EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$Co_2C_{45}H_{58}N_{24}O_5$
Formula Weight	1132.98
Crystal Color, Habit	red, prismatic
Crystal Dimensions	0.24 X 0.18 X 0.21 mm
Crystal System	orthorhombic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (57.1 - 59.3°)
Omega Scan Peak Width at Half-height	0.30°
Lattice Parameters	a = 13.917(4) $\AA$ b = 31.216(8) $\AA$ c = 12.721(5) $\AA$ V = 5526(2) $\AA^3$
Space Group	$P2_12_12_1$ (#19)
Z value	4
D_{calc}	1.362 g/cm^3
F_{000}	2360.00
μ(CuKα)	52.54 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	(0.73 + 0.30 tan θ)°
$2\theta_{max}$	120.2°
No. of Reflections Measured	Total: 4530 Unique: 4528 (R_{int} = 0.034)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.6697 - 0.9979) Decay (1.92% increase) Secondary Extinction (coefficient: 1.79293e-06)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
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	0.0500
Anomalous Dispersion	All non-hydrogen atoms
No. of Observations (I>3.00σ(I), 2θ<120.19°)	2913
No. Variables	686
Reflection/Parameter Ratio	4.25
Residuals: R; Rw	0.044 ; 0.051

Residuals: R1	0.044
No. of Reflections to calc R1	2913
Goodness of Fit Indicator	1.25
Max Shift/Error in Final Cycle	0.034
Maximum peak in Final Diff. Map	0.38 $e^-/\mathring{A}^3$
Minimum peak in Final Diff. Map	-0.31 $e^-/\mathring{A}^3$

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

atom	x	y	z	B_{eq}
Co(1)	0.15568(9)	-0.44457(4)	0.1145(1)	2.18(3)
Co(2)	0.09998(10)	0.18939(4)	0.0026(1)	2.59(3)
O(1)	0.7359(4)	0.4089(2)	0.3763(5)	3.5(1)
O(2)	0.4052(5)	0.1711(3)	0.3953(6)	6.8(2)
O(3)	0.3409(5)	0.0792(2)	0.2375(6)	5.2(2)
O(4)	0.2329(5)	0.1619(2)	0.4851(5)	4.2(2)
O(5)	0.3108(4)	0.0518(2)	0.4434(5)	4.5(2)
N(1)	0.1771(5)	-0.3849(2)	0.0864(5)	2.3(1)
N(2)	0.2427(5)	-0.3232(2)	0.1416(6)	2.8(2)
N(3)	0.2130(5)	-0.4300(2)	0.2493(5)	2.0(2)
N(4)	0.2771(5)	-0.3816(2)	0.3527(5)	2.4(2)
N(5)	0.2800(4)	-0.4576(2)	0.0552(5)	2.1(1)
N(6)	0.4014(5)	-0.5016(2)	0.0474(6)	2.6(2)
N(7)	0.1579(5)	-0.5046(2)	0.1492(5)	2.5(2)
N(8)	0.2464(5)	-0.5650(2)	0.1641(5)	2.7(2)
N(9)	0.0284(5)	-0.4372(2)	0.1698(6)	2.4(2)
N(10)	-0.1266(4)	-0.4372(2)	0.1447(6)	2.6(2)
N(11)	0.0873(5)	-0.4510(2)	-0.0151(5)	2.4(2)
N(12)	-0.0535(5)	-0.4422(2)	-0.1006(6)	3.3(2)
N(13)	0.1073(5)	0.1287(2)	-0.0206(5)	2.5(2)
N(14)	0.0300(5)	0.0675(2)	-0.0588(5)	2.2(2)
N(15)	-0.0290(5)	0.1817(2)	-0.0471(6)	2.7(2)
N(16)	-0.1394(5)	0.1369(2)	-0.1076(6)	2.9(2)
N(17)	0.1452(5)	0.2035(2)	-0.1364(5)	2.8(2)

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

atom	x	y	z	B_{eq}
N(18)	0.1954(5)	0.2532(2)	-0.2472(5)	2.8(2)
N(19)	0.0915(5)	0.2506(2)	0.0166(6)	2.2(2)
N(20)	0.1256(5)	0.3144(2)	-0.0542(6)	2.5(2)
N(21)	0.0667(5)	0.1812(2)	0.1480(6)	2.6(2)
N(22)	0.1117(5)	0.1733(2)	0.3128(6)	3.1(2)
N(23)	0.2274(5)	0.1878(2)	0.0567(5)	2.4(2)
N(24)	0.3236(5)	0.1736(2)	0.1960(6)	3.2(2)
C(1)	0.1701(6)	-0.3559(3)	0.0078(7)	2.6(2)
C(2)	0.2102(7)	-0.3188(3)	0.0407(7)	3.2(2)
C(3)	0.2325(6)	-0.4501(3)	0.3423(7)	2.5(2)
C(4)	0.2738(7)	-0.4202(3)	0.4073(7)	2.9(2)
C(5)	0.2217(6)	-0.3636(3)	0.1662(7)	2.5(2)
C(6)	0.2394(6)	-0.3892(3)	0.2566(7)	2.3(2)
C(7)	0.3539(6)	-0.4379(3)	0.0041(7)	2.8(2)
C(8)	0.4288(6)	-0.4647(3)	-0.0010(8)	2.7(2)
C(9)	0.1017(6)	-0.5351(3)	0.1970(7)	2.7(2)
C(10)	0.1565(7)	-0.5715(3)	0.2049(7)	2.6(2)
C(11)	0.3116(6)	-0.4969(2)	0.0803(6)	2.1(2)
C(12)	0.2423(5)	-0.5243(3)	0.1334(6)	2.1(2)
C(13)	-0.0165(7)	-0.4327(3)	0.2664(7)	2.6(2)
C(14)	-0.1119(7)	-0.4328(3)	0.2513(7)	2.8(2)
C(15)	0.1045(6)	-0.4516(3)	-0.1212(7)	2.5(2)
C(16)	0.0195(7)	-0.4469(3)	-0.1712(7)	3.4(2)
C(17)	-0.0407(6)	-0.4400(3)	0.0990(7)	2.3(2)

