)	0.068(5)	0.053(5)	-0.006(4)	0.001(4)	0.007(4)
C(24)	0.048(6)	0.082(6)	0.047(5)	-0.005(5)	-0.001(5)	-0.003(5)
C(25)	0.018(4)	0.074(5)	0.053(5)	0.003(4)	0.007(4)	-0.015(5)
C(26)	0.027(5)	0.077(6)	0.053(5)	-0.004(4)	0.001(4)	-0.001(5)
C(27)	0.034(4)	0.075(5)	0.032(4)	-0.001(4)	-0.003(4)	-0.004(4)
C(28)	0.017(4)	0.078(5)	0.050(5)	-0.004(4)	-0.002(4)	0.005(5)
C(29)	0.030(4)	0.082(6)	0.045(5)	-0.015(4)	0.018(4)	-0.008(4)
C(30)	0.024(4)	0.066(5)	0.079(6)	0.005(4)	0.000(5)	0.005(5)
C(31)	0.037(5)	0.064(5)	0.060(5)	-0.012(4)	0.010(5)	-0.002(4)
C(32)	0.024(4)	0.082(6)	0.052(5)	-0.006(4)	0.021(4)	-0.001(5)
C(33)	0.024(4)	0.067(5)	0.044(5)	0.002(4)	-0.003(4)	0.004(4)
C(34)	0.042(5)	0.083(6)	0.035(4)	-0.004(5)	0.015(4)	-0.003(4)
C(35)	0.029(4)	0.069(5)	0.047(5)	0.005(4)	-0.002(4)	-0.003(4)
C(36)	0.019(4)	0.074(5)	0.046(5)	-0.004(4)	0.003(4)	0.003(4)
C(37)	0.041(5)	0.069(5)	0.057(5)	0.008(4)	0.011(5)	-0.001(5)
C(38)	0.032(5)	0.077(6)	0.101(8)	0.012(5)	-0.014(5)	-0.004(6)
C(39)	0.045(6)	0.100(7)	0.095(8)	0.008(5)	-0.020(6)	0.003(6)
C(40)	0.053(6)	0.085(7)	0.084(7)	0.012(5)	-0.008(6)	0.007(6)
C(41)	0.067(7)	0.071(6)	0.100(8)	0.021(6)	0.004(7)	0.009(6)
C(42)	0.033(5)	0.120(9)	0.091(8)	0.003(6)	-0.006(6)	-0.021(7)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(43)	0.039(6)	0.19(1)	0.11(1)	-0.033(8)	-0.019(7)	0.04(1)
C(44)	0.10(1)	0.54(5)	0.11(1)	-0.05(2)	0.04(1)	0.06(2)
C(45)	0.09(1)	0.18(2)	0.25(2)	-0.03(1)	-0.03(1)	0.09(2)
C(46)	0.019(4)	0.065(5)	0.040(4)	-0.001(4)	-0.001(4)	0.001(4)

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
Co(1)	N(4)	1.918(7)	Co(1)	N(8)	1.904(6)
Co(1)	N(12)	1.934(7)	Co(1)	N(13)	1.918(7)
Co(1)	N(20)	1.922(7)	Co(1)	N(24)	1.921(7)
Co(2)	N(6)	1.913(6)	Co(2)	N(7)	1.930(6)
Co(2)	N(11)	1.929(6)	Co(2)	N(14)	1.915(7)
Co(2)	N(26)	1.897(6)	Co(2)	N(27)	1.921(7)
O(1)	C(24)	1.43(1)	O(1)	H(56)	0.94
O(4)	H(57)	1.08	O(4)	H(58)	1.22
O(6)	H(53)	0.73	O(6)	H(54)	0.80
O(7)	C(38)	1.45(1)	O(7)	H(55)	1.14
O(8)	C(43)	1.45(1)	O(8)	H(52)	0.95
N(1)	C(3)	1.33(1)	N(1)	C(20)	1.37(1)
N(1)	H(1)	0.98	N(2)	C(10)	1.36(1)
N(2)	C(11)	1.374(10)	N(3)	C(35)	1.355(10)
N(3)	C(46)	1.347(10)	N(3)	H(2)	0.95
N(4)	C(9)	1.337(10)	N(4)	C(36)	1.38(1)
N(5)	C(23)	1.34(1)	N(5)	C(30)	1.37(1)
N(5)	H(3)	1.02	N(6)	C(17)	1.368(10)
N(6)	C(46)	1.334(9)	N(7)	C(6)	1.331(9)
N(7)	C(14)	1.365(9)	N(8)	C(5)	1.345(10)
N(8)	C(28)	1.368(10)	N(9)	C(6)	1.347(9)
N(9)	C(27)	1.38(1)	N(10)	C(9)	1.34(1)
N(10)	C(26)	1.38(1)	N(10)	H(4)	0.99
N(11)	C(1)	1.357(10)	N(11)	C(3)	1.389(10)

