Electronic Supplementary Information for Dalton Transactions

Supporting Information for:

On the mechanism of isospecific epoxide polymerization by salen cobalt (III) complexes: Evidence for solid-state catalysis

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General Procedures. All air or water sensitive reactions were carried out under nitrogen in Braun Labmaster dryboxes or using standard Schlenk-line techniques. Propylene oxide (PO) was dried over calcium hydride and vacuum transferred before use. Toluene, tetrahydrofuran, methylene chloride, diethyl ether, and hexanes were dried by passing through a column of activated alumina and degassed by sparging with dry nitrogen prior to use. Absolute ethanol was degassed by sparing with dry nitrogen and used without further purification. All other reagents were purchased from commercial sources and used as received. *N,N'*-Bis-(3,5-di-*tert*-butylsalicylidene)-1,2-benzenediamine was prepared according to literature procedure (J. Woltinger, J. E. Backvall, A. Zsigmond, *Chem. Eur. J.* 1999, **5**, 1460-1467), and complexes **1-9** were synthesized using reported procedures (K. L. Peretti, H. Ajiro, C. T. Cohen, E. B. Lobkovsky, and G. W. Coates, *J. Am. Chem. Soc.*, 2005, **127**, 11566-11567).

NMR spectroscopy was performed using Varian Unity (500 MHz), INOVA (400 MHz), and Mercury (300 MHz) spectrometers. All spectra were referenced by residual solvent shifts. PPO isotacticity (isotactic triad: [*mm*] and dyad: [*m*]), was determined by inspection of the methine peaks in the $^{13}C\{^1H\}$ NMR spectra of polymer samples (W. Hirahata, R. M. Thomas, E. B. Lobkovsky, and G. W. Coates, *J. Am. Chem. Soc.*, 2008, **130**, 17658-17659). Crystallographic data were collected at 173(2) K using a Siemens SMART CCD Area Detector System (M_o K_α, λ = 0.71073) and frames were integrated with the Siemens SAINT program. M_n and molecular weight distributions (M_w/M_n) were measured by high temperature gel-permeation chromatography. Data were collected using a Waters Alliance GPCV 2000 size exclusion chromatograph equipped with a Waters DRI detector and viscometer. The column set (four Waters HT 6E and one Waters HT 2) was eluted with 1,2,4-trichlorobenzene containing approximately 0.01 wt% di-*tert*-butylhydroxytoluene (BHT) at 1.0 mL/min, at 140 °C calibrated with polystyrene standards.

Synthesis of (salph)Co(μ-MeOH)OMe•(μ-MeOH) (10). A 2 L round bottom flask was charged with (salph)Co (2.0 g, 3.3 mmol) and KOH (0.21 g, 3.7 mmol). Methanol (2 L) was then added, and the mixture was stirred overnight, open to air. The mixture was filtered through a Büchner funnel, and the filtrate solution was transferred into a glass bottle which was allowed to sit open to air for 7 days. After approximately half of the methanol evaporated, filtration gave dark red crystals of **10** (1.6 g, 68%). ^1H NMR (anhydrous DMSO-d_6, 300 MHz): δ 1.15 (s, 3H, OCH_3), 1.32 (s, 18H, ^{t}Bu), 1.67 (s, 18H, ^{t}Bu), 7.36 (d, J = 2.7 Hz, 2H, Ar), 7.39 (dd, J = 3.6 Hz and 6.3 Hz, 2H, Ar), 7.44 (d, J = 2.7 Hz, 2H, Ar), 8.42 (dd, J = 3.6 Hz and 6.2 Hz, 2H, Ar), 8.73 (s, 2H, Ar). IR (KBr, cm^{-1}): 743, 1031 1172, 1360, 1388, 1429, 1463, 1521, 1579, 1613, 2868, 2905, 2955.

