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Copolymerization of cyclohexene oxide and carbon dioxide using (salen)Co(III) complexes: synthesis and characterization of syndiotactic poly(cyclohexene carbonate)

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Table 1. Crystal data and structure refinement for (*R,R*)-(salen-**1**)CoCl.

Identification code	(*R,R*)-(salen-**1**)CoCl	
Empirical formula	C96 H128 Cl2 Co2 N4 O4	
Formula weight	1590.78	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 14.5088(11) Å	α= 90°.
	b = 10.1068(6) Å	β= 93.639(3)°.
	c = 29.765(2) Å	γ = 90°.
Volume	4355.9(5) Å^3	
Z	2	
Density (calculated)	1.213 Mg/m^3	
Absorption coefficient	0.494 mm^{-1}	
F(000)	1704	
Crystal size	0.20 x 0.05 x 0.04 mm^3	
Theta range for data collection	1.52 to 20.87°.	
Index ranges	-14<=h<=14, -10<=k<=10, -26<=l<=29	
Reflections collected	23614	
Independent reflections	8926 [R(int) = 0.0679]	
Completeness to theta = 20.87°	99.6 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9805 and 0.9076
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8926 / 955 / 973
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0589, wR2 = 0.1325
R indices (all data)	R1 = 0.0808, wR2 = 0.1408
Absolute structure parameter	0.02(2)
Largest diff. peak and hole	0.546 and -0.376 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R,R*)-(salen-**1**)CoCl. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	11018(1)	8151(1)	5370(1)	20(1)
Cl(1)	11598(1)	10266(2)	5257(1)	33(1)
O(1)	10657(3)	8235(5)	5953(2)	23(1)
O(2)	12090(3)	7366(5)	5604(2)	22(1)
N(1)	9832(4)	8562(6)	5114(2)	16(1)
N(2)	11243(4)	7510(6)	4792(2)	15(2)
C(1)	9822(5)	8646(8)	4621(3)	20(2)
C(2)	8883(5)	8696(8)	4365(3)	19(2)
C(3)	9025(6)	8644(8)	3857(3)	29(2)
C(4)	9554(5)	7427(8)	3730(3)	24(2)
C(5)	10509(5)	7380(8)	3985(3)	20(2)
C(6)	10382(5)	7454(7)	4484(3)	15(2)
C(7)	9097(5)	8783(7)	5337(3)	15(2)
C(8)	9052(5)	8807(7)	5811(3)	18(2)
C(9)	8191(5)	9067(7)	5977(3)	18(2)
C(10)	8081(5)	9134(7)	6427(3)	19(2)
C(11)	8874(5)	8891(7)	6716(3)	22(2)
C(12)	9742(5)	8578(7)	6576(3)	20(2)
C(13)	9860(5)	8525(8)	6109(3)	20(2)
C(14)	7172(5)	9466(8)	6632(3)	23(2)
C(15)	6936(5)	8365(9)	6957(3)	38(2)
C(16)	6368(5)	9575(10)	6268(3)	42(3)
C(17)	7262(6)	10772(9)	6886(3)	49(3)
C(18)	10543(5)	8260(8)	6915(3)	26(2)
C(19)	10260(5)	8295(10)	7408(3)	39(2)
C(20)	11288(6)	9343(9)	6881(3)	35(2)
C(21)	10950(6)	6918(8)	6838(3)	31(2)
C(22)	12046(5)	7310(7)	4650(3)	17(2)
C(23)	12882(5)	7274(7)	4933(3)	21(2)
C(24)	12854(5)	7201(7)	5402(3)	17(2)
C(25)	13708(5)	6953(7)	5669(3)	20(2)

C(26)	14509(5)	6884(7)	5437(3)	17(2)
C(27)	14551(5)	7046(7)	4971(3)	20(2)
C(28)	13732(5)	7171(7)	4721(3)	17(2)
C(29)	13709(5)	6808(8)	6177(3)	22(2)
C(30)	13064(5)	5690(9)	6299(3)	34(2)
C(31)	13426(5)	8120(9)	6373(3)	38(2)
C(32)	14675(5)	6452(9)	6381(3)	32(2)
C(33)	15498(5)	6965(8)	4753(3)	25(2)
C(34)	15750(6)	5523(9)	4703(4)	56(3)
C(35)	15439(5)	7595(12)	4293(3)	58(3)
C(36)	16250(5)	7632(10)	5057(3)	45(3)
C(7S)	6824(7)	4427(10)	6520(5)	64(3)
C(8S)	6953(7)	4824(9)	6079(4)	53(3)
C(9S)	7769(7)	5421(9)	5984(4)	47(2)
C(10S)	8436(6)	5603(8)	6325(4)	44(2)
C(11S)	8294(7)	5185(9)	6757(4)	50(3)
C(12S)	7497(8)	4594(10)	6851(4)	60(3)
Co(1')	9046(1)	7789(1)	330(1)	19(1)
Cl(1')	8490(1)	5647(2)	221(1)	31(1)
O(1')	9552(3)	7742(5)	918(2)	19(1)
O(2')	8015(3)	8548(5)	559(2)	20(1)
N(1')	10159(4)	7401(6)	80(2)	18(1)
N(2')	8671(4)	8418(6)	-259(2)	15(1)
C(1')	10061(5)	7314(8)	-418(3)	18(2)
C(2')	10946(5)	7287(8)	-676(3)	26(2)
C(3')	10675(5)	7322(9)	-1183(3)	33(2)
C(4')	10102(5)	8526(8)	-1299(3)	28(2)
C(5')	9215(5)	8582(8)	-1052(3)	24(2)
C(6')	9459(5)	8508(7)	-555(3)	15(2)
C(7')	10953(5)	7189(8)	295(3)	18(2)
C(8')	11110(5)	7148(7)	773(3)	16(2)
C(9')	12011(5)	6893(7)	950(3)	19(2)
C(10')	12238(5)	6776(8)	1395(3)	21(2)
C(11')	11528(5)	7011(7)	1684(3)	20(2)
C(12')	10615(5)	7340(8)	1544(3)	20(2)
C(13')	10394(5)	7415(7)	1062(3)	15(2)

C(14')	13211(5)	6458(8)	1596(3)	23(2)
C(15')	13530(5)	7470(8)	1959(3)	29(2)
C(16')	13176(6)	5075(8)	1795(3)	46(3)
C(17')	13924(5)	6467(9)	1239(3)	33(2)
C(18')	9888(5)	7639(8)	1885(3)	26(2)
C(19')	10291(5)	7504(9)	2373(3)	36(2)
C(20')	9087(5)	6651(8)	1828(3)	28(2)
C(21')	9523(5)	9050(8)	1819(3)	27(2)
C(22')	7822(5)	8628(7)	-392(3)	20(2)
C(23')	7066(5)	8670(7)	-123(3)	17(2)
C(24')	7192(5)	8731(7)	354(3)	19(2)
C(25')	6428(5)	9009(7)	609(3)	20(2)
C(26')	5580(5)	9104(7)	381(3)	20(2)
C(27')	5404(5)	8956(7)	-91(3)	17(2)
C(28')	6150(5)	8777(7)	-336(3)	22(2)
C(29')	6545(5)	9135(8)	1120(3)	22(2)
C(30')	7254(5)	10211(8)	1253(3)	30(2)
C(31')	6842(5)	7793(8)	1321(3)	30(2)
C(32')	5644(5)	9553(9)	1327(3)	29(2)
C(33')	4424(5)	9051(8)	-308(3)	24(2)
C(34')	4109(6)	10470(9)	-288(3)	35(2)
C(35')	4357(6)	8613(9)	-792(3)	41(2)
C(36')	3759(5)	8204(9)	-39(3)	39(2)
C(1S)	6006(8)	6938(12)	3188(4)	73(3)
C(2S)	5470(7)	7818(12)	2942(4)	65(3)
C(3S)	5872(8)	8700(11)	2666(4)	66(3)
C(4S)	6815(9)	8680(11)	2628(4)	70(3)
C(5S)	7339(7)	7759(14)	2889(4)	75(3)
C(6S)	6918(9)	6917(12)	3151(4)	76(4)
C(13S)	5575(8)	4371(12)	2382(4)	67(3)
C(14S)	5636(8)	3053(13)	2379(4)	73(3)
C(15S)	6338(9)	2482(11)	2182(5)	85(4)
C(16S)	7010(8)	3216(14)	1969(4)	88(4)
C(17S)	6891(8)	4567(11)	1965(4)	65(3)
C(18S)	6198(8)	5098(11)	2173(4)	65(3)
C(19S)	7828(7)	5734(10)	-1785(4)	58(3)

