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Table 1. Crystal data and structure refinement for Co(tmmda)(3,6-DBSQ)(3,6-DBCat).

Empirical formula	$C_{33}H_{54}CoN_2O_4$
Formula weight	601.71
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 17.916(6) A alpha = 90.00(2) deg. b = 10.525(2) A beta = 104.51(3) deg. c = 19.174(5) A gamma = 90.00(2) deg.
Volume	3500(2) A^3
Z	4
Density (calculated)	1.142 Mg/m^3
Absorption coefficient	0.525 mm^{-1}
F(000)	1300
Crystal size	0.54 x 0.42 x 0.41
Theta range for data collection	2.19 to 24.98 deg.
Index ranges	$-21 \le h \le 20, 0 \le k \le 12, 0 \le l \le 22$
Reflections collected	4221
Independent reflections	4094 [R(int) = 0.0269]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4094 / 0 / 361
Goodness-of-fit on F^2	1.012
Final R indices [I>2sigma(I)]	R(F) = 0.0435, $wR(F^2)$ = 0.1026
R indices (all data)	R(F) = 0.0461, $wR(F^2)$ = 0.1046
Largest diff. peak and hole	0.402 and -0.174 e/A^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Co(tmmda)(3,6-DBSQ)(3,6-DBCat). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Co	2860(1)	1438(1)	9016(1)	40(1)
O(1)	2028(1)	602(2)	8361(1)	46(1)
O(2)	2096(1)	2214(2)	9372(1)	45(1)
O(3)	2905(1)	81(2)	9630(1)	47(1)
O(4)	3614(1)	2216(2)	9737(1)	44(1)
N(1)	2982(2)	2765(3)	8304(2)	55(1)
N(2)	3658(2)	844(3)	8531(2)	61(1)
C(1)	1412(2)	688(3)	8603(2)	40(1)
C(2)	1446(2)	1598(3)	9168(2)	38(1)
C(3)	817(2)	1826(3)	9472(2)	44(1)
C(4)	177(2)	1103(4)	9189(2)	59(1)
C(5)	140(2)	216(4)	8636(2)	58(1)
C(6)	730(2)	-49(3)	8326(2)	47(1)
C(7)	874(2)	2800(3)	10074(2)	54(1)
C(8)	1079(3)	4088(4)	9831(2)	81(1)
C(9)	1496(2)	2371(4)	10741(2)	77(1)
C(10)	106(2)	2907(5)	10288(2)	84(1)
C(11)	691(2)	-1048(4)	7743(2)	63(1)
C(12)	862(3)	-463(5)	7075(2)	86(1)
C(13)	1279(3)	-2088(4)	8043(3)	95(2)
C(14)	-118(3)	-1650(5)	7514(3)	99(2)
C(15)	3288(2)	412(3)	10305(2)	41(1)
C(16)	3682(2)	1583(3)	10359(2)	39(1)
C(17)	4132(2)	2025(3)	11025(2)	41(1)
C(18)	4143(2)	1256(3)	11612(2)	50(1)
C(19)	3742(2)	127(4)	11558(2)	53(1)
C(20)	3298(2)	-346(3)	10905(2)	46(1)
C(21)	4558(2)	3296(3)	11076(2)	53(1)
C(22)	5053(2)	3557(4)	11840(2)	77(1)
C(23)	3967(2)	4357(4)	10875(3)	80(1)
C(24)	5100(2)	3319(4)	10570(2)	66(1)
C(25)	2859(2)	-1600(3)	10837(2)	59(1)
C(26)	1994(2)	-1354(4)	10559(3)	89(1)
C(27)	3115(3)	-2468(4)	10294(3)	91(1)
C(28)	2991(3)	-2316(5)	11545(3)	103(2)
C(29)	3672(3)	2087(5)	8198(3)	97(2)
C(30)	3187(3)	4051(4)	8599(2)	87(1)
C(31)	2353(3)	2900(5)	7651(2)	93(2)
C(32)	4422(2)	532(5)	9020(3)	93(2)
C(33)	3420(3)	-220(5)	8027(3)	92(2)

Table 3. Bond lengths [A] and angles [deg] for Co(tmmda)(3,6-DBSQ)(3,6-DBCat).

Co-O(3)	1.840(2)
Co-O(4)	1.863(2)
Co-O(2)	1.864(2)
Co-O(1)	1.906(2)
Co-N(2)	1.993(3)
Co-N(1)	2.003(3)
Co-C(29)	2.487(4)
O(1)-C(1)	1.303(4)
O(2)-C(2)	1.304(3)
O(3)-C(15)	1.349(4)
O(4)-C(16)	1.345(3)
N(1)-C(31)	1.466(4)
N(1)-C(30)	1.477(5)
N(1)-C(29)	1.485(5)
N(2)-C(29)	1.458(6)
N(2)-C(33)	1.470(5)
N(2)-C(32)	1.489(5)
C(1)-C(6)	1.431(4)
C(1)-C(2)	1.437(4)
C(2)-C(3)	1.414(4)
C(3)-C(4)	1.370(5)
C(3)-C(7)	1.528(5)
C(4)-C(5)	1.401(5)
C(5)-C(6)	1.365(5)
C(6)-C(11)	1.523(5)
C(7)-C(8)	1.509(6)
C(7)-C(10)	1.535(5)
C(7)-C(9)	1.538(5)
C(11)-C(12)	1.521(6)
C(11)-C(13)	1.527(6)
C(11)-C(14)	1.543(5)
C(15)-C(20)	1.395(4)
C(15)-C(16)	1.411(4)
C(16)-C(17)	1.407(4)
C(17)-C(18)	1.383(4)
C(17)-C(21)	1.531(5)
C(18)-C(19)	1.378(5)
C(19)-C(20)	1.397(5)
C(20)-C(25)	1.526(5)
C(21)-C(23)	1.520(5)
C(21)-C(22)	1.536(5)
C(21)-C(24)	1.536(5)
C(25)-C(28)	1.518(5)
C(25)-C(26)	1.529(5)
C(25)-C(27)	1.539(6)

O(3)-Co-O(4)	87.64(9)
O(3)-Co-O(2)	91.37(10)
O(4)-Co-O(2)	89.93(9)
O(3)-Co-O(1)	87.99(10)
O(4)-Co-O(1)	173.46(9)
O(2)-Co-O(1)	85.32(9)
O(3)-Co-N(2)	97.71(12)
O(4)-Co-N(2)	90.72(11)
O(2)-Co-N(2)	170.92(12)
O(1)-Co-N(2)	94.69(11)
O(3)-Co-N(1)	169.36(11)
O(4)-Co-N(1)	90.97(11)
O(2)-Co-N(1)	99.18(11)
O(1)-Co-N(1)	94.21(10)
N(2)-Co-N(1)	71.75(13)
O(3)-Co-C(29)	132.69(14)
O(4)-Co-C(29)	85.3(2)
O(2)-Co-C(29)	135.23(14)
O(1)-Co-C(29)	101.3(2)
N(2)-Co-C(29)	35.9(2)
N(1)-Co-C(29)	36.67(14)
C(1)-O(1)-Co	109.1(2)
C(2)-O(2)-Co	110.8(2)
C(15)-O(3)-Co	110.1(2)
C(16)-O(4)-Co	109.1(2)
C(31)-N(1)-C(30)	107.7(3)
C(31)-N(1)-C(29)	114.7(4)
C(30)-N(1)-C(29)	110.9(3)
C(31)-N(1)-Co	117.2(2)
C(30)-N(1)-Co	115.9(2)
C(29)-N(1)-Co	89.7(2)
C(29)-N(2)-C(33)	115.5(4)
C(29)-N(2)-C(32)	111.2(4)
C(33)-N(2)-C(32)	108.4(3)
C(29)-N(2)-Co	90.9(2)
C(33)-N(2)-Co	114.9(2)
C(32)-N(2)-Co	115.3(3)
O(1)-C(1)-C(6)	123.5(3)
O(1)-C(1)-C(2)	115.7(3)
C(6)-C(1)-C(2)	120.8(3)
O(2)-C(2)-C(3)	122.4(3)
O(2)-C(2)-C(1)	115.1(3)
C(3)-C(2)-C(1)	122.5(3)
C(4)-C(3)-C(2)	114.6(3)
C(4)-C(3)-C(7)	124.3(3)
C(2)-C(3)-C(7)	121.1(3)
C(3)-C(4)-C(5)	123.1(3)
C(6)-C(5)-C(4)	124.8(3)
C(5)-C(6)-C(1)	114.2(3)
C(5)-C(6)-C(11)	124.2(3)
C(1)-C(6)-C(11)	121.6(3)
C(8)-C(7)-C(3)	110.1(3)