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

atom	atom	distance	atom	atom	distance
N(12)	C(4)	1.39(1)	N(12)	C(23)	1.33(1)
N(13)	C(13)	1.37(1)	N(13)	C(21)	1.330(10)
N(14)	C(7)	1.319(10)	N(14)	C(8)	1.375(9)
N(16)	C(21)	1.33(1)	N(16)	C(31)	1.36(1)
N(16)	H(5)	0.99	N(17)	C(2)	1.316(9)
N(17)	C(18)	1.379(10)	N(17)	H(6)	0.97
N(18)	C(5)	1.323(10)	N(18)	C(33)	1.39(1)
N(20)	C(15)	1.31(1)	N(20)	C(32)	1.40(1)
N(21)	C(16)	1.346(10)	N(21)	C(37)	1.40(1)
N(22)	C(15)	1.35(1)	N(22)	C(29)	1.43(1)
N(24)	C(16)	1.340(10)	N(24)	C(34)	1.356(10)
N(25)	C(7)	1.352(9)	N(25)	C(25)	1.398(10)
N(26)	C(2)	1.363(10)	N(26)	C(12)	1.388(10)
N(27)	C(11)	1.313(9)	N(27)	C(19)	1.373(10)
C(1)	C(20)	1.37(1)	C(1)	H(7)	0.99
C(2)	C(7)	1.45(1)	C(3)	C(11)	1.40(1)
C(4)	C(30)	1.36(1)	C(4)	H(8)	0.98
C(5)	C(23)	1.44(1)	C(6)	C(46)	1.43(1)
C(8)	C(25)	1.36(1)	C(8)	H(9)	1.01
C(9)	C(16)	1.43(1)	C(10)	C(19)	1.38(1)
C(10)	H(10)	0.99	C(12)	C(18)	1.37(1)
C(12)	H(11)	1.01	C(13)	C(31)	1.35(1)
C(13)	H(12)	1.04	C(14)	C(27)	1.34(1)
C(14)	H(13)	1.00	C(15)	C(21)	1.46(1)

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

atom	atom	distance	atom	atom	distance
C(17)	C(35)	1.37(1)	C(17)	H(14)	1.00
C(18)	H(15)	1.01	C(19)	H(16)	1.03
C(20)	H(17)	1.01	C(24)	C(39)	1.51(1)
C(24)	C(40)	1.48(1)	C(24)	H(31)	0.99
C(25)	H(18)	0.98	C(26)	C(36)	1.38(1)
C(26)	H(19)	0.99	C(27)	H(20)	0.97
C(28)	C(33)	1.41(1)	C(28)	H(21)	1.01
C(29)	C(32)	1.33(1)	C(29)	H(22)	0.99
C(30)	H(23)	0.97	C(31)	H(24)	0.98
C(32)	H(25)	0.96	C(33)	H(26)	1.01
C(34)	C(37)	1.35(1)	C(34)	H(27)	1.03
C(35)	H(28)	0.98	C(36)	H(29)	1.02
C(37)	H(30)	1.01	C(38)	C(41)	1.51(2)
C(38)	C(42)	1.48(1)	C(38)	H(32)	1.04
C(39)	H(33)	0.98	C(39)	H(34)	0.94
C(39)	H(35)	0.99	C(40)	H(36)	0.99
C(40)	H(37)	0.98	C(40)	H(38)	0.97
C(41)	H(39)	0.94	C(41)	H(40)	0.97
C(41)	H(41)	1.01	C(42)	H(42)	0.95
C(42)	H(43)	0.92	C(42)	H(44)	0.94
C(43)	C(44)	1.49(2)	C(43)	C(45)	1.47(2)
C(43)	H(45)	0.96	C(44)	H(46)	0.96
C(44)	H(47)	0.98	C(44)	H(48)	0.98
C(45)	H(49)	1.01	C(45)	H(50)	0.96