C(20S)	6967(8)	6373(10)	-1874(4)	57(3)
C(21S)	6388(7)	6484(9)	-1544(4)	49(3)
C(22S)	6637(6)	6109(9)	-1117(4)	45(2)
C(23S)	7489(6)	5486(9)	-1013(4)	45(2)
C(24S)	8074(7)	5325(9)	-1355(4)	51(3)

Table 3. Bond lengths [Å] and angles [°] for (*R,R*)-(salen-**1**)CoCl.

Co(1)-O(2)	1.844(5)
Co(1)-O(1)	1.845(5)
Co(1)-N(1)	1.882(6)
Co(1)-N(2)	1.887(6)
Co(1)-Cl(1)	2.330(2)
O(1)-C(13)	1.307(8)
O(2)-C(24)	1.305(9)
N(1)-C(7)	1.311(9)
N(1)-C(1)	1.468(10)
N(2)-C(22)	1.280(9)
N(2)-C(6)	1.503(9)
C(1)-C(2)	1.520(10)
C(1)-C(6)	1.524(10)
C(2)-C(3)	1.540(11)
C(3)-C(4)	1.510(10)
C(4)-C(5)	1.538(9)
C(5)-C(6)	1.508(10)
C(7)-C(8)	1.415(11)
C(8)-C(9)	1.397(10)
C(8)-C(13)	1.452(10)
C(9)-C(10)	1.361(11)
C(10)-C(11)	1.415(10)
C(10)-C(14)	1.526(11)
C(11)-C(12)	1.388(10)
C(12)-C(13)	1.413(11)
C(12)-C(18)	1.526(10)
C(14)-C(17)	1.522(12)
C(14)-C(15)	1.527(11)
C(14)-C(16)	1.544(11)
C(18)-C(21)	1.503(11)
C(18)-C(20)	1.546(11)
C(18)-C(19)	1.548(11)
C(22)-C(23)	1.432(10)
C(23)-C(24)	1.401(11)

C(23)-C(28)	1.425(10)
C(24)-C(25)	1.451(10)
C(25)-C(26)	1.390(10)
C(25)-C(29)	1.520(11)
C(26)-C(27)	1.402(11)
C(27)-C(28)	1.367(10)
C(27)-C(33)	1.557(11)
C(29)-C(31)	1.516(11)
C(29)-C(30)	1.525(11)
C(29)-C(32)	1.535(10)
C(33)-C(35)	1.508(12)
C(33)-C(34)	1.512(12)
C(33)-C(36)	1.528(11)
C(7S)-C(12S)	1.352(14)
C(7S)-C(8S)	1.398(15)
C(8S)-C(9S)	1.375(13)
C(9S)-C(10S)	1.369(12)
C(10S)-C(11S)	1.381(13)
C(11S)-C(12S)	1.347(13)
Co(1')-O(2')	1.848(5)
Co(1')-O(1')	1.856(5)
Co(1')-N(1')	1.863(6)
Co(1')-N(2')	1.912(6)
Co(1')-Cl(1')	2.326(2)
O(1')-C(13')	1.311(8)
O(2')-C(24')	1.319(8)
N(1')-C(7')	1.299(9)
N(1')-C(1')	1.482(10)
N(2')-C(22')	1.287(8)
N(2')-C(6')	1.488(9)
C(1')-C(6')	1.531(10)
C(1')-C(2')	1.537(10)
C(2')-C(3')	1.536(11)
C(3')-C(4')	1.501(11)
C(4')-C(5')	1.523(10)
C(5')-C(6')	1.502(10)

C(7')-C(8')	1.427(11)
C(8')-C(9')	1.403(10)
C(8')-C(13')	1.417(11)
C(9')-C(10')	1.347(11)
C(10')-C(11')	1.405(10)
C(10')-C(14')	1.532(10)
C(11')-C(12')	1.403(10)
C(12')-C(13')	1.452(11)
C(12')-C(18')	1.540(10)
C(14')-C(16')	1.520(12)
C(14')-C(17')	1.529(11)
C(14')-C(15')	1.537(11)
C(18')-C(21')	1.530(11)
C(18')-C(20')	1.532(11)
C(18')-C(19')	1.537(11)
C(22')-C(23')	1.399(10)
C(23')-C(24')	1.421(11)
C(23')-C(28')	1.440(10)
C(24')-C(25')	1.411(11)
C(25')-C(26')	1.370(10)
C(25')-C(29')	1.525(11)
C(26')-C(27')	1.421(11)
C(27')-C(28')	1.355(11)
C(27')-C(33')	1.526(10)
C(29')-C(30')	1.532(11)
C(29')-C(31')	1.533(11)
C(29')-C(32')	1.538(11)
C(33')-C(35')	1.507(11)
C(33')-C(34')	1.508(11)
C(33')-C(36')	1.550(11)
C(1S)-C(6S)	1.336(15)
C(1S)-C(2S)	1.363(15)
C(2S)-C(3S)	1.369(15)
C(3S)-C(4S)	1.380(15)
C(4S)-C(5S)	1.405(16)
C(5S)-C(6S)	1.329(16)

C(13S)-C(14S)	1.335(16)
C(13S)-C(18S)	1.348(14)
C(14S)-C(15S)	1.338(15)
C(15S)-C(16S)	1.407(16)
C(16S)-C(17S)	1.376(16)
C(17S)-C(18S)	1.327(14)
C(19S)-C(24S)	1.372(14)
C(19S)-C(20S)	1.416(14)
C(20S)-C(21S)	1.338(13)
C(21S)-C(22S)	1.353(13)
C(22S)-C(23S)	1.404(12)
C(23S)-C(24S)	1.375(13)

O(2)-Co(1)-O(1)	87.0(2)
O(2)-Co(1)-N(1)	167.3(2)
O(1)-Co(1)-N(1)	93.7(2)
O(2)-Co(1)-N(2)	90.4(2)
O(1)-Co(1)-N(2)	161.7(2)
N(1)-Co(1)-N(2)	85.0(3)
O(2)-Co(1)-Cl(1)	98.34(17)
O(1)-Co(1)-Cl(1)	102.69(18)
N(1)-Co(1)-Cl(1)	93.94(18)
N(2)-Co(1)-Cl(1)	95.64(19)
C(13)-O(1)-Co(1)	130.9(5)
C(24)-O(2)-Co(1)	127.0(5)
C(7)-N(1)-C(1)	122.6(6)
C(7)-N(1)-Co(1)	125.8(6)
C(1)-N(1)-Co(1)	111.6(4)
C(22)-N(2)-C(6)	122.1(6)
C(22)-N(2)-Co(1)	124.7(5)
C(6)-N(2)-Co(1)	112.6(4)
N(1)-C(1)-C(2)	117.1(6)
N(1)-C(1)-C(6)	104.5(6)
C(2)-C(1)-C(6)	111.5(6)
C(1)-C(2)-C(3)	108.7(6)
C(4)-C(3)-C(2)	112.0(7)