C(8)-C(7)-C(10)	108.7(3)
C(3)-C(7)-C(10)	110.9(3)
C(8)-C(7)-C(9)	109.8(3)
C(3)-C(7)-C(9)	109.2(3)
C(10)-C(7)-C(9)	108.1(3)
C(12)-C(11)-C(6)	110.9(3)
C(12)-C(11)-C(13)	110.0(4)
C(6)-C(11)-C(13)	108.6(3)
C(12)-C(11)-C(14)	107.4(3)
C(6)-C(11)-C(14)	111.1(3)
C(13)-C(11)-C(14)	108.9(4)
O(3)-C(15)-C(20)	122.8(3)
O(3)-C(15)-C(16)	114.9(3)
C(20)-C(15)-C(16)	122.4(3)
O(4)-C(16)-C(17)	123.0(3)
O(4)-C(16)-C(15)	115.8(3)
C(17)-C(16)-C(15)	121.2(3)
C(18)-C(17)-C(16)	115.6(3)
C(18)-C(17)-C(21)	123.7(3)
C(16)-C(17)-C(21)	120.6(3)
C(19)-C(18)-C(17)	122.9(3)
C(18)-C(19)-C(20)	122.9(3)
C(15)-C(20)-C(19)	115.0(3)
C(15)-C(20)-C(25)	121.6(3)
C(19)-C(20)-C(25)	123.4(3)
C(23)-C(21)-C(17)	108.8(3)
C(23)-C(21)-C(22)	108.0(3)
C(17)-C(21)-C(22)	112.1(3)
C(23)-C(21)-C(24)	109.8(3)
C(17)-C(21)-C(24)	111.0(3)
C(22)-C(21)-C(24)	107.1(3)
C(28)-C(25)-C(20)	113.0(3)
C(28)-C(25)-C(26)	108.3(4)
C(20)-C(25)-C(26)	109.8(3)
C(28)-C(25)-C(27)	107.7(4)
C(20)-C(25)-C(27)	109.6(3)
C(26)-C(25)-C(27)	108.3(4)
N(2)-C(29)-N(1)	105.4(3)
N(2)-C(29)-Co	53.2(2)
N(1)-C(29)-Co	53.7(2)

Table 4. Anisotropic displacement parameters ($A^2 \times 10^3$) for Co(tmmda)(3,6-DBSQ)(3,6-DBCat).

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co	36(1)	47(1)	36(1)	-1(1)	7(1)	-2(1)
O(1)	43(1)	55(1)	38(1)	-8(1)	9(1)	-6(1)
O(2)	40(1)	46(1)	46(1)	-5(1)	7(1)	-1(1)
O(3)	52(1)	43(1)	43(1)	1(1)	5(1)	-4(1)
O(4)	41(1)	49(1)	38(1)	6(1)	2(1)	-7(1)
N(1)	50(2)	66(2)	48(2)	11(2)	9(1)	-7(2)
N(2)	51(2)	73(2)	64(2)	-6(2)	23(2)	1(2)
C(1)	39(2)	43(2)	37(2)	6(1)	5(1)	-1(1)
C(2)	38(2)	38(2)	35(2)	4(1)	2(1)	1(1)
C(3)	41(2)	49(2)	41(2)	5(1)	8(1)	9(2)
C(4)	45(2)	76(3)	60(2)	6(2)	20(2)	3(2)
C(5)	43(2)	67(2)	62(2)	-2(2)	11(2)	-16(2)
C(6)	44(2)	49(2)	44(2)	2(2)	3(1)	-8(2)
C(7)	56(2)	59(2)	47(2)	-4(2)	13(2)	14(2)
C(8)	88(3)	63(3)	89(3)	-16(2)	19(3)	14(2)
C(9)	82(3)	97(3)	47(2)	-10(2)	7(2)	26(2)
C(10)	73(3)	101(4)	85(3)	-19(3)	30(2)	27(3)
C(11)	69(2)	61(2)	54(2)	-14(2)	9(2)	-21(2)
C(12)	103(3)	107(4)	47(2)	-22(2)	16(2)	-28(3)
C(13)	117(4)	62(3)	102(4)	-21(3)	19(3)	1(3)
C(14)	93(3)	111(4)	92(3)	-37(3)	21(3)	-52(3)
C(15)	32(2)	46(2)	42(2)	2(2)	6(1)	7(1)
C(16)	30(1)	46(2)	39(2)	2(2)	6(1)	7(1)
C(17)	31(2)	52(2)	40(2)	-2(2)	8(1)	9(1)
C(18)	44(2)	65(2)	38(2)	-3(2)	7(1)	10(2)
C(19)	49(2)	67(2)	45(2)	12(2)	15(2)	9(2)
C(20)	36(2)	53(2)	51(2)	11(2)	13(1)	11(2)
C(21)	47(2)	55(2)	54(2)	-7(2)	5(2)	-3(2)
C(22)	76(3)	90(3)	57(2)	-17(2)	4(2)	-24(2)
C(23)	78(3)	52(2)	104(3)	-13(2)	12(2)	5(2)
C(24)	56(2)	75(3)	65(2)	-1(2)	14(2)	-21(2)
C(25)	52(2)	54(2)	70(2)	16(2)	14(2)	1(2)
C(26)	55(2)	75(3)	131(4)	20(3)	15(2)	-15(2)
C(27)	111(4)	47(2)	119(4)	11(3)	35(3)	6(2)
C(28)	116(4)	92(4)	95(4)	44(3)	15(3)	-27(3)
C(29)	92(3)	111(4)	106(4)	29(3)	57(3)	7(3)
C(30)	109(4)	66(3)	75(3)	18(2)	5(3)	-24(3)
C(31)	89(3)	115(4)	57(2)	33(3)	-17(2)	-33(3)
C(32)	47(2)	113(4)	119(4)	-27(3)	19(2)	18(2)
C(33)	76(3)	117(4)	91(3)	-49(3)	37(2)	-3(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Co(tmmda)(3,6-DBSQ)(3,6-DBCat).