Representative Procedure for PO Polymerization. In the glovebox, a Schlenk tube was charged with **10** (20 mg, 0.029 mmol) and a Teflon-coated stir bar, then sealed and removed from the glovebox. Toluene (1.85 mL) was added under N_2 and the solution was brought to 0 °C. PO (1.0 mL, 0.812 g, 14 mmol) was added *via* airtight syringe, and was stirred for 10 h at 0 °C. An aliquot was taken from the reaction mixture for NMR spectroscopic analysis before it was quenched with 1N HCl_{aq} (5.0 mL). Unreacted PO was removed under vacuum, and CH_2Cl_2 (20 mL) was added to dissolve the precipitated polymer. The organic layer was separated and solvent was removed by rotary evaporation at 22 °C (620 mg, 76%). The polymer was purified by dissolving in acetone at 50 °C (10 mL) then adding the resulting solution dropwise to acetone (500 mL) at 25 °C. The polymer solution was cooled to 0 °C for 3 h. The white precipitate was filtered and dried in vacuo to constant weight (600 mg, 74%).

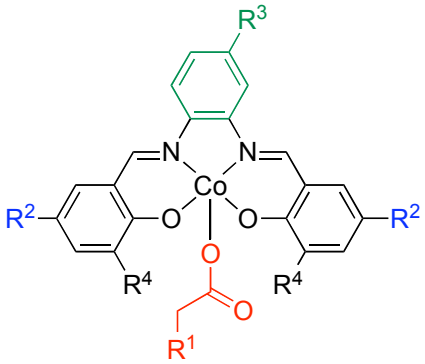

Table S1. Polymerization of *rac*-Propylene Oxide using Cobalt Carboxylate Catalysts (1-9).

cplx.	R^1	R^2	R^3	R^4	T_{rxn} (h)	Conv. (%)	*[mm]* (%)	M_n (g mol^{-1})	PDI (M_w/M_n)
1	H	^{t}Bu	H	^{t}Bu	2	89	> 99	287 000	1.40
2	H	^{t}Bu	H	^{i}Pr	10	11	69	184 000	1.22
3	Ph	^{t}Bu	H	^{t}Bu	4	89	> 99	423 000	1.40
4	1-Nap	^{t}Bu	H	^{t}Bu	10	16	> 99	28 000	1.59
5	H	Me	H	^{t}Bu	24	< 1	ND	ND	ND
6	H	$CMe_2CH_2{}^t$Bu	H	^{t}Bu	24	< 1	ND	ND	ND
7	H	^{t}Bu	OMe	^{t}Bu	18	79	> 99	71 900	4.09
8	H	^{t}Bu	Me	^{t}Bu	18	< 1	ND	ND	ND
9	H	^{t}Bu	Cl	^{t}Bu	18	< 1	ND	ND	ND

Crystal data and structure refinement for (salph)Co(μ-MeOH)OMe•(μ-MeOH) (10)

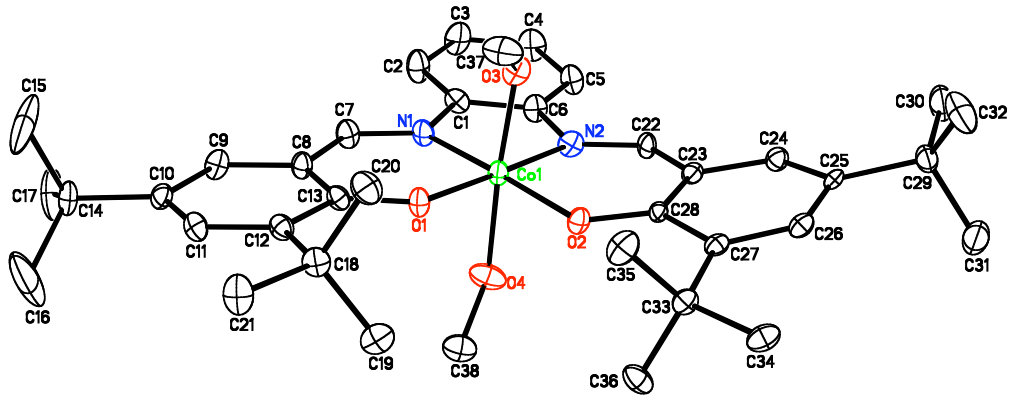

Table S2. Crystal data and structure refinement for **10**.