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

atom	x	y	z	B_{eq}
C(18)	-0.0089(6)	-0.4446(3)	-0.0074(7)	2.6(2)
C(19)	0.1717(6)	0.0961(3)	-0.0083(7)	2.9(2)
C(20)	0.1231(6)	0.0588(3)	-0.0321(6)	2.6(2)
C(21)	-0.1077(6)	0.2051(3)	-0.0737(7)	3.3(2)
C(22)	-0.1771(6)	0.1781(3)	-0.1126(9)	3.6(2)
C(23)	0.0246(6)	0.1099(3)	-0.0493(7)	2.5(2)
C(24)	-0.0500(6)	0.1402(3)	-0.0693(7)	2.6(2)
C(25)	0.1739(7)	0.1833(3)	-0.2267(8)	3.8(2)
C(26)	0.2054(7)	0.2134(3)	-0.2949(7)	3.2(2)
C(27)	0.0642(6)	0.2815(3)	0.0867(7)	2.6(2)
C(28)	0.0861(6)	0.3206(3)	0.0429(7)	2.6(2)
C(29)	0.1583(6)	0.2450(3)	-0.1513(7)	2.5(2)
C(30)	0.1274(6)	0.2729(3)	-0.0665(6)	2.2(2)
C(31)	-0.0133(6)	0.1799(3)	0.2095(8)	3.1(2)
C(32)	0.0141(6)	0.1750(3)	0.3106(8)	3.1(2)
C(33)	0.3200(6)	0.1864(3)	0.0228(7)	2.8(2)
C(34)	0.3765(6)	0.1784(3)	0.1059(8)	3.4(2)
C(35)	0.1409(7)	0.1772(3)	0.2111(7)	2.7(2)
C(36)	0.2344(6)	0.1797(3)	0.1610(7)	2.5(2)
C(37)	0.7819(7)	0.4200(3)	0.2790(8)	3.6(2)
C(38)	0.7970(8)	0.4667(3)	0.2703(10)	5.4(3)
C(39)	0.8742(8)	0.3950(3)	0.2738(9)	5.1(3)
C(40)	0.4865(10)	0.1971(6)	0.411(1)	8.7(5)
C(41)	0.513(1)	0.1949(10)	0.522(1)	19.5(9)

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

atom	x	y	z	B_{eq}
C(42)	0.464(1)	0.2417(6)	0.372(2)	12.4(7)
C(43)	0.4255(7)	0.0570(4)	0.2012(10)	4.9(3)
C(44)	0.5119(8)	0.0787(4)	0.241(1)	6.1(3)
C(45)	0.4279(9)	0.0550(4)	0.084(1)	6.3(3)
H(1)	0.1418	-0.3608	-0.0589	3.2
H(2)	0.2146	-0.2939	-0.0009	4.1
H(3)	0.2201	-0.4790	0.3593	3.0
H(4)	0.2961	-0.4250	0.4763	3.6
H(5)	0.2730	-0.3026	0.1843	3.4
H(6)	0.3516	-0.4095	-0.0238	3.4
H(7)	0.4897	-0.4589	-0.0324	3.2
H(8)	0.0372	-0.5319	0.2198	3.2
H(9)	0.1346	-0.5976	0.2356	3.1
H(10)	0.4401	-0.5265	0.0559	3.2
H(11)	0.0148	-0.4303	0.3326	3.2
H(12)	-0.1600	-0.4302	0.3047	3.4
H(13)	0.1656	-0.4547	-0.1533	3.0
H(14)	0.0120	-0.4467	-0.2456	4.1
H(15)	-0.1870	-0.4379	0.1099	3.3
H(16)	0.2372	0.0986	0.0131	3.4
H(17)	0.1505	0.0310	-0.0303	3.2
H(18)	-0.1122	0.2346	-0.0662	4.3
H(19)	-0.2387	0.1861	-0.1369	4.5
H(20)	-0.1706	0.1104	-0.1289	3.5