C(3)-C(4)-C(5)	111.0(7)
C(6)-C(5)-C(4)	108.8(6)
N(2)-C(6)-C(5)	116.9(6)
N(2)-C(6)-C(1)	104.1(6)
C(5)-C(6)-C(1)	113.8(6)
N(1)-C(7)-C(8)	126.7(7)
C(9)-C(8)-C(7)	117.0(7)
C(9)-C(8)-C(13)	121.7(8)
C(7)-C(8)-C(13)	121.2(7)
C(10)-C(9)-C(8)	121.4(8)
C(9)-C(10)-C(11)	116.6(7)
C(9)-C(10)-C(14)	124.3(7)
C(11)-C(10)-C(14)	119.0(8)
C(12)-C(11)-C(10)	125.1(8)
C(11)-C(12)-C(13)	118.3(7)
C(11)-C(12)-C(18)	121.1(7)
C(13)-C(12)-C(18)	120.6(6)
O(1)-C(13)-C(12)	121.5(7)
O(1)-C(13)-C(8)	121.7(7)
C(12)-C(13)-C(8)	116.8(7)
C(17)-C(14)-C(10)	109.9(7)
C(17)-C(14)-C(15)	109.5(7)
C(10)-C(14)-C(15)	109.1(6)
C(17)-C(14)-C(16)	108.9(7)
C(10)-C(14)-C(16)	111.6(7)
C(15)-C(14)-C(16)	107.8(7)
C(21)-C(18)-C(12)	112.2(7)
C(21)-C(18)-C(20)	110.3(6)
C(12)-C(18)-C(20)	108.3(7)
C(21)-C(18)-C(19)	107.3(7)
C(12)-C(18)-C(19)	112.7(6)
C(20)-C(18)-C(19)	106.0(7)
N(2)-C(22)-C(23)	124.3(8)
C(24)-C(23)-C(28)	121.1(7)
C(24)-C(23)-C(22)	120.7(7)
C(28)-C(23)-C(22)	117.8(8)

O(2)-C(24)-C(23)	122.1(7)
O(2)-C(24)-C(25)	119.4(7)
C(23)-C(24)-C(25)	118.5(7)
C(26)-C(25)-C(24)	116.7(8)
C(26)-C(25)-C(29)	122.8(7)
C(24)-C(25)-C(29)	120.5(7)
C(25)-C(26)-C(27)	125.1(7)
C(28)-C(27)-C(26)	117.3(7)
C(28)-C(27)-C(33)	122.6(8)
C(26)-C(27)-C(33)	120.0(7)
C(27)-C(28)-C(23)	120.9(8)
C(31)-C(29)-C(25)	108.4(7)
C(31)-C(29)-C(30)	111.8(7)
C(25)-C(29)-C(30)	110.3(7)
C(31)-C(29)-C(32)	108.4(7)
C(25)-C(29)-C(32)	111.0(6)
C(30)-C(29)-C(32)	106.9(7)
C(35)-C(33)-C(34)	108.5(8)
C(35)-C(33)-C(36)	110.3(7)
C(34)-C(33)-C(36)	108.3(7)
C(35)-C(33)-C(27)	110.8(7)
C(34)-C(33)-C(27)	108.5(6)
C(36)-C(33)-C(27)	110.3(7)
C(12S)-C(7S)-C(8S)	121.1(11)
C(9S)-C(8S)-C(7S)	119.1(10)
C(10S)-C(9S)-C(8S)	119.0(10)
C(9S)-C(10S)-C(11S)	120.6(9)
C(12S)-C(11S)-C(10S)	120.7(10)
C(11S)-C(12S)-C(7S)	119.5(12)
O(2')-Co(1')-O(1')	86.8(2)
O(2')-Co(1')-N(1')	167.7(2)
O(1')-Co(1')-N(1')	94.0(2)
O(2')-Co(1')-N(2')	90.6(2)
O(1')-Co(1')-N(2')	161.2(2)
N(1')-Co(1')-N(2')	84.6(3)
O(2')-Co(1')-Cl(1')	98.99(16)

O(1')-Co(1')-Cl(1')	102.76(17)
N(1')-Co(1')-Cl(1')	92.85(19)
N(2')-Co(1')-Cl(1')	96.05(18)
C(13')-O(1')-Co(1')	128.3(5)
C(24')-O(2')-Co(1')	128.2(5)
C(7')-N(1')-C(1')	120.5(6)
C(7')-N(1')-Co(1')	127.1(6)
C(1')-N(1')-Co(1')	112.4(4)
C(22')-N(2')-C(6')	124.4(6)
C(22')-N(2')-Co(1')	123.2(5)
C(6')-N(2')-Co(1')	112.2(4)
N(1')-C(1')-C(6')	103.6(6)
N(1')-C(1')-C(2')	118.1(6)
C(6')-C(1')-C(2')	111.2(6)
C(3')-C(2')-C(1')	108.7(6)
C(4')-C(3')-C(2')	110.4(7)
C(3')-C(4')-C(5')	113.0(7)
C(6')-C(5')-C(4')	108.7(6)
N(2')-C(6')-C(5')	116.3(6)
N(2')-C(6')-C(1')	104.0(6)
C(5')-C(6')-C(1')	113.3(6)
N(1')-C(7')-C(8')	125.2(7)
C(9')-C(8')-C(13')	120.5(8)
C(9')-C(8')-C(7')	117.9(7)
C(13')-C(8')-C(7')	121.6(7)
C(10')-C(9')-C(8')	123.4(7)
C(9')-C(10')-C(11')	116.4(7)
C(9')-C(10')-C(14')	124.4(7)
C(11')-C(10')-C(14')	119.2(8)
C(12')-C(11')-C(10')	125.0(8)
C(11')-C(12')-C(13')	116.8(7)
C(11')-C(12')-C(18')	121.6(7)
C(13')-C(12')-C(18')	121.6(6)
O(1')-C(13')-C(8')	123.6(7)
O(1')-C(13')-C(12')	118.6(6)
C(8')-C(13')-C(12')	117.8(7)

C(16')-C(14')-C(17')	108.5(7)
C(16')-C(14')-C(10')	107.0(6)
C(17')-C(14')-C(10')	111.9(7)
C(16')-C(14')-C(15')	110.7(7)
C(17')-C(14')-C(15')	107.3(6)
C(10')-C(14')-C(15')	111.4(6)
C(21')-C(18')-C(20')	109.9(6)
C(21')-C(18')-C(19')	108.2(7)
C(20')-C(18')-C(19')	106.7(7)
C(21')-C(18')-C(12')	110.1(7)
C(20')-C(18')-C(12')	110.2(7)
C(19')-C(18')-C(12')	111.7(6)
N(2')-C(22')-C(23')	126.8(8)
C(22')-C(23')-C(24')	121.2(7)
C(22')-C(23')-C(28')	119.1(8)
C(24')-C(23')-C(28')	119.5(7)
O(2')-C(24')-C(25')	119.9(8)
O(2')-C(24')-C(23')	120.7(7)
C(25')-C(24')-C(23')	119.4(7)
C(26')-C(25')-C(24')	117.3(8)
C(26')-C(25')-C(29')	121.9(7)
C(24')-C(25')-C(29')	120.8(7)
C(25')-C(26')-C(27')	125.6(7)
C(28')-C(27')-C(26')	116.5(7)
C(28')-C(27')-C(33')	122.5(8)
C(26')-C(27')-C(33')	121.0(7)
C(27')-C(28')-C(23')	121.4(8)
C(25')-C(29')-C(30')	110.3(7)
C(25')-C(29')-C(31')	109.1(7)
C(30')-C(29')-C(31')	111.1(6)
C(25')-C(29')-C(32')	112.2(7)
C(30')-C(29')-C(32')	106.0(7)
C(31')-C(29')-C(32')	108.2(7)
C(35')-C(33')-C(34')	108.4(7)
C(35')-C(33')-C(27')	112.9(7)
C(34')-C(33')-C(27')	108.6(6)