Table 3. Bond Lengths($\mathring{A}$) (continued)

atom	atom	distance	atom	atom	distance
C(45)	H(51)	0.87			

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(4)	Co(1)	N(8)	175.7(3)	N(4)	Co(1)	N(12)	96.1(3)
N(4)	Co(1)	N(13)	92.8(3)	N(4)	Co(1)	N(20)	91.7(3)
N(4)	Co(1)	N(24)	82.7(3)	N(8)	Co(1)	N(12)	81.6(3)
N(8)	Co(1)	N(13)	89.6(3)	N(8)	Co(1)	N(20)	92.2(3)
N(8)	Co(1)	N(24)	93.6(3)	N(12)	Co(1)	N(13)	170.6(3)
N(12)	Co(1)	N(20)	95.1(3)	N(12)	Co(1)	N(24)	91.5(3)
N(13)	Co(1)	N(20)	81.9(3)	N(13)	Co(1)	N(24)	92.4(3)
N(20)	Co(1)	N(24)	171.8(3)	N(6)	Co(2)	N(7)	82.6(3)
N(6)	Co(2)	N(11)	91.3(3)	N(6)	Co(2)	N(14)	90.5(3)
N(6)	Co(2)	N(26)	170.2(3)	N(6)	Co(2)	N(27)	94.9(3)
N(7)	Co(2)	N(11)	171.6(3)	N(7)	Co(2)	N(14)	90.8(3)
N(7)	Co(2)	N(26)	90.5(3)	N(7)	Co(2)	N(27)	91.8(3)
N(11)	Co(2)	N(14)	95.2(3)	N(11)	Co(2)	N(26)	96.2(3)
N(11)	Co(2)	N(27)	82.9(3)	N(14)	Co(2)	N(26)	82.5(3)
N(14)	Co(2)	N(27)	174.3(3)	N(26)	Co(2)	N(27)	92.4(3)
C(24)	O(1)	H(56)	118.0	H(57)	O(4)	H(58)	75.6
H(53)	O(6)	H(54)	119.5	C(38)	O(7)	H(55)	119.2
C(43)	O(8)	H(52)	109.8	C(3)	N(1)	C(20)	105.1(6)
C(3)	N(1)	H(1)	128.2	C(20)	N(1)	H(1)	126.6
C(10)	N(2)	C(11)	106.8(7)	C(35)	N(3)	C(46)	103.4(6)
C(35)	N(3)	H(2)	127.2	C(46)	N(3)	H(2)	129.3
Co(1)	N(4)	C(9)	114.7(5)	Co(1)	N(4)	C(36)	139.6(6)
C(9)	N(4)	C(36)	105.4(7)	C(23)	N(5)	C(30)	108.0(7)
C(23)	N(5)	H(3)	125.0	C(30)	N(5)	H(3)	127.0