	x	y	z	U(eq)
H(4)	-254(2)	1205(4)	9371(2)	71
H(5)	-320(2)	-225(4)	8469(2)	70
H(8A)	1114(3)	4692(4)	10213(2)	121
H(8B)	688(3)	4353(4)	9417(2)	121
H(8C)	1566(3)	4038(4)	9709(2)	121
H(9A)	1362(2)	1552(4)	10894(2)	116
H(9B)	1529(2)	2974(4)	11123(2)	116
H(9C)	1984(2)	2319(4)	10622(2)	116
H(10A)	-31(2)	2092(5)	10445(2)	127
H(10B)	-290(2)	3185(5)	9880(2)	127
H(10C)	157(2)	3510(5)	10672(2)	127
H(12A)	834(3)	-1108(5)	6715(2)	129
H(12B)	1369(3)	-99(5)	7197(2)	129
H(12C)	490(3)	188(5)	6889(2)	129
H(13A)	1167(3)	-2451(4)	8465(3)	143
H(13B)	1787(3)	-1729(4)	8167(3)	143
H(13C)	1251(3)	-2737(4)	7685(3)	143
H(14A)	-244(3)	-2028(5)	7925(3)	148
H(14B)	-124(3)	-2291(5)	7156(3)	148
H(14C)	-491(3)	-1006(5)	7316(3)	148
H(18)	4433(2)	1511(3)	12063(2)	60
H(19)	3768(2)	-340(4)	11975(2)	64
H(22A)	5432(2)	2898(4)	11978(2)	115
H(22B)	4730(2)	3576(4)	12170(2)	115
H(22C)	5308(2)	4362(4)	11848(2)	115
H(23A)	4228(2)	5159(4)	10905(3)	120
H(23B)	3639(2)	4353(4)	11200(3)	120
H(23C)	3662(2)	4228(4)	10391(3)	120
H(24A)	5472(2)	2648(4)	10699(2)	99
H(24B)	5362(2)	4122(4)	10612(2)	99
H(24C)	4806(2)	3201(4)	10082(2)	99
H(26A)	1898(2)	-903(4)	10110(3)	133
H(26B)	1816(2)	-856(4)	10905(3)	133
H(26C)	1723(2)	-2150(4)	10487(3)	133
H(27A)	3037(3)	-2038(4)	9839(3)	137
H(27B)	2818(3)	-3236(4)	10231(3)	137
H(27C)	3652(3)	-2670(4)	10472(3)	137
H(28A)	2702(3)	-3094(5)	11471(3)	155
H(28B)	2825(3)	-1802(5)	11891(3)	155
H(28C)	3530(3)	-2504(5)	11720(3)	155
H(29A)	3646(3)	1999(5)	7689(3)	116
H(29B)	4139(3)	2543(5)	8428(3)	116
H(30A)	3599(3)	3991(4)	9029(2)	130
H(30B)	2746(3)	4436(4)	8712(2)	130
H(30C)	3350(3)	4560(4)	8249(2)	130
H(31A)	2208(3)	2076(5)	7447(2)	139

H(31B)	2522(3)	3419(5)	7308(2)	139
H(31C)	1918(3)	3292(5)	7771(2)	139
H(32A)	4397(2)	-288(5)	9232(3)	140
H(32B)	4554(2)	1161(5)	9393(3)	140
H(32C)	4807(2)	521(5)	8751(3)	140
H(33A)	3429(3)	-994(5)	8294(3)	137
H(33B)	3769(3)	-291(5)	7722(3)	137
H(33C)	2908(3)	-70(5)	7737(3)	137

Table 1s. Crystal Data, Data Collection Conditions, and Solution and Refinement Details for Co(tmpda)(3,6-DBSQ)$_2$

Crystal Data

formula	$C_{35}\ H_{58}\ N_2\ O_4\ Co$
color; habit	blue-green prism
crystal dimensions	0.64 0.38 0.27 mm
space group[a]	P2(1)/c
crystal system	monoclinic
unit cell dimensions[b,c]	a = 16.987(2) Å
	b = 11.771(2) Å
	c = 19.723(3) Å
	β = 111.820(10)°
volume	3661.1(9) Å^3
formula units / cell	Z = 4
formula weight	629.8 amu
density(calc.)	1.143 g/cm^3
absorption coefficient	0.501 mm^{-1}
F(000)	1364 e$^-$

Data Collection

diffractometer used	Siemens P3/F
radiation	Mo-K_α (λ = 0.71073 Å)
temperature	23-26°C
monochromator	highly oriented graphite crystal
mosaic character[d]	0.20°
2θ range	3.0 to 45.0°
scan type	θ-2θ
scan speed	variable; 4.00 to 30.00°/min.
scan range	from 0.90° below 2θ for $K_{\alpha 1}$ to 0.90° above 2θ for $K_{\alpha 2}$
background measurement	stationary crystal and stationary counter at beginning and end of scan, each for 50% of total scan time
standard reflections	3 measured every 97 reflections
index ranges	$-20 \leq h \leq 0$, $-19 \leq k \leq 3$, $12 \leq l \leq 19$
reflections collected	7204
unique reflections[e]	5682 (R_{int} = 2.00%)
observed reflections	2242 ($F > 4.0\sigma(F)$)

Solution and Refinement

system used[f]	Siemens SHELXTL PLUS (MicroVAX II)
solution	Patterson techniques
refinement method[g]	full-matrix least-squares
scattering factors	neutral atoms[h]
hydrogen atoms	riding model, fixed isotropic U
weighting scheme	$w = 1.0 / [\sigma^2(F) + 0.0010F^2]$
final residuals (obs. data)	R = 8.03%, wR = 9.96%
residuals (all data)	R = 17.81%, wR = 13.00%
goodness-of-fit	1.36
largest and mean Δ/σ	0.118, 0.009
data-to-parameter ratio	5.9:1
largest difference peak	0.67 $e^-/Å^3$
largest difference hole	-0.34 $e^-/Å^3$

(a) "International Tables for X-ray Crystallography", Vol. A., D. Reidel Publishing, Dordrecht, Holland/ Boston, U.S.A , 1983.

(b) Cell dimensions were determined by least-squares fit of the setting angles for 25 reflections with 2θ in the range 21.0 - 38.0°. Angle tolerances for centering, 2θ, ω and, χ; 0.02, 0.01 and, 0.04 .

(c) Estimated standard deviations in the least significant figure(s) are given in parentheses in this and all subsequent tables.

(d) Crystal mosaic character was determined from the width at half height of ω scans.

(e) $R_{int} = [\Sigma N(\Sigma w(F_{mean} - F)^2)/\Sigma(N-1)\Sigma wF^2]^{1/2}$

(f) G. M. Sheldrick, SHELXTL-PLUS, A Program For Crystal Structure Determination, Version 4.1, 1990, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

(g) The quantity minimized in the least-squares procedures is:

$$\Sigma w(|F_o|-|F_c|)^2 .$$

$$R = R_1 = \Sigma||F_o|-|F_c|| \; / \; \Sigma|F_o|$$

$$wR = R_2 = [\Sigma w(|F_o|-|F_c|)^2 \; / \; \Sigma w(F_o)^2]^{1/2}$$

(h) "International Tables for X-ray Crystallography", Vol. 4., Kynoch Press, Birmingham, England, 1974.

(i) Rogers, D., Acta Cryst., (1981), A37, 734-741.