C(35')-C(33')-C(36')	109.0(7)
C(34')-C(33')-C(36')	107.8(7)
C(27')-C(33')-C(36')	110.0(7)
C(6S)-C(1S)-C(2S)	120.0(12)
C(1S)-C(2S)-C(3S)	119.8(11)
C(2S)-C(3S)-C(4S)	120.2(11)
C(3S)-C(4S)-C(5S)	117.9(12)
C(6S)-C(5S)-C(4S)	119.8(11)
C(5S)-C(6S)-C(1S)	122.2(12)
C(14S)-C(13S)-C(18S)	119.6(12)
C(13S)-C(14S)-C(15S)	119.1(12)
C(14S)-C(15S)-C(16S)	122.6(11)
C(17S)-C(16S)-C(15S)	115.9(11)
C(18S)-C(17S)-C(16S)	119.7(11)
C(17S)-C(18S)-C(13S)	123.0(11)
C(24S)-C(19S)-C(20S)	119.1(10)
C(21S)-C(20S)-C(19S)	119.2(11)
C(20S)-C(21S)-C(22S)	121.6(11)
C(21S)-C(22S)-C(23S)	120.7(10)
C(24S)-C(23S)-C(22S)	117.8(10)
C(19S)-C(24S)-C(23S)	121.3(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R,R*)-(salen-**1**)CoCl. 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(1)	13(1)	20(1)	25(1)	-1(1)	1(1)	1(1)
Cl(1)	23(1)	25(1)	52(2)	-7(1)	6(1)	-3(1)
O(1)	13(3)	32(3)	26(3)	-6(3)	6(2)	1(3)
O(2)	19(3)	24(3)	23(3)	7(3)	0(2)	12(2)
N(1)	10(3)	18(4)	20(4)	-1(3)	-1(3)	-6(3)
N(2)	8(3)	24(4)	14(3)	1(3)	-1(3)	-1(3)
C(1)	16(4)	17(4)	26(4)	1(4)	2(3)	4(3)
C(2)	13(4)	21(5)	23(5)	2(4)	-6(3)	3(3)
C(3)	24(5)	35(5)	28(5)	0(4)	-7(4)	8(4)
C(4)	18(4)	37(5)	17(5)	-3(4)	-2(3)	5(4)
C(5)	7(4)	29(5)	23(4)	0(4)	1(3)	2(3)
C(6)	14(4)	12(4)	18(4)	-2(4)	-8(3)	-6(3)
C(7)	6(4)	14(5)	25(4)	-2(4)	-9(3)	2(4)
C(8)	18(4)	11(4)	25(4)	2(4)	0(3)	0(4)
C(9)	5(4)	17(4)	31(5)	3(4)	-2(3)	-5(3)
C(10)	20(4)	9(4)	30(5)	0(4)	6(3)	1(3)
C(11)	22(4)	20(5)	23(5)	5(4)	7(3)	-3(4)
C(12)	20(4)	21(5)	18(4)	-4(4)	0(3)	-3(3)
C(13)	10(4)	23(5)	26(4)	5(4)	1(3)	-1(4)
C(14)	15(4)	31(5)	24(5)	5(4)	3(3)	2(4)
C(15)	19(5)	48(5)	49(6)	10(5)	17(4)	6(4)
C(16)	15(4)	79(7)	33(6)	11(5)	15(4)	6(5)
C(17)	41(6)	38(5)	69(8)	-16(5)	21(5)	8(5)
C(18)	24(4)	31(5)	22(4)	6(4)	2(3)	5(4)
C(19)	33(5)	54(6)	28(5)	10(5)	0(4)	-2(5)
C(20)	32(5)	44(5)	29(6)	-4(5)	-2(4)	-9(4)
C(21)	19(5)	39(5)	35(6)	9(4)	-1(4)	0(4)
C(22)	17(4)	18(5)	16(5)	1(4)	-4(3)	-2(4)
C(23)	16(4)	12(4)	34(5)	-1(4)	-1(3)	2(4)
C(24)	19(4)	10(4)	21(4)	-9(4)	0(3)	2(4)
C(25)	12(4)	19(4)	29(4)	7(4)	-2(3)	-7(4)

C(26)	8(4)	20(5)	23(4)	1(4)	-1(3)	2(3)
C(27)	13(4)	16(4)	30(5)	0(4)	-3(3)	-2(3)
C(28)	15(4)	13(5)	24(5)	-3(4)	5(3)	-1(4)
C(29)	5(4)	34(5)	27(5)	-3(4)	1(4)	3(3)
C(30)	17(4)	41(5)	43(6)	21(5)	-9(4)	-4(4)
C(31)	32(5)	37(5)	46(6)	-11(5)	-1(4)	6(4)
C(32)	13(4)	43(6)	39(6)	9(5)	-6(4)	3(4)
C(33)	14(4)	28(5)	32(5)	5(4)	6(4)	-10(4)
C(34)	16(5)	41(5)	114(10)	-6(5)	31(5)	-6(4)
C(35)	24(5)	96(8)	57(6)	23(6)	21(4)	11(6)
C(36)	9(4)	55(6)	71(7)	-9(6)	11(4)	-16(4)
C(7S)	36(6)	43(6)	113(9)	28(7)	7(6)	0(5)
C(8S)	45(6)	23(6)	87(7)	-3(6)	-24(6)	1(4)
C(9S)	53(6)	33(6)	57(7)	-2(5)	10(5)	11(5)
C(10S)	30(5)	20(5)	81(7)	0(6)	0(5)	3(4)
C(11S)	43(5)	37(6)	67(7)	-10(6)	-12(5)	11(5)
C(12S)	64(7)	46(7)	72(8)	7(6)	12(6)	1(6)
Co(1')	12(1)	21(1)	23(1)	1(1)	0(1)	2(1)
Cl(1')	21(1)	22(1)	50(2)	6(1)	-5(1)	-3(1)
O(1')	7(3)	30(3)	20(3)	3(3)	-1(2)	4(2)
O(2')	10(3)	28(3)	21(3)	-1(3)	0(2)	6(2)
N(1')	17(3)	13(4)	23(4)	1(3)	3(3)	2(3)
N(2')	13(3)	17(4)	15(3)	-8(3)	-5(3)	-7(3)
C(1')	18(4)	16(4)	21(4)	1(4)	-2(3)	-3(3)
C(2')	20(4)	35(5)	23(5)	2(4)	2(4)	4(4)
C(3')	16(5)	57(6)	25(5)	0(5)	2(4)	4(4)
C(4')	27(5)	36(5)	22(5)	6(4)	1(4)	-3(4)
C(5')	25(4)	21(5)	27(5)	5(4)	0(4)	-2(4)
C(6')	14(4)	12(4)	20(4)	0(4)	0(3)	-4(3)
C(7')	21(4)	19(5)	14(4)	-2(4)	11(3)	2(4)
C(8')	10(4)	18(4)	21(4)	1(4)	1(3)	1(4)
C(9')	12(4)	20(5)	24(5)	-4(4)	4(3)	5(3)
C(10')	9(4)	25(5)	29(5)	7(4)	-2(3)	-4(3)
C(11')	12(4)	21(5)	26(5)	5(4)	-1(3)	-2(4)
C(12')	16(4)	23(5)	20(4)	6(4)	0(3)	0(3)
C(13')	6(4)	18(5)	22(4)	0(4)	4(3)	-4(3)