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

atom	x	y	z	B_{eq}
H(21)	0.1708	0.1534	-0.2395	4.5
H(22)	0.2307	0.2080	-0.3633	3.9
H(23)	0.0357	0.2772	0.1537	3.1
H(24)	0.0760	0.3478	0.0751	3.0
H(25)	0.1475	0.3363	-0.1031	3.0
H(26)	-0.0778	0.1820	0.1859	3.7
H(27)	-0.0276	0.1730	0.3701	3.7
H(28)	0.3411	0.1903	-0.0479	3.4
H(29)	0.4441	0.1757	0.1038	4.1
H(30)	0.1516	0.1702	0.3731	3.7
H(31)	0.7423	0.4109	0.2227	4.4
H(32)	0.8279	0.4726	0.2046	6.6
H(33)	0.8369	0.4761	0.3258	6.6
H(34)	0.7372	0.4808	0.2725	6.6
H(35)	0.8612	0.3654	0.2766	6.1
H(36)	0.9071	0.4017	0.2102	6.1
H(37)	0.9142	0.4028	0.3319	6.1
H(38)	0.6667	0.4151	0.4025	4.5
H(39)	0.5371	0.1839	0.3712	10.8
H(40)	0.5735	0.2076	0.5309	25.2
H(41)	0.4662	0.2060	0.5636	25.2
H(42)	0.5214	0.1638	0.5412	25.2
H(43)	0.4466	0.2391	0.3020	15.9
H(44)	0.5213	0.2573	0.3806	15.9

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

atom	x	y	z	B_{eq}
H(45)	0.4148	0.2522	0.4144	15.9
H(46)	0.3679	0.1458	0.3537	4.5
H(47)	0.4240	0.0286	0.2283	5.9
H(48)	0.5091	0.0813	0.3157	7.3
H(49)	0.5678	0.0635	0.2218	7.3
H(50)	0.5157	0.1072	0.2118	7.3
H(51)	0.4819	0.0389	0.0615	7.7
H(52)	0.3706	0.0417	0.0582	7.7
H(53)	0.4317	0.0832	0.0556	7.7
H(54)	0.3395	0.1049	0.2053	4.5