Table 2s. Atomic Coordinates[a] ($x10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 x10^3$)

for **Co(tmpda)(3,6-DBSQ)$_2$**

	x/a	y/b	z/c	U(eq)[b]
Co	1757(1)	356(1)	2188(1)	55(1)*
O1	2179(5)	1591(7)	2997(4)	68(4)*
O2	2232(5)	-661(6)	3076(5)	73(4)*
O3	2939(5)	416(7)	2140(4)	69(4)*
O4	1568(6)	1673(7)	1495(5)	74(4)*
N1	479(7)	427(14)	2205(7)	92(6)*
N2	1467(9)	-1062(12)	1398(8)	99(7)*
C1	2670(9)	1179(11)	3575(10)	80(8)*
C2	2691(8)	-110(12)	3669(8)	77(7)*
C3	3211(10)	-693(13)	4334(8)	98(8)*
C4	3759(10)	35(15)	4856(9)	119(9)*
C5	3781(10)	1240(13)	4785(8)	102(8)*
C6	3279(10)	1849(12)	4211(8)	82(7)*
C7	3216(11)	-1950(13)	4407(8)	95(8)*
C8	3745(10)	-2357(13)	5146(9)	157(11)*
C9	2326(12)	-2347(13)	4240(9)	152(13)*
C10	3485(12)	-2566(15)	3890(9)	153(12)*
C11	3210(11)	3122(13)	4137(7)	77(8)*
C12	2358(10)	3506(12)	4069(10)	137(12)*
C13	3859(11)	3691(14)	4798(10)	159(13)*
C14	3498(10)	3466(14)	3553(11)	141(13)*
C15	3057(9)	1318(14)	1863(7)	75(7)*
C16	2278(10)	2056(13)	1492(7)	75(7)*
C17	2362(10)	3153(13)	1182(8)	83(8)*
C18	3212(12)	3464(14)	1290(9)	106(10)*
C19	3936(10)	2759(15)	1652(9)	100(9)*
C20	3905(10)	1735(14)	1937(8)	85(8)*
C21	1590(10)	3914(11)	834(8)	78(7)*
C22	1794(11)	5010(13)	551(9)	129(10)*
C23	987(11)	3335(13)	244(9)	161(11)*
C24	1351(12)	4187(14)	1456(11)	149(14)*
C25	4664(8)	982(13)	2311(10)	77(7)*

C26	5475(9)	1514(15)	2394(12)	183(15)*
C27	4571(10)	-75(14)	1863(8)	110(9)*
C28	4693(9)	598(15)	3041(9)	139(10)*
C34	2189(12)	-1847(16)	1605(11)	168(13)*
C29	24(15)	-612(23)	2104(18)	226(27)*
C30	-1(13)	-1230(22)	1368(15)	188(18)*
C35	1276(16)	-666(17)	711(9)	263(23)*
C31	817(17)	-1783(18)	1463(13)	189(18)*
C32	526(12)	704(23)	2915(12)	213(19)*
C33	-9(14)	1209(26)	1773(17)	363(33)*

(a) Atoms have occupancies of 1.0.

(b) For atoms marked with *, the equivalent isotropic U is defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 3s. Bond Lengths (Å)
for Co(tmpda)(3,6-DBSQ)$_2$

Co-O1	2.080 (8)	Co-O2	2.025 (8)
Co-O3	2.046 (9)	Co-O4	2.012 (9)
Co-N1	2.185 (14)	Co-N2	2.210 (14)
O1-C1	1.234 (16)	O2-C2	1.312 (15)
O3-C15	1.245 (18)	O4-C16	1.290 (19)
N1-C29	1.420 (31)	N1-C32	1.411 (29)
N1-C33	1.318 (30)	N2-C34	1.467 (23)
N2-C35	1.354 (24)	N2-C31	1.435 (32)
C1-C2	1.527 (19)	C1-C6	1.518 (19)
C2-C3	1.452 (18)	C3-C4	1.395 (21)
C3-C7	1.487 (21)	C4-C5	1.427 (23)
C5-C6	1.344 (19)	C6-C11	1.506 (21)
C7-C8	1.478 (20)	C7-C9	1.496 (27)
C7-C10	1.458 (28)	C11-C12	1.474 (25)
C11-C13	1.515 (20)	C11-C14	1.465 (29)
C15-C16	1.523 (20)	C15-C20	1.476 (23)
C16-C17	1.458 (22)	C17-C18	1.427 (27)
C17-C21	1.525 (21)	C18-C19	1.434 (22)
C19-C20	1.340 (24)	C20-C25	1.511 (20)
C21-C22	1.496 (23)	C21-C23	1.407 (20)
C21-C24	1.464 (30)	C25-C26	1.466 (22)
C25-C27	1.499 (23)	C25-C28	1.494 (26)
C29-C30	1.609 (45)	C30-C31	1.482 (36)

Table 4s. Bond Angles (°)
for Co(tmpda)(3,6-DBSQ)$_2$

O1-Co-O2	80.6(3)	O1-Co-O3	87.0(4)
O2-Co-O3	88.7(4)	O1-Co-O4	84.5(3)
O2-Co-O4	162.6(3)	O3-Co-O4	81.6(4)
O1-Co-N1	91.3(5)	O2-Co-N1	95.1(5)
O3-Co-N1	175.5(5)	O4-Co-N1	94.2(5)
O1-Co-N2	172.7(4)	O2-Co-N2	94.3(4)
O3-Co-N2	87.6(5)	O4-Co-N2	99.6(5)
N1-Co-N2	94.5(6)	Co-O1-C1	110.8(8)
Co-O2-C2	113.1(8)	Co-O3-C15	111.8(8)
Co-O4-C16	111.0(8)	Co-N1-C29	117.1(15)
Co-N1-C32	109.5(10)	C29-N1-C32	99.6(21)
Co-N1-C33	113.9(16)	C29-N1-C33	109.4(17)
C32-N1-C33	105.7(20)	Co-N2-C34	109.6(10)
Co-N2-C35	110.7(12)	C34-N2-C35	111.1(19)
Co-N2-C31	111.2(14)	C34-N2-C31	101.2(15)
C35-N2-C31	112.7(16)	O1-C1-C2	118.7(12)
O1-C1-C6	125.3(12)	C2-C1-C6	115.9(12)
O2-C2-C1	113.8(11)	O2-C2-C3	122.1(12)
C1-C2-C3	123.9(12)	C2-C3-C4	113.0(13)
C2-C3-C7	122.5(12)	C4-C3-C7	124.1(13)
C3-C4-C5	124.9(13)	C4-C5-C6	125.6(13)
C1-C6-C5	116.3(13)	C1-C6-C11	115.6(11)
C5-C6-C11	128.0(12)	C3-C7-C8	113.4(12)
C3-C7-C9	108.8(14)	C8-C7-C9	108.1(15)
C3-C7-C10	114.7(16)	C8-C7-C10	107.2(14)
C9-C7-C10	104.1(13)	C6-C11-C12	110.6(14)
C6-C11-C13	110.5(11)	C12-C11-C13	108.6(15)
C6-C11-C14	108.3(14)	C12-C11-C14	116.5(13)
C13-C11-C14	101.9(15)	O3-C15-C16	116.3(13)
O3-C15-C20	123.5(12)	C16-C15-C20	120.0(14)
O4-C16-C15	116.5(13)	O4-C16-C17	123.2(13)
C15-C16-C17	120.2(14)	C16-C17-C18	114.6(13)
C16-C17-C21	120.5(15)	C18-C17-C21	124.7(14)
C17-C18-C19	124.0(15)	C18-C19-C20	124.7(16)

C15-C20-C19	116.6(14)	C15-C20-C25	118.5(14)
C19-C20-C25	124.9(15)	C17-C21-C22	113.3(14)
C17-C21-C23	109.1(13)	C22-C21-C23	107.9(13)
C17-C21-C24	102.2(13)	C22-C21-C24	107.4(13)
C23-C21-C24	117.1(16)	C20-C25-C26	113.6(14)
C20-C25-C27	108.4(11)	C26-C25-C27	108.0(15)
C20-C25-C28	111.4(15)	C26-C25-C28	109.2(13)
C27-C25-C28	106.0(13)	N1-C29-C30	110.4(25)
C29-C30-C31	112.1(18)	N2-C31-C30	116.5(18)