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Co(2)	N(6)	C(17)	140.0(5)	Co(2)	N(6)	C(46)	114.3(5)
C(17)	N(6)	C(46)	105.1(6)	Co(2)	N(7)	C(6)	113.8(5)
Co(2)	N(7)	C(14)	139.0(5)	C(6)	N(7)	C(14)	107.2(6)
Co(1)	N(8)	C(5)	116.5(5)	Co(1)	N(8)	C(28)	138.4(5)
C(5)	N(8)	C(28)	104.8(6)	C(6)	N(9)	C(27)	105.6(7)
C(9)	N(10)	C(26)	102.9(7)	C(9)	N(10)	H(4)	130.2
C(26)	N(10)	H(4)	126.8	Co(2)	N(11)	C(1)	139.8(5)
Co(2)	N(11)	C(3)	112.8(5)	C(1)	N(11)	C(3)	105.6(6)
Co(1)	N(12)	C(4)	138.2(6)	Co(1)	N(12)	C(23)	114.5(5)
C(4)	N(12)	C(23)	107.1(7)	Co(1)	N(13)	C(13)	138.4(5)
Co(1)	N(13)	C(21)	114.8(5)	C(13)	N(13)	C(21)	105.7(7)
Co(2)	N(14)	C(7)	114.4(5)	Co(2)	N(14)	C(8)	138.2(5)
C(7)	N(14)	C(8)	107.0(6)	C(21)	N(16)	C(31)	104.2(7)
C(21)	N(16)	H(5)	128.3	C(31)	N(16)	H(5)	127.5
C(2)	N(17)	C(18)	103.8(6)	C(2)	N(17)	H(6)	129.5
C(18)	N(17)	H(6)	126.6	C(5)	N(18)	C(33)	103.4(7)
Co(1)	N(20)	C(15)	115.8(5)	Co(1)	N(20)	C(32)	138.1(6)
C(15)	N(20)	C(32)	106.1(7)	C(16)	N(21)	C(37)	105.5(7)
C(15)	N(22)	C(29)	103.7(7)	Co(1)	N(24)	C(16)	113.2(5)
Co(1)	N(24)	C(34)	139.8(6)	C(16)	N(24)	C(34)	106.8(7)
C(7)	N(25)	C(25)	104.9(7)	Co(2)	N(26)	C(2)	115.6(5)
Co(2)	N(26)	C(12)	141.3(5)	C(2)	N(26)	C(12)	102.8(6)
Co(2)	N(27)	C(11)	113.5(5)	Co(2)	N(27)	C(19)	138.2(5)
C(11)	N(27)	C(19)	108.1(6)	N(11)	C(1)	C(20)	107.6(7)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(11)	C(1)	H(7)	127.8	C(20)	C(1)	H(7)	124.6
N(17)	C(2)	N(26)	115.6(6)	N(17)	C(2)	C(7)	133.1(7)
N(26)	C(2)	C(7)	111.1(7)	N(1)	C(3)	N(11)	111.5(7)
N(1)	C(3)	C(11)	135.6(7)	N(11)	C(3)	C(11)	112.7(7)
N(12)	C(4)	C(30)	107.5(7)	N(12)	C(4)	H(8)	126.9
C(30)	C(4)	H(8)	125.5	N(8)	C(5)	N(18)	115.8(7)
N(8)	C(5)	C(23)	111.9(7)	N(18)	C(5)	C(23)	132.3(7)
N(7)	C(6)	N(9)	110.5(7)	N(7)	C(6)	C(46)	114.7(6)
N(9)	C(6)	C(46)	134.8(7)	N(14)	C(7)	N(25)	112.3(7)
N(14)	C(7)	C(2)	115.4(6)	N(25)	C(7)	C(2)	132.3(7)
N(14)	C(8)	C(25)	107.9(7)	N(14)	C(8)	H(9)	128.4
C(25)	C(8)	H(9)	123.6	N(4)	C(9)	N(10)	114.6(7)
N(4)	C(9)	C(16)	113.2(7)	N(10)	C(9)	C(16)	132.2(7)
N(2)	C(10)	C(19)	107.4(7)	N(2)	C(10)	H(10)	126.2
C(19)	C(10)	H(10)	126.2	N(2)	C(11)	N(27)	110.2(7)
N(2)	C(11)	C(3)	132.1(7)	N(27)	C(11)	C(3)	117.7(7)
N(26)	C(12)	C(18)	108.3(7)	N(26)	C(12)	H(11)	124.9
C(18)	C(12)	H(11)	126.7	N(13)	C(13)	C(31)	107.1(7)
N(13)	C(13)	H(12)	128.1	C(31)	C(13)	H(12)	124.6
N(7)	C(14)	C(27)	107.9(7)	N(7)	C(14)	H(13)	126.5
C(27)	C(14)	H(13)	125.6	N(20)	C(15)	N(22)	113.4(7)
N(20)	C(15)	C(21)	113.5(7)	N(22)	C(15)	C(21)	132.8(7)
N(21)	C(16)	N(24)	110.9(7)	N(21)	C(16)	C(9)	133.5(7)
N(24)	C(16)	C(9)	115.5(7)	N(6)	C(17)	C(35)	107.3(7)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(6)	C(17)	H(14)	126.7	C(35)	C(17)	H(14)	125.9
N(17)	C(18)	C(12)	109.4(7)	N(17)	C(18)	H(15)	125.4
C(12)	C(18)	H(15)	125.2	N(27)	C(19)	C(10)	107.5(7)