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co(1)	0.0284(7)	0.0328(7)	0.0215(7)	0.0009(7)	-0.0004(7)	-0.0020(7)
Co(2)	0.0322(7)	0.0328(7)	0.0336(8)	-0.0016(7)	0.0032(8)	0.0019(8)
O(1)	0.036(3)	0.057(4)	0.039(4)	0.002(3)	0.013(3)	0.002(4)
O(2)	0.053(5)	0.145(8)	0.060(5)	-0.016(5)	-0.006(5)	0.000(6)
O(3)	0.032(4)	0.066(5)	0.098(6)	0.005(4)	0.002(4)	0.013(5)
O(4)	0.062(4)	0.069(4)	0.026(4)	-0.002(4)	-0.005(4)	-0.003(4)
O(5)	0.038(4)	0.072(5)	0.059(5)	0.006(4)	-0.006(4)	0.003(4)
N(1)	0.028(4)	0.040(4)	0.019(4)	0.004(3)	0.001(3)	-0.002(3)
N(2)	0.037(4)	0.036(4)	0.034(5)	-0.006(4)	-0.005(4)	-0.002(4)
N(3)	0.033(4)	0.027(4)	0.018(4)	-0.001(3)	-0.001(3)	-0.001(3)
N(4)	0.035(4)	0.039(4)	0.019(4)	-0.001(3)	0.001(3)	-0.001(3)
N(5)	0.020(3)	0.037(4)	0.023(4)	-0.005(3)	0.001(3)	-0.004(3)
N(6)	0.029(4)	0.036(4)	0.034(4)	0.002(3)	-0.005(4)	0.002(4)
N(7)	0.030(4)	0.042(4)	0.021(4)	-0.012(4)	0.004(3)	-0.001(3)
N(8)	0.043(5)	0.041(5)	0.018(4)	0.000(4)	-0.001(4)	-0.001(4)
N(9)	0.032(4)	0.026(4)	0.034(4)	0.004(3)	0.006(4)	0.007(4)
N(10)	0.013(3)	0.043(4)	0.044(5)	0.003(3)	0.000(3)	0.002(4)
N(11)	0.035(4)	0.035(4)	0.021(4)	0.001(3)	-0.001(4)	-0.005(3)
N(12)	0.040(4)	0.045(4)	0.039(5)	0.005(4)	0.002(4)	-0.002(4)
N(13)	0.027(4)	0.035(4)	0.033(5)	-0.007(3)	-0.001(4)	0.003(4)
N(14)	0.031(4)	0.030(4)	0.024(4)	-0.001(3)	0.000(3)	-0.003(3)
N(15)	0.030(4)	0.033(4)	0.039(5)	0.005(3)	0.007(4)	0.002(4)
N(16)	0.033(4)	0.033(4)	0.045(5)	0.000(3)	-0.003(4)	0.008(4)
N(17)	0.041(4)	0.035(4)	0.030(5)	-0.012(4)	0.003(4)	-0.003(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(18)	0.050(5)	0.031(4)	0.025(4)	0.001(4)	0.002(4)	-0.007(4)
N(19)	0.029(4)	0.034(3)	0.022(4)	0.002(3)	0.001(4)	0.002(3)
N(20)	0.035(4)	0.027(4)	0.034(4)	-0.003(3)	-0.002(4)	0.007(4)
N(21)	0.029(4)	0.030(4)	0.040(5)	-0.004(3)	0.000(4)	-0.004(4)
N(22)	0.046(5)	0.038(4)	0.035(5)	-0.004(4)	0.003(4)	0.002(4)
N(23)	0.033(4)	0.024(4)	0.035(4)	-0.003(3)	0.008(4)	-0.003(4)
N(24)	0.036(4)	0.044(5)	0.043(5)	0.003(4)	0.006(4)	0.005(4)
C(1)	0.028(4)	0.040(5)	0.032(5)	-0.001(4)	0.001(5)	0.011(5)
C(2)	0.051(6)	0.042(6)	0.030(5)	0.003(5)	-0.001(5)	0.012(5)
C(3)	0.030(5)	0.039(5)	0.025(5)	-0.009(4)	-0.004(4)	0.008(4)
C(4)	0.043(5)	0.044(5)	0.025(5)	-0.004(5)	-0.002(5)	0.008(4)
C(5)	0.026(4)	0.037(5)	0.030(5)	-0.003(4)	0.001(4)	-0.002(4)
C(6)	0.029(5)	0.037(5)	0.022(5)	0.002(4)	0.009(4)	0.006(4)
C(7)	0.030(4)	0.043(5)	0.034(5)	-0.004(4)	0.002(5)	0.004(5)
C(8)	0.026(4)	0.042(5)	0.034(5)	-0.003(4)	0.007(5)	0.013(5)
C(9)	0.025(4)	0.049(5)	0.027(5)	0.001(4)	0.000(4)	-0.001(4)
C(10)	0.037(5)	0.034(5)	0.026(5)	-0.007(4)	0.002(5)	-0.003(4)
C(11)	0.027(5)	0.023(4)	0.028(5)	0.004(4)	-0.007(4)	-0.008(4)
C(12)	0.022(4)	0.041(5)	0.016(5)	-0.001(4)	-0.006(4)	0.006(4)
C(13)	0.045(6)	0.032(5)	0.021(5)	0.003(4)	0.005(4)	-0.004(4)
C(14)	0.043(6)	0.039(5)	0.023(5)	0.010(4)	0.005(5)	-0.004(4)
C(15)	0.032(5)	0.038(5)	0.023(5)	0.002(4)	0.007(5)	-0.002(4)
C(16)	0.052(6)	0.047(6)	0.031(5)	0.002(5)	-0.013(5)	-0.001(5)
C(17)	0.030(5)	0.029(5)	0.030(5)	0.002(4)	0.004(4)	0.001(4)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(18)	0.032(5)	0.040(5)	0.027(5)	-0.006(4)	0.000(4)	0.001(5)
C(19)	0.041(5)	0.037(5)	0.034(5)	0.005(4)	0.005(5)	0.009(5)
C(20)	0.039(5)	0.034(5)	0.028(5)	-0.001(4)	0.007(4)	0.007(4)
C(21)	0.031(5)	0.052(6)	0.042(6)	0.001(5)	0.004(5)	0.001(5)
C(22)	0.027(5)	0.046(5)	0.065(7)	0.003(4)	0.004(5)	0.004(6)
C(23)	0.032(5)	0.039(5)	0.023(5)	0.000(4)	0.001(4)	0.001(4)
C(24)	0.029(5)	0.045(5)	0.026(5)	0.002(4)	0.005(4)	0.002(4)
C(25)	0.056(7)	0.047(6)	0.040(6)	0.003(5)	0.016(5)	-0.014(5)
C(26)	0.056(6)	0.043(5)	0.021(5)	0.001(5)	0.010(5)	-0.004(5)
C(27)	0.021(4)	0.049(5)	0.029(5)	0.004(4)	0.006(4)	-0.007(5)
C(28)	0.035(5)	0.032(5)	0.032(5)	0.005(4)	0.000(4)	0.002(4)
C(29)	0.032(5)	0.032(5)	0.031(5)	-0.014(4)	0.006(5)	-0.001(4)
C(30)	0.031(5)	0.031(5)	0.022(5)	-0.001(4)	0.002(4)	0.002(4)
C(31)	0.026(5)	0.039(6)	0.053(7)	-0.006(4)	0.009(5)	-0.003(5)
C(32)	0.035(5)	0.043(6)	0.041(6)	-0.007(5)	0.019(5)	-0.007(5)
C(33)	0.026(5)	0.041(5)	0.038(6)	-0.005(4)	0.004(4)	-0.008(5)
C(34)	0.038(6)	0.043(5)	0.049(6)	-0.008(4)	0.008(5)	-0.003(5)
C(35)	0.039(5)	0.029(5)	0.033(5)	-0.004(4)	0.007(5)	0.001(4)
C(36)	0.032(5)	0.036(5)	0.027(5)	-0.002(4)	0.004(4)	-0.003(4)
C(37)	0.039(6)	0.059(6)	0.039(6)	-0.001(5)	0.015(5)	-0.005(5)
C(38)	0.068(8)	0.050(6)	0.088(10)	-0.001(6)	0.011(7)	0.020(7)
C(39)	0.058(7)	0.063(7)	0.073(8)	0.000(6)	0.022(6)	-0.013(6)
C(40)	0.055(8)	0.18(2)	0.09(1)	-0.02(1)	0.003(8)	-0.06(1)
C(41)	0.09(1)	0.55(4)	0.09(1)	-0.06(2)	-0.05(1)	-0.05(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(42)	0.13(1)	0.16(2)	0.18(2)	-0.03(1)	0.05(2)	-0.07(2)
C(43)	0.040(6)	0.064(7)	0.082(9)	-0.003(6)	0.007(6)	0.005(7)
C(44)	0.042(7)	0.098(9)	0.09(1)	0.014(7)	0.015(7)	0.016(9)
C(45)	0.087(9)	0.065(7)	0.087(10)	0.012(7)	-0.025(8)	-0.016(8)