Table 5s. Anisotropic Displacement Parameters[a] ($Å^2 x 10^3$) for Co(tmpda)(3,6-DBSQ)$_2$

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co	46(1)	52(1)	52(1)	-6(1)	3(1)	3(1)
O1	64(6)	69(6)	43(5)	-11(5)	-11(4)	8(4)
O2	71(6)	53(6)	65(6)	-20(4)	-10(5)	8(4)
O3	75(6)	43(5)	86(6)	-3(5)	25(5)	27(5)
O4	53(6)	71(6)	78(6)	-19(5)	2(5)	14(5)
N1	63(8)	105(10)	94(9)	-19(9)	12(7)	-5(9)
N2	76(10)	83(10)	116(12)	-13(9)	8(9)	-42(9)
C1	89(12)	55(10)	107(13)	-19(9)	51(11)	-10(10)
C2	67(9)	73(10)	74(10)	-18(8)	8(8)	0(8)
C3	105(12)	86(13)	62(10)	6(9)	-16(9)	-10(9)
C4	106(13)	125(17)	85(12)	16(11)	-13(10)	9(11)
C5	140(15)	64(10)	71(11)	-20(10)	4(10)	-6(9)
C6	112(13)	63(10)	57(9)	17(10)	14(9)	11(9)
C7	115(14)	52(10)	65(10)	-20(10)	-27(10)	19(8)
C8	158(17)	92(14)	148(16)	-13(12)	-28(13)	52(13)
C9	228(25)	72(12)	112(14)	-25(14)	11(15)	34(11)
C10	204(23)	122(16)	96(14)	71(15)	12(14)	17(14)
C11	98(12)	88(12)	52(9)	-38(11)	36(9)	-16(9)
C12	104(15)	66(11)	237(24)	3(10)	58(14)	-46(13)
C13	176(19)	117(16)	173(20)	-46(14)	52(16)	-77(15)
C14	109(15)	94(13)	223(24)	-30(11)	65(16)	-69(15)
C15	57(10)	93(12)	65(9)	8(9)	10(8)	-6(9)
C16	84(12)	81(11)	48(8)	3(9)	9(8)	9(8)
C17	93(12)	70(11)	87(11)	-9(10)	34(10)	5(9)
C18	129(16)	76(12)	116(14)	-18(12)	49(12)	9(10)
C19	73(11)	98(13)	123(14)	17(10)	28(10)	21(11)
C20	80(12)	92(12)	94(12)	13(10)	42(9)	15(10)
C21	99(12)	52(9)	69(10)	3(9)	16(9)	29(8)
C22	163(17)	102(15)	118(14)	19(11)	47(12)	25(11)
C23	218(22)	84(13)	92(13)	-4(13)	-45(14)	14(10)
C24	187(21)	113(16)	193(21)	0(13)	124(18)	2(15)
C25	43(9)	80(10)	112(13)	13(8)	34(9)	23(10)
C26	68(12)	196(22)	302(29)	42(14)	90(16)	-6(20)

C27	109(13)	117(14)	96(12)	37(11)	27(10)	1(11)
C28	82(12)	182(20)	114(14)	66(12)	-7(10)	-30(15)
C34	151(19)	117(16)	185(22)	-16(16)	4(16)	-77(15)
C29	131(22)	174(28)	430(57)	11(19)	168(29)	38(30)
C30	88(16)	198(27)	285(34)	-84(18)	79(21)	-106(24)
C35	532(54)	137(20)	46(11)	54(24)	23(19)	-22(13)
C31	231(29)	151(21)	209(25)	-116(24)	108(24)	-123(19)
C32	103(16)	367(42)	192(25)	-80(20)	83(16)	-79(28)
C33	179(27)	500(59)	495(57)	201(34)	222(34)	332(53)

(a)The anisotropic displacement exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2klb^*c^*U_{23})$

Table 6s. Hydrogen Atom Coordinates[a] ($x10^4$) and Isotropic Displacement Parameters ($Å^2x10^3$) for Co(tmpda)(3,6-DBSQ)$_2$

	x/a	y/b	z/c	U
H4A	4145	-313	5294	80
H5A	4164	1657	5193	80
H8A	4326	-2141	5268	80
H8B	3528	-2001	5479	80
H8C	3708	-3167	5180	80
H9A	1970	-2127	3754	80
H9B	2308	-3158	4286	80
H9C	2129	-1992	4585	80
H10A	4057	-2339	3978	80
H10B	3465	-3373	3952	80
H10C	3127	-2365	3400	80
H12A	1945	3170	3640	80
H12B	2255	3260	4493	80
H12C	2315	4319	4032	80
H13A	3733	3517	5222	80
H13B	4402	3378	4855	80
H13C	3871	4500	4742	80
H14A	3094	3168	3106	80
H14B	3517	4278	3521	80
H14C	4048	3156	3634	80
H18A	3294	4198	1114	80
H19A	4475	3027	1664	80
H22A	1301	5475	324	80
H22B	2189	5406	962	80
H22C	2054	4848	205	80
H23A	506	3823	21	80
H23B	1218	3115	-112	80
H23C	812	2670	433	80
H24A	861	4671	1289	80
H24B	1217	3501	1655	80
H24C	1808	4572	1828	80
H26A	5447	1729	1916	80

H26B	5524	2182	2685	80
H26C	5960	1035	2621	80
H27A	4571	130	1392	80
H27B	5020	-606	2093	80
H27C	4037	-416	1807	80
H28A	4175	198	2970	80
H28B	5167	106	3277	80
H28C	4731	1254	3341	80
H34A	2069	-2470	1267	80
H34B	2676	-1441	1599	80
H34C	2300	-2133	2088	80
H29A	-520	-546	2144	80
H29B	373	-1112	2480	80
H30A	-26	-623	1036	80
H30B	-491	-1707	1162	80
H35A	1157	-1297	379	80
H35B	785	-187	584	80
H35C	1742	-237	680	80
H31A	1008	-2015	1965	80
H31B	729	-2449	1163	80
H32A	-25	737	2945	80
H32B	857	121	3235	80
H32C	806	1423	3058	80
H33A	-569	1249	1783	80
H33B	264	1934	1904	80
H33C	-46	1008	1290	80

(a) Atoms have occupancies of 1.0.

Table 1s. Crystal Data, Data Collection Conditions, and Solution and Refinement Details for **Co(tmpda)(3,6-DBSQ)$_2$**

Crystal Data

formula	$C_{35}H_{59}N_2O_4Co$
color; habit	dark blue prism
crystal dimensions	0.64 x 0.38 x 0.27 mm
space group[a]	P2(1)/c
crystal system	monoclinic
unit cell dimensions[b,c]	a = 16.804(2) Å
	b = 11.691(2) Å
	c = 19.415(3) Å
	β = 111.520(10)°
volume	3548.3(9) Å^3
formula units / cell	Z = 4
formula weight	630.8 amu
density(calc.)	1.181 g/cm^3
absorption coefficient	0.517 mm^{-1}
F(000)	1368 e$^-$