Identification code	ha4	
Empirical formula	C39 H57 Co N2 O5	
Formula weight	692.80	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Iba2	
Unit cell dimensions	a = 23.9083(10) Å	α= 90°
	b = 26.4057(10) Å	β= 90°
	c = 11.6690(7) Å	γ = 90°
Volume	7366.8(6) $Å^3$	
Z	8	
Density (calculated)	1.249 Mg/m^3	
Absorption coefficient	0.510 mm^{-1}	
F(000)	2976	
Crystal size	0.20 x 0.10 x 0.03 mm^3	
Theta range for data collection	1.70 to 24.70°	
Index ranges	-19<=h<=28, -30<=k<=29, -13<=l<=11	
Reflections collected	15844	
Independent reflections	5578 [R(int) = 0.0404]	
Completeness to theta = 24.70°	99.1 %	
Absorption correction	Semiempirical by SADABS	
Max. and min. transmission	0.9874 and 0.9049	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5578 / 1 / 510	
Goodness-of-fit on F^2	0.920	
Final R indices [I>2sigma(I)]	R1 = 0.0381, wR2 = 0.0868	
R indices (all data)	R1 = 0.0571, wR2 = 0.0942	
Absolute structure parameter	0.507(15)	
Largest diff. peak and hole	0.474 and -0.345 e $Å^{-3}$	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **10**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	2393(1)	1728(1)	1551(1)	17(1)
O(1)	2882(1)	1189(1)	1950(2)	19(1)
O(2)	1900(1)	1214(1)	1023(2)	19(1)
O(3)	2696(1)	1809(1)	115(2)	25(1)
O(4)	2014(1)	1688(1)	3049(3)	33(1)
N(1)	2861(1)	2239(1)	2140(3)	21(1)
N(2)	1918(1)	2275(1)	1146(3)	22(1)
C(1)	2660(2)	2739(1)	1939(3)	21(1)
C(2)	2942(2)	3186(1)	2218(4)	32(1)
C(3)	2700(2)	3649(1)	1936(4)	33(1)
C(4)	2185(2)	3665(1)	1404(5)	33(1)
C(5)	1901(2)	3220(1)	1149(4)	26(1)
C(6)	2142(1)	2756(1)	1415(4)	23(1)
C(7)	3325(2)	2161(1)	2672(4)	24(1)
C(8)	3575(1)	1681(1)	2921(3)	21(1)
C(9)	4070(1)	1693(1)	3587(4)	22(1)
C(10)	4340(1)	1263(1)	3916(3)	21(1)
C(11)	4120(2)	807(1)	3481(4)	20(1)
C(12)	3656(1)	765(1)	2799(3)	20(1)
C(13)	3347(2)	1215(1)	2534(3)	19(1)
C(14)	4863(1)	1271(1)	4668(4)	26(1)
C(15)	5375(2)	1237(2)	3910(5)	72(2)
C(16)	4859(3)	830(2)	5512(6)	99(3)
C(17)	4910(2)	1753(1)	5385(5)	52(1)
C(18)	3466(2)	245(1)	2346(4)	21(1)
C(19)	2881(1)	122(1)	2765(4)	28(1)
C(20)	3481(2)	241(1)	1035(4)	29(1)
C(21)	3857(2)	-182(1)	2750(4)	31(1)
C(22)	1475(1)	2226(1)	510(3)	20(1)
C(23)	1255(1)	1763(1)	76(3)	18(1)
C(24)	809(1)	1815(1)	-721(3)	20(1)
C(25)	568(1)	1410(1)	-1260(3)	18(1)
C(26)	761(1)	926(1)	-879(3)	19(1)
C(27)	1176(1)	843(1)	-89(3)	16(1)
C(28)	1466(1)	1279(1)	369(3)	14(1)
C(29)	121(1)	1455(1)	-2186(3)	24(1)
C(30)	35(2)	2008(1)	-2567(4)	39(1)
C(31)	-434(2)	1258(1)	-1722(4)	37(1)
C(32)	294(2)	1150(2)	-3251(4)	47(1)
C(33)	1327(1)	306(1)	296(3)	19(1)
C(34)	945(1)	-94(1)	-245(4)	26(1)
C(35)	1934(1)	181(1)	-77(4)	29(1)
C(36)	1265(2)	258(1)	1590(5)	26(1)
C(37)	2969(2)	1397(2)	-439(5)	40(1)
C(38)	2009(2)	1252(1)	3766(4)	33(1)
O(1S)	3201(1)	2584(1)	-636(3)	47(1)
C(1S)	3750(2)	2535(2)	-295(6)	73(2)