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(1)	1.919(7)	Co(1)	N(3)	1.945(7)
Co(1)	N(5)	1.931(6)	Co(1)	N(7)	1.925(7)
Co(1)	N(9)	1.921(7)	Co(1)	N(11)	1.913(7)
Co(2)	N(13)	1.919(7)	Co(2)	N(15)	1.918(7)
Co(2)	N(17)	1.929(7)	Co(2)	N(19)	1.922(7)
Co(2)	N(21)	1.923(8)	Co(2)	N(23)	1.903(7)
O(1)	C(37)	1.44(1)	O(1)	H(38)	1.04
O(2)	C(40)	1.41(1)	O(2)	H(46)	1.08
O(3)	C(43)	1.44(1)	O(3)	H(54)	0.90
N(1)	C(1)	1.353(10)	N(1)	C(5)	1.363(10)
N(2)	C(2)	1.37(1)	N(2)	C(5)	1.334(10)
N(2)	H(5)	0.94	N(3)	C(3)	1.367(10)
N(3)	C(6)	1.330(10)	N(4)	C(4)	1.390(10)
N(4)	C(6)	1.35(1)	N(5)	C(7)	1.362(10)
N(5)	C(11)	1.344(9)	N(6)	C(8)	1.361(10)
N(6)	C(11)	1.326(10)	N(6)	H(10)	0.95
N(7)	C(9)	1.375(10)	N(7)	C(12)	1.341(10)
N(8)	C(10)	1.37(1)	N(8)	C(12)	1.331(10)
N(9)	C(13)	1.38(1)	N(9)	C(17)	1.32(1)
N(10)	C(14)	1.38(1)	N(10)	C(17)	1.332(10)
N(10)	H(15)	0.95	N(11)	C(15)	1.37(1)
N(11)	C(18)	1.357(10)	N(12)	C(16)	1.36(1)
N(12)	C(18)	1.34(1)	N(13)	C(19)	1.367(10)
N(13)	C(23)	1.344(10)	N(14)	C(20)	1.37(1)

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

atom	atom	distance	atom	atom	distance
N(14)	C(23)	1.330(10)	N(15)	C(21)	1.36(1)
N(15)	C(24)	1.36(1)	N(16)	C(22)	1.39(1)
N(16)	C(24)	1.34(1)	N(16)	H(20)	0.97
N(17)	C(25)	1.37(1)	N(17)	C(29)	1.321(9)
N(18)	C(26)	1.39(1)	N(18)	C(29)	1.35(1)
N(19)	C(27)	1.37(1)	N(19)	C(30)	1.361(10)
N(20)	C(28)	1.37(1)	N(20)	C(30)	1.304(10)
N(20)	H(25)	0.97	N(21)	C(31)	1.36(1)
N(21)	C(35)	1.31(1)	N(22)	C(32)	1.36(1)
N(22)	C(35)	1.36(1)	N(22)	H(30)	0.95
N(23)	C(33)	1.360(10)	N(23)	C(36)	1.35(1)
N(24)	C(34)	1.37(1)	N(24)	C(36)	1.33(1)
C(1)	C(2)	1.35(1)	C(1)	H(1)	0.95
C(2)	H(2)	0.94	C(3)	C(4)	1.37(1)
C(3)	H(3)	0.94	C(4)	H(4)	0.94
C(5)	C(6)	1.42(1)	C(7)	C(8)	1.34(1)
C(7)	H(6)	0.95	C(8)	H(7)	0.95
C(9)	C(10)	1.37(1)	C(9)	H(8)	0.95
C(10)	H(9)	0.95	C(11)	C(12)	1.45(1)
C(13)	C(14)	1.34(1)	C(13)	H(11)	0.95
C(14)	H(12)	0.96	C(15)	C(16)	1.35(1)
C(15)	H(13)	0.95	C(16)	H(14)	0.95
C(17)	C(18)	1.43(1)	C(19)	C(20)	1.38(1)
C(19)	H(16)	0.95	C(20)	H(17)	0.95