Data Collection

diffractometer used	Siemens P3/F
radiation	Mo-K_α (λ = 0.71073 Å)
temperature	-125°C
monochromator	highly oriented graphite crystal
mosaic character[d]	0.10°
2θ range	3.0 to 45.0°
scan type	θ-2θ
scan speed	variable; 4.00 to 30.00°/min.
scan range	from 1.00° below 2θ for $K_{\alpha 1}$ to 1.00° above 2θ for $K_{\alpha 2}$
background measurement	stationary crystal and stationary counter at beginning and end of scan, each for 50% of total scan time
standard reflections	3 measured every 97 reflections
index ranges	$-18 \leq h \leq 12$, $-11 \leq k \leq 11$, $-17 \leq l \leq 20$
reflections collected	4746
unique reflections[e]	4083 (R_{int} = 3.08%)
observed reflections	2753 ($F > 4.0\sigma(F)$)

Solution and Refinement

system used[f]	Siemens SHELXTL PLUS (MicroVAX II)
solution	Patterson techniques
refinement method[g]	full-matrix least-squares
scattering factors	neutral atoms[h]
hydrogen atoms	riding model, fixed isotropic U
weighting scheme	$w = 1.0 / [\sigma^2(F) + 0.0010F^2]$
final residuals (obs. data)	R = 7.43%, wR = 10.50%
residuals (all data)	R = 11.79%, wR = 11.10%
goodness-of-fit	2.27
largest and mean Δ/σ	0.010, 0.002
data-to-parameter ratio	7.2:1
largest difference peak	0.77 $e^-/Å^3$
largest difference hole	-0.36 $e^-/Å^3$

(a) "International Tables for X-ray Crystallography", Vol. A., D. Reidel Publishing, Dordrecht, Holland/ Boston, U.S.A , 1983.

(b) Cell dimensions were determined by least-squares fit of the setting angles for 25 reflections with 2θ in the range 21.0 - 38.0°. Angle tolerances for centering, 2θ, ω and, χ; 0.02, 0.01 and, 0.04 .

(c) Estimated standard deviations in the least significant figure(s) are given in parentheses in this and all subsequent tables.

(d) Crystal mosaic character was determined from the width at half height of ω scans.

(e) $R_{int} = [\Sigma N(\Sigma w(F_{mean} - F)^2)/\Sigma(N-1)\Sigma wF^2]^{1/2}$

(f) G. M. Sheldrick, SHELXTL-PLUS, A Program For Crystal Structure Determination, Version 4.1, 1990, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

(g) The quantity minimized in the least-squares procedures is:

$$\Sigma w(|F_o|-|F_c|)^2 .$$

$$R = R_1 = \Sigma||F_o|-|F_c|| \; / \; \Sigma|F_o|$$

$$wR = R_2 = [\Sigma w(|F_o|-|F_c|)^2 \; / \; \Sigma w(F_o)^2]^{1/2}$$

(h) "International Tables for X-ray Crystallography", Vol. 4., Kynoch Press, Birmingham, England, 1974.

Table 2s. Atomic Coordinates[a] ($x10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2x10^3$)

for Co(tmpda)(3,6-DBSQ)$_2$

	x/a	y/b	z/c	U(eq)[b]
Co	1750(1)	338(1)	2187(1)	31(1)*
O1	2185(4)	1554(5)	2992(3)	40(3)*
O2	2208(4)	-689(5)	3074(3)	43(3)*
O3	2923(4)	387(6)	2123(3)	44(3)*
O4	1563(4)	1648(5)	1477(3)	44(3)*
N1	472(5)	410(9)	2230(5)	55(4)*
N2	1465(6)	-1090(9)	1411(5)	62(4)*
C1	2703(7)	1140(9)	3592(6)	49(5)*
C2	2702(7)	-138(10)	3663(6)	55(5)*
C3	3228(7)	-702(10)	4339(6)	63(5)*
C4	3779(8)	24(11)	4870(7)	80(6)*
C5	3796(7)	1233(10)	4799(6)	64(6)*
C6	3287(7)	1843(9)	4214(5)	46(5)*
C7	3201(8)	-1998(9)	4422(6)	58(5)*
C8	3793(9)	-2396(10)	5179(7)	109(7)*
C9	2279(8)	-2390(10)	4268(7)	84(7)*
C10	3525(8)	-2589(11)	3901(7)	85(7)*
C11	3248(7)	3126(9)	4138(5)	43(5)*
C12	2387(8)	3521(10)	4064(8)	84(7)*
C13	3886(8)	3685(10)	4814(7)	84(7)*
C14	3510(7)	3486(10)	3502(6)	67(6)*
C15	3066(6)	1314(11)	1866(6)	51(5)*
C16	2299(6)	2064(10)	1494(5)	47(5)*
C17	2381(7)	3162(9)	1191(6)	48(5)*
C18	3211(8)	3457(10)	1284(7)	67(6)*
C19	3948(7)	2738(10)	1658(6)	61(6)*
C20	3903(7)	1715(10)	1940(6)	50(5)*
C21	1584(7)	3915(9)	821(6)	52(5)*
C22	1812(9)	5024(10)	518(7)	83(7)*
C23	962(8)	3319(10)	205(6)	84(6)*
C24	1290(8)	4223(11)	1425(7)	84(7)*
C25	4675(6)	952(9)	2323(7)	53(5)*

C26	5486(7)	1529(13)	2407(9)	120(9)*
C27	4591(8)	-97(11)	1855(6)	75(6)*
C28	4694(8)	591(11)	3083(6)	80(6)*
C34	2189(9)	-1893(11)	1600(8)	99(8)*
C29	7(9)	-660(13)	2093(9)	105(9)*
C30	-48(8)	-1239(14)	1364(9)	120(9)*
C35	1263(13)	-696(12)	685(7)	101(14)*
C31	803(12)	-1859(14)	1473(10)	140(12)*
C32	544(8)	772(15)	2963(8)	126(10)*
C33	-42(9)	1258(16)	1740(10)	160(12)*

(a) Atoms have occupancies of 1.0.

(b) For atoms marked with *, the equivalent isotropic U is defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 3s. Bond Lengths (Å)
for Co(tmpda)(3,6-DBSQ)$_2$

Co-O1	2.040 (6)	Co-O2	2.007 (6)
Co-O3	2.021 (7)	Co-O4	2.007 (6)
Co-N1	2.180 (10)	Co-N2	2.182 (10)
O1-C1	1.267 (11)	O2-C2	1.310 (11)
O3-C15	1.253 (14)	O4-C16	1.318 (13)
N1-C29	1.447 (18)	N1-C32	1.447 (18)
N1-C33	1.425 (19)	N2-C34	1.472 (17)
N2-C35	1.400 (16)	N2-C31	1.469 (22)
C1-C2	1.501 (15)	C1-C6	1.493 (13)
C2-C3	1.445 (14)	C3-C4	1.393 (15)
C3-C7	1.526 (15)	C4-C5	1.421 (17)
C5-C6	1.349 (14)	C6-C11	1.506 (14)
C7-C8	1.515 (14)	C7-C9	1.537 (18)
C7-C10	1.482 (20)	C11-C12	1.476 (17)
C11-C13	1.507 (14)	C11-C14	1.514 (18)
C15-C16	1.507 (14)	C15-C20	1.438 (16)
C16-C17	1.439 (16)	C17-C18	1.383 (18)
C17-C21	1.543 (15)	C18-C19	1.451 (16)
C19-C20	1.329 (17)	C20-C25	1.525 (14)
C21-C22	1.530 (17)	C21-C23	1.447 (14)
C21-C24	1.474 (20)	C25-C26	1.474 (17)
C25-C27	1.502 (17)	C25-C28	1.524 (18)
C29-C30	1.542 (25)	C30-C31	1.547 (24)