C(14')	11(4)	26(5)	31(5)	5(4)	-5(3)	6(4)
C(15')	9(4)	37(5)	39(6)	-8(4)	-7(4)	2(4)
C(16')	41(6)	32(5)	62(8)	2(5)	-7(5)	15(4)
C(17')	11(4)	45(6)	41(6)	-8(5)	-7(4)	1(4)
C(18')	20(4)	40(5)	18(4)	6(4)	0(3)	6(4)
C(19')	30(5)	61(6)	18(4)	6(5)	3(4)	15(5)
C(20')	12(4)	38(5)	35(6)	-1(5)	13(4)	4(4)
C(21')	4(4)	37(5)	41(6)	1(4)	2(4)	3(4)
C(22')	16(4)	18(5)	26(5)	2(4)	-5(3)	1(4)
C(23')	15(4)	12(4)	25(4)	4(4)	-1(3)	-3(3)
C(24')	16(4)	12(4)	29(4)	8(4)	-2(3)	5(4)
C(25')	19(4)	12(4)	29(4)	-1(4)	2(3)	-3(4)
C(26')	10(4)	13(4)	37(5)	3(4)	6(3)	-1(3)
C(27')	13(4)	8(4)	29(5)	4(4)	-3(3)	-4(3)
C(28')	21(4)	13(5)	31(5)	-1(4)	-6(3)	3(4)
C(29')	13(4)	23(4)	28(5)	5(4)	1(4)	-3(3)
C(30')	27(5)	30(5)	31(6)	-12(4)	-2(4)	-2(4)
C(31')	28(5)	37(5)	25(5)	5(4)	-4(4)	-1(4)
C(32')	20(4)	39(6)	30(6)	-3(5)	6(4)	-5(4)
C(33')	13(4)	27(5)	32(5)	-1(4)	1(4)	2(4)
C(34')	27(5)	36(5)	39(6)	9(4)	-14(4)	8(4)
C(35')	26(5)	57(6)	39(5)	-10(5)	-14(4)	-2(5)
C(36')	7(4)	45(6)	64(6)	25(5)	-12(4)	0(4)
C(1S)	78(7)	69(8)	72(9)	-2(6)	15(7)	2(6)
C(2S)	51(6)	74(8)	71(9)	-32(6)	13(5)	14(5)
C(3S)	84(7)	54(7)	57(8)	-9(5)	-19(6)	20(6)
C(4S)	90(7)	62(8)	59(8)	-15(6)	6(7)	-25(7)
C(5S)	50(6)	97(10)	77(9)	-29(7)	-3(5)	-5(6)
C(6S)	79(7)	67(8)	83(10)	-5(6)	4(7)	38(7)
C(13S)	56(7)	67(6)	78(9)	-7(7)	0(6)	5(6)
C(14S)	79(8)	72(6)	67(8)	-6(7)	8(6)	-30(7)
C(15S)	122(10)	33(6)	100(11)	-12(6)	17(8)	-6(6)
C(16S)	85(8)	86(7)	97(10)	-22(9)	30(7)	16(7)
C(17S)	64(7)	59(6)	73(9)	-18(6)	14(6)	-31(6)
C(18S)	77(8)	50(6)	67(9)	13(6)	7(6)	15(5)
C(19S)	55(6)	41(6)	79(7)	-8(6)	28(6)	-15(5)

C(20S)	70(7)	42(7)	60(7)	13(6)	6(5)	-24(5)
C(21S)	35(6)	36(6)	74(8)	9(6)	0(5)	-6(5)
C(22S)	42(5)	36(6)	58(6)	-4(5)	10(5)	-15(4)
C(23S)	41(6)	27(6)	66(7)	-1(5)	-1(5)	-15(4)
C(24S)	43(6)	25(6)	85(8)	-4(6)	13(5)	-13(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R,R*)-(salen-**1**)CoCl.

	x	y	z	U(eq)
H(1)	10168	9462	4544	24
H(2B)	8557	9522	4438	23
H(2A)	8502	7936	4451	23
H(3B)	8415	8649	3687	35
H(3A)	9366	9443	3770	35
H(4B)	9631	7431	3402	29
H(4A)	9199	6626	3802	29
H(5B)	10829	6548	3914	23
H(5A)	10890	8133	3893	23
H(6)	10033	6644	4566	18
H(7)	8537	8944	5163	19
H(9)	7672	9200	5771	21
H(11)	8808	8947	7031	26
H(15C)	6354	8575	7091	57
H(15B)	7431	8287	7195	57
H(15A)	6872	7526	6793	57
H(16C)	6497	10287	6058	63
H(16B)	5794	9770	6412	63
H(16A)	6302	8736	6104	63
H(17C)	7416	11478	6677	73
H(17B)	7752	10699	7126	73
H(17A)	6676	10980	7016	73
H(19C)	9788	7619	7450	58
H(19B)	10009	9169	7474	58
H(19A)	10802	8118	7613	58
H(20C)	11498	9359	6574	53
H(20B)	11812	9152	7095	53
H(20A)	11025	10207	6951	53
H(21C)	10469	6242	6856	47
H(21B)	11449	6745	7067	47

H(21A)	11196	6892	6539	47
H(22)	12090	7176	4336	21
H(26)	15072	6715	5608	21
H(28)	13730	7190	4402	21
H(30C)	12433	5896	6184	51
H(30B)	13081	5594	6627	51
H(30A)	13264	4862	6164	51
H(31C)	12805	8354	6250	58
H(31B)	13863	8808	6294	58
H(31A)	13426	8045	6701	58
H(32C)	15113	7149	6310	49
H(32B)	14872	5609	6255	49
H(32A)	14659	6369	6708	49
H(34C)	16350	5456	4570	83
H(34B)	15278	5081	4507	83
H(34A)	15788	5098	5000	83
H(35C)	16043	7543	4164	87
H(35B)	15258	8524	4319	87
H(35A)	14979	7126	4097	87
H(36C)	16841	7573	4916	67
H(36B)	16301	7185	5350	67
H(36A)	16090	8563	5099	67
H(7SA)	6255	4034	6589	76
H(8SA)	6482	4683	5847	64
H(9SA)	7870	5703	5687	57
H(10A)	9001	6020	6264	53
H(11C)	8764	5315	6990	60
H(12A)	7408	4297	7148	72
H(1')	9700	6496	-499	22
H(2D)	11337	8060	-590	31
H(2C)	11302	6473	-600	31
H(3D)	11239	7335	-1353	39
H(3C)	10319	6516	-1270	39
H(4C)	9943	8535	-1627	34
H(4D)	10474	9327	-1224	34
H(5D)	8881	9416	-1125	29

H(5C)	8808	7832	-1147	29
H(6')	9817	9324	-467	18
H(7')	11470	7051	120	21
H(9')	12486	6798	747	22
H(11')	11678	6942	1999	24
H(15F)	14152	7240	2082	43
H(15E)	13103	7459	2201	43
H(15D)	13538	8356	1825	43
H(16F)	13787	4838	1930	68
H(16E)	12993	4441	1557	68
H(16D)	12725	5056	2027	68
H(17F)	14536	6268	1381	49
H(17E)	13933	7341	1097	49
H(17D)	13759	5796	1010	49
H(19F)	9808	7681	2580	54
H(19E)	10795	8142	2427	54
H(19E)	10529	6605	2423	54
H(20F)	8632	6847	2048	41
H(20D)	9324	5751	1877	41
H(20E)	8795	6725	1523	41
H(21F)	9055	9227	2035	41
H(21E)	9247	9150	1512	41
H(21D)	10034	9679	1868	41
H(22')	7696	8770	-705	24
H(26')	5066	9285	554	24
H(28')	6067	8721	-654	26
H(30F)	7318	10287	1582	44
H(30E)	7046	11059	1123	44
H(30D)	7852	9976	1140	44
H(31F)	6915	7865	1650	45
H(31E)	7431	7528	1204	45
H(31D)	6371	7128	1238	45
H(32F)	5751	9624	1654	44
H(32E)	5165	8890	1255	44
H(32D)	5443	10412	1203	44
H(34F)	4528	11032	-449	52