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

atom	atom	distance	atom	atom	distance
C(21)	C(22)	1.37(1)	C(21)	H(18)	0.93
C(22)	H(19)	0.95	C(23)	C(24)	1.43(1)
C(25)	C(26)	1.35(1)	C(25)	H(21)	0.95
C(26)	H(22)	0.95	C(27)	C(28)	1.37(1)
C(27)	H(23)	0.95	C(28)	H(24)	0.95
C(29)	C(30)	1.45(1)	C(31)	C(32)	1.35(1)
C(31)	H(26)	0.95	C(32)	H(27)	0.96
C(33)	C(34)	1.34(1)	C(33)	H(28)	0.95
C(34)	H(29)	0.94	C(35)	C(36)	1.45(1)
C(37)	C(38)	1.48(1)	C(37)	C(39)	1.50(1)
C(37)	H(31)	0.95	C(38)	H(32)	0.96
C(38)	H(33)	0.95	C(38)	H(34)	0.94
C(39)	H(35)	0.94	C(39)	H(36)	0.95
C(39)	H(37)	0.96	C(40)	C(41)	1.47(2)
C(40)	C(42)	1.51(2)	C(40)	H(39)	0.96
C(41)	H(40)	0.94	C(41)	H(41)	0.91
C(41)	H(42)	1.01	C(42)	H(43)	0.92
C(42)	H(44)	0.94	C(42)	H(45)	0.93
C(43)	C(44)	1.47(2)	C(43)	C(45)	1.50(2)
C(43)	H(47)	0.95	C(44)	H(48)	0.96
C(44)	H(49)	0.94	C(44)	H(50)	0.97
C(45)	H(51)	0.95	C(45)	H(52)	0.96
C(45)	H(53)	0.95			

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Co(1)	N(3)	82.8(3)	N(1)	Co(1)	N(5)	89.6(3)
N(1)	Co(1)	N(7)	169.9(3)	N(1)	Co(1)	N(9)	95.4(3)
N(1)	Co(1)	N(11)	91.0(3)	N(3)	Co(1)	N(5)	91.5(3)
N(3)	Co(1)	N(7)	91.1(3)	N(3)	Co(1)	N(9)	91.5(3)
N(3)	Co(1)	N(11)	171.0(3)	N(5)	Co(1)	N(7)	82.6(3)
N(5)	Co(1)	N(9)	174.5(3)	N(5)	Co(1)	N(11)	95.0(3)
N(7)	Co(1)	N(9)	92.7(3)	N(7)	Co(1)	N(11)	96.0(3)
N(9)	Co(1)	N(11)	82.5(3)	N(13)	Co(2)	N(15)	82.8(3)
N(13)	Co(2)	N(17)	93.9(3)	N(13)	Co(2)	N(19)	176.4(3)
N(13)	Co(2)	N(21)	91.7(3)	N(13)	Co(2)	N(23)	88.9(3)
N(15)	Co(2)	N(17)	91.8(3)	N(15)	Co(2)	N(19)	95.6(3)
N(15)	Co(2)	N(21)	94.3(3)	N(15)	Co(2)	N(23)	171.1(3)
N(17)	Co(2)	N(19)	83.0(3)	N(17)	Co(2)	N(21)	172.2(3)
N(17)	Co(2)	N(23)	91.9(3)	N(19)	Co(2)	N(21)	91.6(3)
N(19)	Co(2)	N(23)	92.8(3)	N(21)	Co(2)	N(23)	82.7(3)
C(37)	O(1)	H(38)	130.2	C(40)	O(2)	H(46)	150.9
C(43)	O(3)	H(54)	107.4	Co(1)	N(1)	C(1)	140.9(6)
Co(1)	N(1)	C(5)	113.9(5)	C(1)	N(1)	C(5)	104.9(7)
C(2)	N(2)	C(5)	104.0(7)	C(2)	N(2)	H(5)	128.5
C(5)	N(2)	H(5)	127.5	Co(1)	N(3)	C(3)	137.5(6)
Co(1)	N(3)	C(6)	113.5(6)	C(3)	N(3)	C(6)	108.9(7)
C(4)	N(4)	C(6)	106.8(7)	Co(1)	N(5)	C(7)	140.1(6)
Co(1)	N(5)	C(11)	113.1(5)	C(7)	N(5)	C(11)	106.2(7)
C(8)	N(6)	C(11)	108.3(7)	C(8)	N(6)	H(10)	125.7