Table 4s. Bond Angles (°)
for Co(tmpda)(3,6-DBSQ)$_2$

O1-Co-O2	81.0(2)	O1-Co-O3	86.8(3)
O2-Co-O3	89.7(3)	O1-Co-O4	85.2(2)
O2-Co-O4	163.8(2)	O3-Co-O4	81.1(3)
O1-Co-N1	91.5(3)	O2-Co-N1	93.6(3)
O3-Co-N1	176.0(3)	O4-Co-N1	95.1(3)
O1-Co-N2	171.5(3)	O2-Co-N2	93.0(3)
O3-Co-N2	87.2(3)	O4-Co-N2	99.8(3)
N1-Co-N2	95.0(4)	Co-O1-C1	111.7(6)
Co-O2-C2	112.1(6)	Co-O3-C15	112.5(6)
Co-O4-C16	110.9(5)	Co-N1-C29	115.6(9)
Co-N1-C32	108.7(7)	C29-N1-C32	106.1(12)
Co-N1-C33	111.5(10)	C29-N1-C33	109.0(10)
C32-N1-C33	105.3(12)	Co-N2-C34	111.3(6)
Co-N2-C35	110.7(8)	C34-N2-C35	109.5(12)
Co-N2-C31	113.1(10)	C34-N2-C31	99.8(11)
C35-N2-C31	111.9(11)	O1-C1-C2	116.2(8)
O1-C1-C6	124.1(9)	C2-C1-C6	119.7(8)
O2-C2-C1	115.5(8)	O2-C2-C3	123.4(10)
C1-C2-C3	121.1(9)	C2-C3-C4	114.4(10)
C2-C3-C7	121.1(9)	C4-C3-C7	124.4(9)
C3-C4-C5	124.5(10)	C4-C5-C6	125.3(9)
C1-C6-C5	114.6(9)	C1-C6-C11	118.4(8)
C5-C6-C11	127.0(9)	C3-C7-C8	111.9(8)
C3-C7-C9	110.0(9)	C8-C7-C9	110.6(11)
C3-C7-C10	111.1(11)	C8-C7-C10	104.2(10)
C9-C7-C10	108.9(9)	C6-C11-C12	109.1(9)
C6-C11-C13	110.8(8)	C12-C11-C13	107.9(10)
C6-C11-C14	110.0(9)	C12-C11-C14	113.7(9)
C13-C11-C14	105.2(10)	O3-C15-C16	116.0(9)
O3-C15-C20	124.5(9)	C16-C15-C20	119.4(10)
O4-C16-C15	115.3(9)	O4-C16-C17	123.3(9)
C15-C16-C17	121.4(10)	C16-C17-C18	114.4(9)
C16-C17-C21	120.2(10)	C18-C17-C21	125.5(10)
C17-C18-C19	123.7(11)	C18-C19-C20	124.1(11)

C15-C20-C19	117.0(10)	C15-C20-C25	118.9(10)
C19-C20-C25	124.1(11)	C17-C21-C22	111.4(10)
C17-C21-C23	110.5(9)	C22-C21-C23	107.3(9)
C17-C21-C24	104.9(9)	C22-C21-C24	107.6(10)
C23-C21-C24	115.1(11)	C20-C25-C26	111.9(10)
C20-C25-C27	108.0(8)	C26-C25-C27	108.6(12)
C20-C25-C28	110.2(10)	C26-C25-C28	109.2(10)
C27-C25-C28	108.9(10)	N1-C29-C30	113.2(14)
C29-C30-C31	109.8(11)	N2-C31-C30	113.0(12)

Table 5s. Anisotropic Displacement Parameters[a] ($Å^2 x 10^3$) for Co(tmpda)(3,6-DBSQ)$_2$

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co	28(1)	30(1)	26(1)	-3(1)	-2(1)	3(1)
O1	39(4)	44(4)	19(4)	-2(3)	-11(3)	2(3)
O2	48(4)	27(4)	32(4)	-17(3)	-12(3)	1(3)
O3	44(4)	31(4)	50(4)	-5(4)	9(3)	23(4)
O4	38(4)	39(4)	41(4)	-5(3)	-3(3)	5(3)
N1	45(5)	65(7)	49(6)	-12(6)	11(4)	-10(6)
N2	41(6)	72(7)	51(7)	1(5)	-9(5)	-23(6)
C1	54(7)	40(8)	61(8)	-10(6)	29(7)	-10(7)
C2	50(7)	44(7)	64(8)	-10(6)	13(6)	6(7)
C3	57(8)	61(9)	45(7)	1(6)	-11(6)	6(6)
C4	79(9)	85(11)	46(8)	0(7)	-13(7)	6(7)
C5	87(9)	37(8)	52(8)	-28(7)	8(7)	-7(7)
C6	61(7)	38(7)	23(6)	14(6)	-1(5)	8(6)
C7	83(9)	24(7)	32(7)	-16(6)	-19(6)	10(6)
C8	143(13)	47(9)	78(10)	-16(8)	-27(9)	29(8)
C9	114(12)	52(9)	67(9)	-21(8)	12(8)	12(7)
C10	107(11)	73(10)	55(8)	24(8)	5(8)	2(8)
C11	59(7)	41(7)	23(6)	-25(6)	9(5)	-7(5)
C12	79(10)	42(8)	127(13)	-13(7)	32(9)	-32(8)
C13	107(11)	56(9)	83(10)	-13(8)	27(9)	-20(8)
C14	73(9)	59(8)	74(9)	-6(6)	34(7)	-7(7)
C15	39(7)	68(9)	38(7)	8(6)	6(5)	-10(7)
C16	42(7)	58(8)	30(6)	3(6)	0(5)	-2(6)
C17	63(8)	32(7)	50(7)	-2(6)	20(6)	9(6)
C18	81(9)	47(8)	77(9)	-20(7)	33(8)	11(7)
C19	55(8)	60(9)	71(8)	-2(7)	25(6)	5(7)
C20	54(7)	50(8)	51(7)	7(6)	24(6)	17(6)
C21	87(9)	28(7)	33(7)	13(6)	13(6)	6(6)
C22	117(11)	55(9)	71(9)	10(7)	25(8)	16(7)
C23	113(11)	59(9)	42(8)	10(8)	-16(7)	6(7)
C24	101(11)	79(10)	83(10)	-22(8)	45(9)	-23(8)
C25	30(6)	43(7)	81(9)	4(5)	16(6)	5(7)
C26	46(8)	125(14)	188(17)	26(9)	43(10)	18(13)

C27	73(8)	100(11)	46(7)	34(8)	14(6)	0(8)
C28	80(9)	104(11)	35(7)	46(8)	-1(6)	-15(8)
C34	116(12)	61(9)	97(11)	-12(9)	10(9)	-42(9)
C29	78(10)	103(13)	146(15)	-29(9)	57(10)	-4(11)
C30	43(8)	137(15)	167(17)	-39(9)	24(10)	-97(14)
C35	176(32)	64(11)	27(9)	37(14)	-4(13)	-11(8)
C31	185(20)	99(13)	167(17)	-90(14)	101(15)	-94(13)
C32	66(9)	210(20)	121(13)	-64(11)	56(9)	-76(14)
C33	95(12)	192(20)	222(21)	90(14)	93(14)	98(18)

(a)The anisotropic displacement exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2klb^*c^*U_{23})$