H(34E)	4113	10755	27	52
H(34D)	3482	10546	-428	52
H(35F)	4570	7696	-812	62
H(35E)	4742	9186	-968	62
H(35D)	3713	8671	-912	62
H(36F)	3948	7274	-47	59
H(36E)	3128	8293	-175	59
H(36D)	3779	8510	273	59
H(1SA)	5730	6339	3386	87
H(2SA)	4819	7818	2962	78
H(3SA)	5502	9329	2500	79
H(4SA)	7101	9270	2431	84
H(5SA)	7992	7739	2879	90
H(6SA)	7278	6278	3318	91
H(13C)	5096	4794	2532	81
H(14A)	5186	2528	2514	87
H(15G)	6385	1544	2186	102
H(16G)	7515	2804	1837	106
H(17G)	7303	5116	1814	78
H(18A)	6138	6034	2174	77
H(19G)	8230	5590	-2020	69
H(20G)	6803	6719	-2165	69
H(21G)	5788	6836	-1610	58
H(22C)	6231	6268	-884	54
H(23A)	7655	5185	-716	54
H(24C)	8659	4922	-1291	61

Table 1. Crystal data and structure refinement for *rac*-(salen-**1**)CoI.

Identification code	*rac*-(salen-**1**)CoI	
Empirical formula	C36 H52 Co I N2 O2 * CH2Cl2, 1/2(C6H14)	
Formula weight	858.64	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.969(4) Å	α= 97.299(9)°.
	b = 12.522(5) Å	β= 105.834(9)°.
	c = 16.694(7) Å	γ = 106.802(9)°.
Volume	2058.3(14) $Å^3$	
Z	2	
Density (calculated)	1.385 Mg/m^3	
Absorption coefficient	1.331 mm^{-1}	
F(000)	890	
Crystal size	0.40 x 0.15 x 0.05 mm^3	
Theta range for data collection	2.04 to 24.71°.	
Index ranges	-12<=h<=11, -14<=k<=11, -19<=l<=19	
Reflections collected	10444	
Independent reflections	6823 [R(int) = 0.0491]	
Completeness to theta = 24.71°	97.2 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9364 and 0.6181	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6823 / 159 / 537	
Goodness-of-fit on F^2	0.881	
Final R indices [I>2sigma(I)]	R1 = 0.0563, wR2 = 0.1322	
R indices (all data)	R1 = 0.0995, wR2 = 0.1537	
Largest diff. peak and hole	0.690 and -0.847 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *rac*-(salen-**1**)CoI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	3723(1)	1632(1)	3717(1)	26(1)
Co(1)	1484(1)	248(1)	3939(1)	17(1)
Cl(1)	4645(2)	637(2)	1075(2)	83(1)
Cl(2)	3442(2)	2401(2)	806(1)	56(1)
O(1)	1086(3)	-1040(3)	3127(2)	20(1)
O(2)	264(3)	640(3)	3121(2)	20(1)
N(1)	2492(4)	-276(4)	4803(3)	21(1)
N(2)	1418(4)	1245(4)	4845(3)	25(1)
C(1)	3159(11)	609(9)	5606(7)	14(3)
C(1)	2605(12)	297(10)	5691(7)	23(3)
C(1S)	3410(6)	1200(6)	1232(4)	44(2)
C(2)	3821(6)	272(5)	6410(4)	25(1)
C(2S)	3930(8)	-2988(7)	605(5)	69(2)
C(3)	4314(11)	1228(10)	7167(7)	23(3)
C(3)	3779(14)	935(11)	7299(8)	28(3)
C(3S)	3863(7)	-4044(7)	-4(5)	56(2)
C(4)	3708(11)	2120(10)	7209(7)	29(3)
C(4)	3173(12)	1637(11)	7271(7)	22(3)
C(4S)	5002(7)	-4511(6)	308(5)	49(2)
C(5)	2490(5)	2033(5)	6462(3)	26(1)
C(6)	1967(10)	955(9)	5711(6)	14(2)
C(6)	2576(10)	1483(9)	5645(6)	17(2)
C(7)	2904(5)	-1148(5)	4702(3)	26(1)
C(8)	2546(5)	-1935(4)	3915(3)	17(1)
C(9)	3082(5)	-2840(4)	3918(3)	19(1)
C(10)	2735(5)	-3677(4)	3208(3)	19(1)
C(11)	1818(5)	-3578(4)	2450(3)	21(1)
C(12)	1259(5)	-2718(4)	2388(3)	19(1)
C(13)	1634(5)	-1854(4)	3154(3)	19(1)
C(14)	3179(5)	-4731(4)	3210(3)	21(1)
C(15)	2011(6)	-5723(5)	3253(5)	54(2)

C(16)	4407(6)	-4548(5)	3976(4)	35(2)
C(17)	3518(6)	-5038(6)	2410(4)	51(2)
C(18)	316(5)	-2665(5)	1544(3)	21(1)
C(19)	97(6)	-3629(5)	807(4)	38(2)
C(20)	914(6)	-1539(5)	1306(3)	29(2)
C(21)	-1088(5)	-2755(5)	1626(4)	28(2)
C(22)	692(5)	1907(5)	4781(3)	26(1)
C(23)	-119(5)	2070(4)	4012(3)	18(1)
C(24)	-230(5)	1475(4)	3206(3)	18(1)
C(25)	-938(5)	1778(4)	2457(3)	18(1)
C(26)	-1520(5)	2590(4)	2584(3)	21(1)
C(27)	-1469(5)	3166(4)	3370(3)	18(1)
C(28)	-768(5)	2888(4)	4092(3)	19(1)
C(29)	-991(5)	1255(5)	1562(3)	23(1)
C(30)	-1762(5)	-47(5)	1322(3)	28(2)
C(31)	441(5)	1457(5)	1528(3)	31(2)
C(32)	-1712(6)	1766(5)	878(3)	31(2)
C(33)	-2082(5)	4142(5)	3418(3)	23(1)
C(34)	-3493(5)	3751(6)	2767(4)	41(2)
C(35)	-1130(6)	5158(5)	3231(4)	43(2)
C(36)	-2194(6)	4481(5)	4302(4)	35(2)

Table 3. Bond lengths [Å] and angles [°] for *rac*-(salen-**1**)CoI.