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(11)	N(6)	H(10)	126.0	Co(1)	N(7)	C(9)	140.1(6)
Co(1)	N(7)	C(12)	115.2(5)	C(9)	N(7)	C(12)	104.3(7)
C(10)	N(8)	C(12)	102.3(7)	Co(1)	N(9)	C(13)	138.9(6)
Co(1)	N(9)	C(17)	114.4(6)	C(13)	N(9)	C(17)	106.5(7)
C(14)	N(10)	C(17)	107.6(7)	C(14)	N(10)	H(15)	126.3
C(17)	N(10)	H(15)	126.0	Co(1)	N(11)	C(15)	139.7(6)
Co(1)	N(11)	C(18)	114.4(6)	C(15)	N(11)	C(18)	104.2(7)
C(16)	N(12)	C(18)	103.3(7)	Co(2)	N(13)	C(19)	138.9(6)
Co(2)	N(13)	C(23)	115.4(5)	C(19)	N(13)	C(23)	105.4(7)
C(20)	N(14)	C(23)	103.2(7)	Co(2)	N(15)	C(21)	140.3(6)
Co(2)	N(15)	C(24)	112.9(5)	C(21)	N(15)	C(24)	106.7(7)
C(22)	N(16)	C(24)	107.2(7)	C(22)	N(16)	H(20)	127.3
C(24)	N(16)	H(20)	125.5	Co(2)	N(17)	C(25)	139.3(6)
Co(2)	N(17)	C(29)	113.6(6)	C(25)	N(17)	C(29)	107.0(7)
C(26)	N(18)	C(29)	105.2(7)	Co(2)	N(19)	C(27)	141.2(6)
Co(2)	N(19)	C(30)	114.5(5)	C(27)	N(19)	C(30)	104.2(6)
C(28)	N(20)	C(30)	104.9(7)	C(28)	N(20)	H(25)	127.2
C(30)	N(20)	H(25)	127.9	Co(2)	N(21)	C(31)	138.9(6)
Co(2)	N(21)	C(35)	114.2(6)	C(31)	N(21)	C(35)	106.8(8)
C(32)	N(22)	C(35)	105.9(8)	C(32)	N(22)	H(30)	127.1
C(35)	N(22)	H(30)	126.9	Co(2)	N(23)	C(33)	140.3(6)
Co(2)	N(23)	C(36)	115.2(6)	C(33)	N(23)	C(36)	103.7(7)
C(34)	N(24)	C(36)	101.9(8)	N(1)	C(1)	C(2)	108.4(8)
N(1)	C(1)	H(1)	125.6	C(2)	C(1)	H(1)	126.0

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(2)	C(2)	C(1)	110.0(8)	N(2)	C(2)	H(2)	125.9
C(1)	C(2)	H(2)	124.1	N(3)	C(3)	C(4)	107.0(7)
N(3)	C(3)	H(3)	126.9	C(4)	C(3)	H(3)	126.1
N(4)	C(4)	C(3)	107.6(7)	N(4)	C(4)	H(4)	126.2
C(3)	C(4)	H(4)	126.2	N(1)	C(5)	N(2)	112.8(8)
N(1)	C(5)	C(6)	114.1(7)	N(2)	C(5)	C(6)	133.1(8)
N(3)	C(6)	N(4)	109.7(7)	N(3)	C(6)	C(5)	115.7(8)
N(4)	C(6)	C(5)	134.6(8)	N(5)	C(7)	C(8)	109.2(7)
N(5)	C(7)	H(6)	124.8	C(8)	C(7)	H(6)	126.0
N(6)	C(8)	C(7)	106.8(7)	N(6)	C(8)	H(7)	126.8
C(7)	C(8)	H(7)	126.4	N(7)	C(9)	C(10)	106.9(7)
N(7)	C(9)	H(8)	126.9	C(10)	C(9)	H(8)	126.2
N(8)	C(10)	C(9)	110.9(7)	N(8)	C(10)	H(9)	125.0
C(9)	C(10)	H(9)	124.1	N(5)	C(11)	N(6)	109.5(7)
N(5)	C(11)	C(12)	115.5(7)	N(6)	C(11)	C(12)	135.0(7)
N(7)	C(12)	N(8)	115.6(7)	N(7)	C(12)	C(11)	112.4(7)
N(8)	C(12)	C(11)	131.9(7)	N(9)	C(13)	C(14)	108.6(8)
N(9)	C(13)	H(11)	125.9	C(14)	C(13)	H(11)	125.5
N(10)	C(14)	C(13)	106.8(8)	N(10)	C(14)	H(12)	127.0
C(13)	C(14)	H(12)	126.2	N(11)	C(15)	C(16)	108.0(8)
N(11)	C(15)	H(13)	125.6	C(16)	C(15)	H(13)	126.4
N(12)	C(16)	C(15)	110.7(8)	N(12)	C(16)	H(14)	124.8
C(15)	C(16)	H(14)	124.5	N(9)	C(17)	N(10)	110.6(7)
N(9)	C(17)	C(18)	115.2(7)	N(10)	C(17)	C(18)	134.2(8)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(11)	C(18)	N(12)	113.7(8)	N(11)	C(18)	C(17)	112.9(8)
N(12)	C(18)	C(17)	133.4(8)	N(13)	C(19)	C(20)	106.4(7)
N(13)	C(19)	H(16)	126.6	C(20)	C(19)	H(16)	127.0
N(14)	C(20)	C(19)	110.6(8)	N(14)	C(20)	H(17)	124.7
C(19)	C(20)	H(17)	124.7	N(15)	C(21)	C(22)	109.1(8)
N(15)	C(21)	H(18)	124.2	C(22)	C(21)	H(18)	126.8
N(16)	C(22)	C(21)	106.6(8)	N(16)	C(22)	H(19)	127.1
C(21)	C(22)	H(19)	126.3	N(13)	C(23)	N(14)	114.3(7)
N(13)	C(23)	C(24)	112.4(7)	N(14)	C(23)	C(24)	133.1(8)
N(15)	C(24)	N(16)	110.4(7)	N(15)	C(24)	C(23)	116.0(7)
N(16)	C(24)	C(23)	133.6(8)	N(17)	C(25)	C(26)	108.2(8)
N(17)	C(25)	H(21)	125.8	C(26)	C(25)	H(21)	126.0
N(18)	C(26)	C(25)	107.9(8)	N(18)	C(26)	H(22)	126.3
C(25)	C(26)	H(22)	125.8	N(19)	C(27)	C(28)	107.5(7)
N(19)	C(27)	H(23)	126.9	C(28)	C(27)	H(23)	125.6
N(20)	C(28)	C(27)	109.2(7)	N(20)	C(28)	H(24)	125.0
C(27)	C(28)	H(24)	125.8	N(17)	C(29)	N(18)	111.6(7)
N(17)	C(29)	C(30)	116.2(7)	N(18)	C(29)	C(30)	132.1(7)
N(19)	C(30)	N(20)	114.1(7)	N(19)	C(30)	C(29)	112.2(7)
N(20)	C(30)	C(29)	133.7(8)	N(21)	C(31)	C(32)	108.6(8)
N(21)	C(31)	H(26)	126.1	C(32)	C(31)	H(26)	125.3
N(22)	C(32)	C(31)	107.9(8)	N(22)	C(32)	H(27)	126.0
C(31)	C(32)	H(27)	126.1	N(23)	C(33)	C(34)	108.1(8)
N(23)	C(33)	H(28)	125.9	C(34)	C(33)	H(28)	125.9