Table 6s. Hydrogen Atom Coordinates[a] ($x10^4$) and Isotropic Displacement Parameters ($Å^2x10^3$)

for Co(tmpda)(3,6-DBSQ)$_2$

	x/a	y/b	z/c	U
H4A	4165	-323	5308	80
H5A	4180	1650	5207	80
H8A	4375	-2181	5301	80
H8B	3576	-2041	5512	80
H8C	3756	-3207	5213	80
H9A	1923	-2170	3781	80
H9B	2261	-3201	4314	80
H9C	2082	-2035	4613	80
H10A	4097	-2362	3989	80
H10B	3505	-3396	3963	80
H10C	3167	-2388	3412	80
H12A	1974	3186	3636	80
H12B	2284	3275	4488	80
H12C	2344	4334	4028	80
H13A	3760	3511	5238	80
H13B	4429	3372	4871	80
H13C	3898	4494	4758	80
H14A	3106	3188	3055	80
H14B	3530	4298	3470	80
H14C	4061	3176	3583	80
H18A	3294	4190	1108	80
H19A	4487	3005	1670	80
H22A	1319	5489	290	80
H22B	2208	5420	929	80
H22C	2073	4862	172	80
H23A	482	3806	-19	80
H23B	1193	3098	-152	80
H23C	787	2654	393	80
H24A	800	4708	1258	80
H24B	1156	3538	1623	80
H24C	1747	4609	1796	80
H26A	5458	1744	1930	80

H26B	5535	2197	2699	80
H26C	5971	1050	2634	80
H27A	4592	108	1384	80
H27B	5041	-628	2085	80
H27C	4057	-438	1799	80
H28A	4177	191	3012	80
H28B	5168	99	3318	80
H28C	4733	1246	3383	80
H34A	2069	-2515	1262	80
H34B	2676	-1486	1594	80
H34C	2300	-2179	2083	80
H29A	-537	-594	2133	80
H29B	356	-1160	2470	80
H30A	-73	-632	1031	80
H30B	-538	-1716	1157	80
H35A	1143	-1326	354	80
H35B	771	-217	559	80
H35C	1729	-267	655	80
H31A	994	-2091	1975	80
H31B	715	-2526	1174	80
H32A	-7	804	2993	80
H32B	875	188	3283	80
H32C	823	1491	3106	80
H33A	-602	1298	1751	80
H33B	230	1984	1871	80
H33C	-79	1057	1257	80

(a) Atoms have occupancies of 1.0.

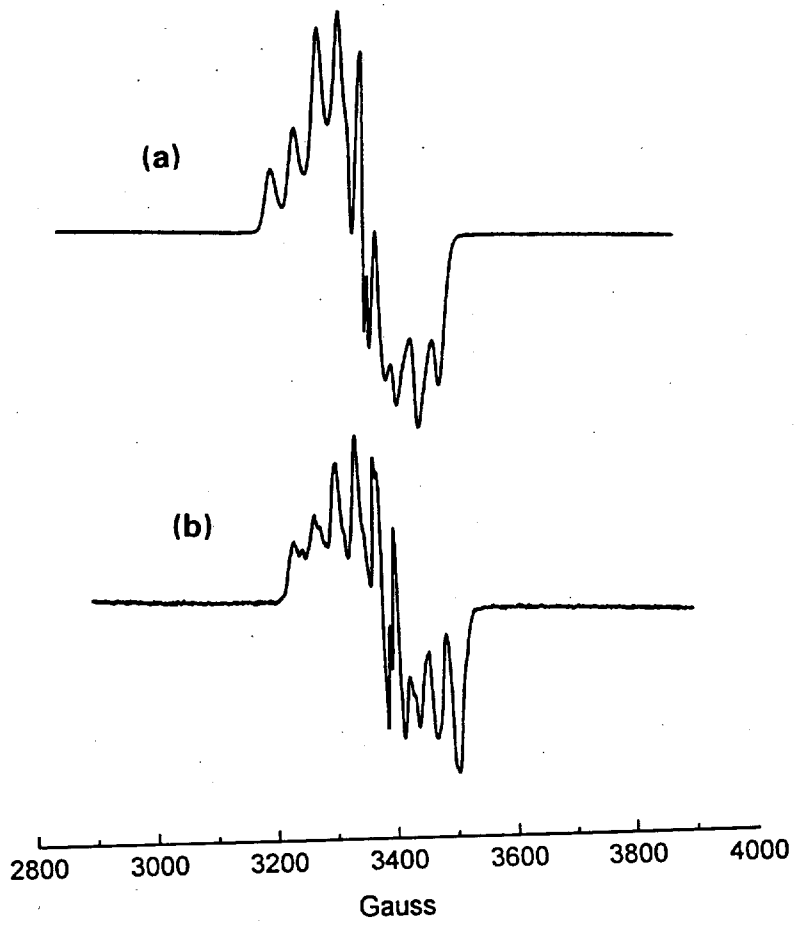

Figure 1S. EPR spectra on Co(tmmda)(3,6-DBSQ)(3,6-DBCat) (a) and Co(tmpda)(3,6-DBSQ)(3,6-DBCat) (b) obtained in toluene glass at 77 K.

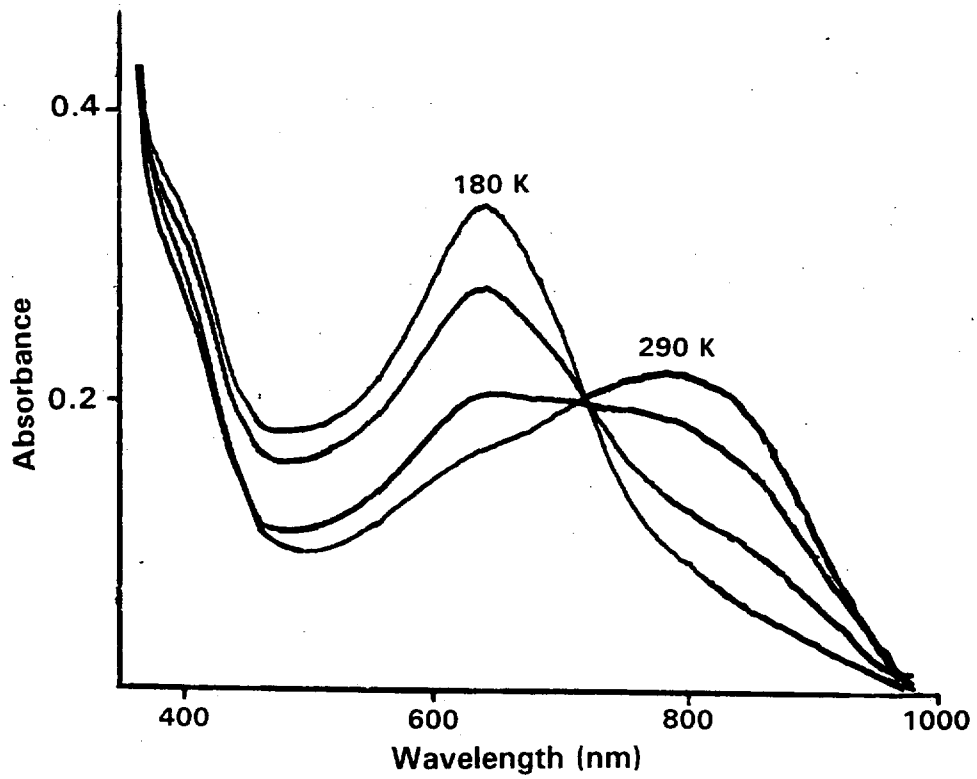

Figure 2S. Changes in intensity of the 650 nm transition of Co^{III}(tmmda)(3,6-DBSQ)(3,6-DBCat) (C = 1.0 x 10^{-4} M) and the 825 nm transition of Co^{II}(tmmda)(3,6-DBSQ)$_2$ in toluene solution at temperatures of 180 K, 230 K, 260 K, and 290 K.