I(1)-Co(1)	2.7144(11)
Co(1)-O(1)	1.828(3)
Co(1)-O(2)	1.858(3)
Co(1)-N(2)	1.866(4)
Co(1)-N(1)	1.877(4)
Cl(1)-C(1S)	1.760(7)
Cl(2)-C(1S)	1.739(8)
O(1)-C(13)	1.325(6)
O(2)-C(24)	1.318(6)
N(1)-C(7)	1.305(7)
N(1)-C(1)	1.476(11)
N(1)-C(1)	1.519(12)
N(2)-C(22)	1.300(7)
N(2)-C(6)	1.497(10)
N(2)-C(6)	1.539(11)
C(1)-C(2)	1.515(12)
C(1)-C(6)	1.537(16)
C(1)-C(6)	1.505(16)
C(1)-C(2)	1.543(12)
C(2)-C(3)	1.480(12)
C(2)-C(3)	1.624(14)
C(2S)-C(3S)	1.533(11)
C(3)-C(4)	1.459(17)
C(3)-C(4)	1.244(18)
C(3S)-C(4S)	1.523(11)
C(4)-C(5)	1.524(12)
C(4)-C(5)	1.569(13)
C(4S)-C(4S)#1	1.495(15)
C(5)-C(6)	1.487(12)
C(5)-C(6)	1.566(11)
C(7)-C(8)	1.421(7)
C(8)-C(9)	1.420(7)
C(8)-C(13)	1.422(7)
C(9)-C(10)	1.363(7)

C(10)-C(11)	1.430(7)
C(10)-C(14)	1.533(7)
C(11)-C(12)	1.387(8)
C(12)-C(13)	1.442(7)
C(12)-C(18)	1.526(7)
C(14)-C(17)	1.515(8)
C(14)-C(16)	1.519(7)
C(14)-C(15)	1.529(8)
C(18)-C(19)	1.524(8)
C(18)-C(20)	1.524(8)
C(18)-C(21)	1.557(7)
C(22)-C(23)	1.425(7)
C(23)-C(24)	1.409(7)
C(23)-C(28)	1.419(7)
C(24)-C(25)	1.440(7)
C(25)-C(26)	1.371(7)
C(25)-C(29)	1.532(7)
C(26)-C(27)	1.394(7)
C(27)-C(28)	1.385(7)
C(27)-C(33)	1.560(7)
C(29)-C(32)	1.525(8)
C(29)-C(31)	1.535(7)
C(29)-C(30)	1.545(7)
C(33)-C(35)	1.522(8)
C(33)-C(34)	1.524(7)
C(33)-C(36)	1.530(8)

O(1)-Co(1)-O(2)	86.13(15)
O(1)-Co(1)-N(2)	161.11(18)
O(2)-Co(1)-N(2)	93.56(18)
O(1)-Co(1)-N(1)	93.04(17)
O(2)-Co(1)-N(1)	171.42(17)
N(2)-Co(1)-N(1)	84.46(19)
O(1)-Co(1)-I(1)	100.62(12)
O(2)-Co(1)-I(1)	95.76(11)
N(2)-Co(1)-I(1)	98.21(14)

N(1)-Co(1)-I(1)	92.79(14)
C(13)-O(1)-Co(1)	129.3(3)
C(24)-O(2)-Co(1)	129.2(3)
C(7)-N(1)-C(1)	119.2(6)
C(7)-N(1)-C(1)	119.9(6)
C(1)-N(1)-C(1)	26.3(5)
C(7)-N(1)-Co(1)	126.8(4)
C(1)-N(1)-Co(1)	111.5(5)
C(1)-N(1)-Co(1)	112.5(5)
C(22)-N(2)-C(6)	119.3(6)
C(22)-N(2)-C(6)	119.6(6)
C(6)-N(2)-C(6)	31.9(5)
C(22)-N(2)-Co(1)	125.8(4)
C(6)-N(2)-Co(1)	112.8(5)
C(6)-N(2)-Co(1)	112.2(5)
N(1)-C(1)-C(2)	118.6(8)
N(1)-C(1)-C(6)	101.0(7)
C(2)-C(1)-C(6)	109.2(9)
C(6)-C(1)-N(1)	106.4(8)
C(6)-C(1)-C(2)	113.9(8)
N(1)-C(1)-C(2)	114.2(8)
Cl(2)-C(1S)-Cl(1)	112.2(4)
C(3)-C(2)-C(1)	111.3(7)
C(3)-C(2)-C(1)	114.0(7)
C(1)-C(2)-C(1)	25.8(5)
C(3)-C(2)-C(3)	25.6(6)
C(1)-C(2)-C(3)	116.3(7)
C(1)-C(2)-C(3)	106.9(7)
C(2)-C(3)-C(4)	122.2(9)
C(4)-C(3)-C(2)	118.7(10)
C(4S)-C(3S)-C(2S)	114.9(6)
C(3)-C(4)-C(5)	118.6(9)
C(3)-C(4)-C(5)	127.2(11)
C(4S)#1-C(4S)-C(3S)	115.2(7)
C(6)-C(5)-C(4)	110.5(7)
C(6)-C(5)-C(6)	31.6(5)

C(4)-C(5)-C(6)	116.3(7)
C(6)-C(5)-C(4)	115.1(7)
C(4)-C(5)-C(4)	28.0(6)
C(6)-C(5)-C(4)	104.8(7)
C(1)-C(6)-N(2)	101.9(8)
C(1)-C(6)-C(5)	109.7(7)
N(2)-C(6)-C(5)	111.2(7)
C(5)-C(6)-N(2)	118.3(7)
C(5)-C(6)-C(1)	109.0(9)
N(2)-C(6)-C(1)	101.6(7)
N(1)-C(7)-C(8)	125.0(5)
C(7)-C(8)-C(9)	117.8(4)
C(7)-C(8)-C(13)	121.4(5)
C(9)-C(8)-C(13)	120.7(4)
C(10)-C(9)-C(8)	122.2(5)
C(9)-C(10)-C(11)	116.0(5)
C(9)-C(10)-C(14)	123.5(5)
C(11)-C(10)-C(14)	120.2(4)
C(12)-C(11)-C(10)	125.5(5)
C(11)-C(12)-C(13)	117.0(4)
C(11)-C(12)-C(18)	121.8(4)
C(13)-C(12)-C(18)	121.2(5)
O(1)-C(13)-C(8)	122.7(4)
O(1)-C(13)-C(12)	118.8(4)
C(8)-C(13)-C(12)	118.4(5)
C(17)-C(14)-C(16)	107.9(5)
C(17)-C(14)-C(15)	109.8(5)
C(16)-C(14)-C(15)	108.3(5)
C(17)-C(14)-C(10)	111.0(5)
C(16)-C(14)-C(10)	112.3(4)
C(15)-C(14)-C(10)	107.5(4)
C(19)-C(18)-C(20)	107.2(5)
C(19)-C(18)-C(12)	112.8(5)
C(20)-C(18)-C(12)	109.6(4)
C(19)-C(18)-C(21)	107.4(4)
C(20)-C(18)-C(21)	109.7(5)