N(27)	C(19)	H(16)	127.6	C(10)	C(19)	H(16)	124.8
N(1)	C(20)	C(1)	110.0(7)	N(1)	C(20)	H(17)	123.6
C(1)	C(20)	H(17)	126.2	N(13)	C(21)	N(16)	113.0(7)
N(13)	C(21)	C(15)	113.8(7)	N(16)	C(21)	C(15)	133.0(7)
N(5)	C(23)	N(12)	110.0(7)	N(5)	C(23)	C(5)	134.9(8)
N(12)	C(23)	C(5)	115.1(7)	O(1)	C(24)	C(39)	107.1(8)
O(1)	C(24)	C(40)	111.1(8)	O(1)	C(24)	H(31)	111.1
C(39)	C(24)	C(40)	111.9(9)	C(39)	C(24)	H(31)	106.8
C(40)	C(24)	H(31)	108.7	N(25)	C(25)	C(8)	107.9(6)
N(25)	C(25)	H(18)	123.9	C(8)	C(25)	H(18)	128.1
N(10)	C(26)	C(36)	110.3(8)	N(10)	C(26)	H(19)	124.9
C(36)	C(26)	H(19)	124.8	N(9)	C(27)	C(14)	108.8(7)
N(9)	C(27)	H(20)	125.0	C(14)	C(27)	H(20)	126.0
N(8)	C(28)	C(33)	107.4(6)	N(8)	C(28)	H(21)	128.7
C(33)	C(28)	H(21)	123.8	N(22)	C(29)	C(32)	107.8(7)
N(22)	C(29)	H(22)	125.0	C(32)	C(29)	H(22)	127.1
N(5)	C(30)	C(4)	107.3(7)	N(5)	C(30)	H(23)	120.7
C(4)	C(30)	H(23)	132.0	N(16)	C(31)	C(13)	109.9(7)
N(16)	C(31)	H(24)	122.9	C(13)	C(31)	H(24)	127.0
N(20)	C(32)	C(29)	108.9(7)	N(20)	C(32)	H(25)	127.0
C(29)	C(32)	H(25)	123.7	N(18)	C(33)	C(28)	108.6(7)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(18)	C(33)	H(26)	126.9	C(28)	C(33)	H(26)	124.5
N(24)	C(34)	C(37)	109.3(8)	N(24)	C(34)	H(27)	127.2
C(37)	C(34)	H(27)	123.5	N(3)	C(35)	C(17)	110.4(7)
N(3)	C(35)	H(28)	127.5	C(17)	C(35)	H(28)	122.1
N(4)	C(36)	C(26)	106.8(7)	N(4)	C(36)	H(29)	126.9
C(26)	C(36)	H(29)	126.2	N(21)	C(37)	C(34)	107.4(7)
N(21)	C(37)	H(30)	126.5	C(34)	C(37)	H(30)	126.1
O(7)	C(38)	C(41)	110.8(9)	O(7)	C(38)	C(42)	110.3(9)
O(7)	C(38)	H(32)	107.8	C(41)	C(38)	C(42)	111.8(9)
C(41)	C(38)	H(32)	105.1	C(42)	C(38)	H(32)	110.8
C(24)	C(39)	H(33)	110.0	C(24)	C(39)	H(34)	116.3
C(24)	C(39)	H(35)	110.8	H(33)	C(39)	H(34)	108.0
H(33)	C(39)	H(35)	104.1	H(34)	C(39)	H(35)	106.7
C(24)	C(40)	H(36)	112.5	C(24)	C(40)	H(37)	116.3
C(24)	C(40)	H(38)	112.6	H(36)	C(40)	H(37)	104.3
H(36)	C(40)	H(38)	104.6	H(37)	C(40)	H(38)	105.4
C(38)	C(41)	H(39)	116.6	C(38)	C(41)	H(40)	109.7
C(38)	C(41)	H(41)	113.2	H(39)	C(41)	H(40)	108.1
H(39)	C(41)	H(41)	105.1	H(40)	C(41)	H(41)	103.2
C(38)	C(42)	H(42)	108.5	C(38)	C(42)	H(43)	108.1
C(38)	C(42)	H(44)	104.2	H(42)	C(42)	H(43)	112.2
H(42)	C(42)	H(44)	110.6	H(43)	C(42)	H(44)	112.9
O(8)	C(43)	C(44)	104(1)	O(8)	C(43)	C(45)	111(1)
O(8)	C(43)	H(45)	112.9	C(44)	C(43)	C(45)	113(1)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(44)	C(43)	H(45)	105.0	C(45)	C(43)	H(45)	108.6
C(43)	C(44)	H(46)	113.7	C(43)	C(44)	H(47)	112.1
C(43)	C(44)	H(48)	114.3	H(46)	C(44)	H(47)	105.8
H(46)	C(44)	H(48)	105.7	H(47)	C(44)	H(48)	104.3
C(43)	C(45)	H(49)	106.5	C(43)	C(45)	H(50)	107.5
C(43)	C(45)	H(51)	111.3	H(49)	C(45)	H(50)	103.9
H(49)	C(45)	H(51)	110.9	H(50)	C(45)	H(51)	116.1
N(3)	C(46)	N(6)	113.8(7)	N(3)	C(46)	C(6)	131.6(7)
N(6)	C(46)	C(6)	114.5(7)				