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(24)	C(34)	C(33)	111.4(8)	N(24)	C(34)	H(29)	123.3
C(33)	C(34)	H(29)	125.3	N(21)	C(35)	N(22)	110.7(8)
N(21)	C(35)	C(36)	115.6(8)	N(22)	C(35)	C(36)	133.6(9)
N(23)	C(36)	N(24)	114.9(8)	N(23)	C(36)	C(35)	112.1(8)
N(24)	C(36)	C(35)	132.9(8)	O(1)	C(37)	C(38)	111.5(8)
O(1)	C(37)	C(39)	107.0(8)	O(1)	C(37)	H(31)	108.7
C(38)	C(37)	C(39)	112.7(9)	C(38)	C(37)	H(31)	108.8
C(39)	C(37)	H(31)	107.9	C(37)	C(38)	H(32)	108.6
C(37)	C(38)	H(33)	109.5	C(37)	C(38)	H(34)	109.4
H(32)	C(38)	H(33)	109.2	H(32)	C(38)	H(34)	109.5
H(33)	C(38)	H(34)	110.6	C(37)	C(39)	H(35)	110.0
C(37)	C(39)	H(36)	109.5	C(37)	C(39)	H(37)	109.3
H(35)	C(39)	H(36)	109.8	H(35)	C(39)	H(37)	109.4
H(36)	C(39)	H(37)	108.7	O(2)	C(40)	C(41)	107(1)
O(2)	C(40)	C(42)	108(1)	O(2)	C(40)	H(39)	105.6
C(41)	C(40)	C(42)	114(1)	C(41)	C(40)	H(39)	107.7
C(42)	C(40)	H(39)	112.4	C(40)	C(41)	H(40)	108.6
C(40)	C(41)	H(41)	111.5	C(40)	C(41)	H(42)	107.9
H(40)	C(41)	H(41)	114.5	H(40)	C(41)	H(42)	105.7
H(41)	C(41)	H(42)	108.2	C(40)	C(42)	H(43)	106.6
C(40)	C(42)	H(44)	104.9	C(40)	C(42)	H(45)	106.9
H(43)	C(42)	H(44)	112.2	H(43)	C(42)	H(45)	113.7
H(44)	C(42)	H(45)	111.8	O(3)	C(43)	C(44)	109.7(9)
O(3)	C(43)	C(45)	111.0(10)	O(3)	C(43)	H(47)	108.2

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(44)	C(43)	C(45)	110(1)	C(44)	C(43)	H(47)	108.9
C(45)	C(43)	H(47)	108.9	C(43)	C(44)	H(48)	110.5
C(43)	C(44)	H(49)	110.7	C(43)	C(44)	H(50)	109.7
H(48)	C(44)	H(49)	109.5	H(48)	C(44)	H(50)	107.8
H(49)	C(44)	H(50)	108.6	C(43)	C(45)	H(51)	109.7
C(43)	C(45)	H(52)	109.8	C(43)	C(45)	H(53)	109.8
H(51)	C(45)	H(52)	109.1	H(51)	C(45)	H(53)	109.6
H(52)	C(45)	H(53)	108.8				