C(12)-C(18)-C(21)	110.0(4)
N(2)-C(22)-C(23)	126.7(5)
C(24)-C(23)-C(28)	121.4(5)
C(24)-C(23)-C(22)	121.3(5)
C(28)-C(23)-C(22)	117.2(5)
O(2)-C(24)-C(23)	122.1(4)
O(2)-C(24)-C(25)	119.7(4)
C(23)-C(24)-C(25)	118.3(5)
C(26)-C(25)-C(24)	116.9(5)
C(26)-C(25)-C(29)	121.5(5)
C(24)-C(25)-C(29)	121.6(5)
C(25)-C(26)-C(27)	126.2(5)
C(28)-C(27)-C(26)	116.8(5)
C(28)-C(27)-C(33)	122.7(5)
C(26)-C(27)-C(33)	120.3(5)
C(27)-C(28)-C(23)	120.2(5)
C(32)-C(29)-C(25)	112.1(5)
C(32)-C(29)-C(31)	108.2(5)
C(25)-C(29)-C(31)	110.2(4)
C(32)-C(29)-C(30)	107.0(4)
C(25)-C(29)-C(30)	110.6(4)
C(31)-C(29)-C(30)	108.6(5)
C(35)-C(33)-C(34)	111.5(5)
C(35)-C(33)-C(36)	109.7(5)
C(34)-C(33)-C(36)	107.8(5)
C(35)-C(33)-C(27)	106.1(4)
C(34)-C(33)-C(27)	110.0(4)
C(36)-C(33)-C(27)	111.7(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y-1,-z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for *rac*-(salen-**1**)CoI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	21(1)	30(1)	28(1)	11(1)	8(1)	10(1)
Co(1)	18(1)	17(1)	16(1)	3(1)	4(1)	10(1)
Cl(1)	54(1)	87(2)	123(2)	30(1)	35(1)	40(1)
Cl(2)	57(1)	49(1)	56(1)	7(1)	16(1)	13(1)
O(1)	23(2)	17(2)	20(2)	0(1)	2(1)	15(1)
O(2)	20(2)	22(2)	20(2)	6(1)	1(1)	16(1)
N(1)	27(2)	18(2)	15(2)	2(2)	1(2)	12(2)
N(2)	23(2)	34(3)	19(2)	-2(2)	2(2)	18(2)
C(1)	17(5)	6(5)	20(4)	2(4)	3(4)	8(4)
C(1)	21(5)	25(5)	24(5)	7(4)	7(4)	10(4)
C(1S)	44(3)	61(4)	38(3)	20(3)	25(3)	20(3)
C(2)	26(3)	30(3)	22(3)	8(2)	1(2)	19(2)
C(2S)	68(5)	86(5)	53(4)	21(4)	1(4)	40(4)
C(3)	30(5)	24(5)	19(5)	5(4)	6(4)	16(4)
C(3)	42(6)	25(6)	21(5)	6(4)	5(5)	21(5)
C(3S)	40(4)	70(5)	57(4)	21(4)	10(3)	16(3)
C(4)	26(5)	26(5)	27(5)	2(4)	-1(4)	7(4)
C(4)	17(5)	33(6)	14(4)	-2(4)	4(4)	11(4)
C(4S)	41(3)	50(4)	49(4)	16(3)	8(3)	8(3)
C(5)	24(3)	36(3)	19(3)	1(2)	5(2)	18(2)
C(6)	14(4)	20(5)	12(4)	12(3)	4(4)	8(4)
C(6)	10(5)	25(5)	16(4)	3(4)	1(4)	11(4)
C(7)	25(3)	30(3)	21(3)	9(2)	5(2)	11(2)
C(8)	17(2)	14(3)	21(3)	4(2)	4(2)	9(2)
C(9)	13(2)	18(3)	22(3)	6(2)	1(2)	4(2)
C(10)	20(2)	14(3)	32(3)	12(2)	12(2)	14(2)
C(11)	24(3)	21(3)	18(3)	-1(2)	5(2)	10(2)
C(12)	16(2)	25(3)	18(2)	4(2)	5(2)	12(2)
C(13)	19(2)	23(3)	18(2)	4(2)	7(2)	14(2)
C(14)	14(2)	19(3)	34(3)	8(2)	7(2)	10(2)
C(15)	37(3)	22(3)	111(6)	20(4)	28(4)	18(3)

C(16)	39(3)	34(3)	36(3)	7(3)	4(3)	27(3)
C(17)	70(4)	77(4)	34(3)	8(3)	22(3)	62(3)
C(18)	23(3)	22(3)	19(3)	4(2)	3(2)	11(2)
C(19)	42(3)	41(4)	26(3)	2(3)	1(3)	21(3)
C(20)	38(3)	38(3)	19(3)	10(2)	7(2)	24(3)
C(21)	21(3)	28(3)	30(3)	1(2)	1(2)	11(2)
C(22)	31(3)	32(3)	18(3)	5(2)	6(2)	19(2)
C(23)	22(2)	17(3)	16(2)	5(2)	5(2)	12(2)
C(24)	12(2)	20(3)	21(3)	7(2)	4(2)	5(2)
C(25)	18(2)	16(3)	24(3)	12(2)	7(2)	9(2)
C(26)	24(3)	22(3)	20(3)	5(2)	3(2)	14(2)
C(27)	14(2)	15(3)	28(3)	8(2)	8(2)	7(2)
C(28)	25(2)	15(3)	24(3)	8(2)	13(2)	12(2)
C(29)	21(2)	24(3)	23(3)	6(2)	9(2)	6(2)
C(30)	29(3)	33(3)	20(3)	0(2)	4(2)	14(2)
C(31)	31(3)	44(4)	25(3)	11(3)	18(2)	15(3)
C(32)	42(3)	41(3)	25(3)	17(2)	15(2)	27(3)
C(33)	22(2)	26(3)	32(3)	11(2)	12(2)	22(2)
C(34)	32(3)	59(4)	38(3)	4(3)	5(3)	33(3)
C(35)	58(3)	34(3)	66(4)	25(3)	41(3)	31(3)
C(36)	42(3)	36(3)	38(3)	8(3)	15(3)	27(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for *rac*-(salen-**1**)CoI.

	x	y	z	U(eq)
H(1A)	3830	1275	5514	17
H(1B)	1772	-127	5809	28
H(1SB)	3730(60)	1310(50)	1920(40)	60(20)
H(1SA)	2660(80)	420(70)	930(50)	90(30)
H(2B)	4660(60)	320(50)	6440(40)	50(20)
H(2A)	3460(80)	-150(70)	6540(50)	80(30)
H(2S1)	3760	-3206	1119	104
H(2S2)	3248	-2677	321	104
H(2S3)	4826	-2406	767	104
H(3SB)	3090(50)	-4490(50)	-10(30)	28(16)
H(3SA)	3760(50)	-4020(50)	-660(40)	36(17)
H(4A)	4416	2861	7287	35
H(4B)	3441	2149	7730	35
H(4C)	3822	2348	7681	26
H(4D)	2455	1346	7521	26
H(4SB)	5790(70)	-3850(60)	550(50)	80(30)
H(4SA)	4960(60)	-4800(60)	860(40)	60(20)
H(5B)	1750(50)	1930(50)	6570(30)	28(16)
H(5A)	2670(80)	2730(70)	6290(50)	100(30)
H(6A)	1276	307	5805	17
H(6B)	3425	1943	5561	20
H(7)	3360(60)	-1380(60)	5270(40)	70(20)
H(9)	3670(40)	-2790(40)	4450(30)	6(12)
H(11)	1650(40)	-4090(40)	1990(30)	8(12)
H(15A)	1304	-6003	2694	80
H(15B)	1646	-5457	3683	80
H(15C)	2336	-6343	3409	80
H(16A)	4710	-5209	3922	52
H(16B)	4172	-4461	4501	52
H(16C)	5131	-3855	4000	52

H(17A)	4243	-4389	2375	77
H(17B)	2719	-5219	1907	77
H(17C)	3813	-5705	2431	77
H(19A)	-505	-3550	281	56
H(19B)	-308	-4367	933	56
H(19C)	964	-3588	733	56
H(20A)	1059	-898	1764	44
H(20B)	292	-1495	774	44
H(20C)	1776	-1503	1225	44
H(21A)	-983	-2136	2090	42
H(21B)	-1489	-3495	1752	42
H(21C)	-1676	-2691	1088	42
H(22)	650(70)	2290(70)	5280(50)	90(30)
H(26)	-2020(40)	2790(40)	2120(30)	1(11)
H(28)	-720(50)	3180(40)	4650(30)	17(14)
H(30A)	-2655	-191	1384	42
H(30B)	-1260	-423	1701	42
H(30C)	-1861	-354	729	42
H(31A)	395	1123	952	46
H(31B)	906	1097	1941	46
H(31C)	937	2282	1668	46
H(32A)	-2631	1644	888	47
H(32B)	-1746	1394	316	47
H(32C)	-1223	2589	991	47
H(34A)	-3842	4388	2769	61
H(34B)	-4088	3115	2916	61
H(34C)	-3455	3498	2196	61
H(35A)	-1042	4932	2671	65
H(35B)	-244	5407	3672	65
H(35C)	-1491	5788	3229	65
H(36A)	-1289	4831	4723	52
H(36B)	-2689	3798	4458	52
H(36C)	-2675	5031	4290	52