Table S4. Bond lengths [Å] and angles [°] for **10**.

Co(1)-O(3)	1.838(3)	N(1)-Co(1)-O(1)	94.67(10)
Co(1)-N(1)	1.883(3)	N(2)-Co(1)-O(1)	178.79(11)
Co(1)-N(2)	1.896(3)	O(3)-Co(1)-O(2)	91.84(11)
Co(1)-O(1)	1.900(2)	N(1)-Co(1)-O(2)	177.24(13)
Co(1)-O(2)	1.899(2)	N(2)-Co(1)-O(2)	95.22(11)
Co(1)-O(4)	1.972(3)	O(1)-Co(1)-O(2)	85.81(8)
O(1)-C(13)	1.305(4)	O(3)-Co(1)-O(4)	174.59(10)
O(2)-C(28)	1.300(4)	N(1)-Co(1)-O(4)	89.31(13)
O(3)-C(37)	1.425(5)	N(2)-Co(1)-O(4)	89.23(12)
O(4)-C(38)	1.422(4)	O(1)-Co(1)-O(4)	91.44(10)
N(1)-C(7)	1.289(5)	O(2)-Co(1)-O(4)	87.95(11)
N(1)-C(1)	1.423(4)	C(13)-O(1)-Co(1)	127.8(2)
N(2)-C(22)	1.300(4)	C(28)-O(2)-Co(1)	126.3(2)
N(2)-C(6)	1.414(4)	C(37)-O(3)-Co(1)	120.3(2)
C(1)-C(6)	1.383(5)	C(38)-O(4)-Co(1)	124.7(2)
C(1)-C(2)	1.398(5)	C(7)-N(1)-C(1)	121.2(3)
C(2)-C(3)	1.391(5)	C(7)-N(1)-Co(1)	125.0(2)
C(3)-C(4)	1.380(5)	C(1)-N(1)-Co(1)	113.8(2)
C(4)-C(5)	1.387(5)	C(22)-N(2)-C(6)	121.6(3)
C(5)-C(6)	1.390(5)	C(22)-N(2)-Co(1)	123.7(2)
C(7)-C(8)	1.431(5)	C(6)-N(2)-Co(1)	113.7(2)
C(8)-C(9)	1.415(5)	C(6)-C(1)-C(2)	120.5(3)
C(8)-C(13)	1.420(5)	C(6)-C(1)-N(1)	113.9(3)
C(9)-C(10)	1.361(5)	C(2)-C(1)-N(1)	125.7(3)
C(10)-C(11)	1.410(5)	C(3)-C(2)-C(1)	119.2(4)
C(10)-C(14)	1.527(5)	C(4)-C(3)-C(2)	120.2(3)
C(11)-C(12)	1.369(5)	C(3)-C(4)-C(5)	120.5(4)
C(12)-C(13)	1.434(5)	C(4)-C(5)-C(6)	119.8(4)
C(12)-C(18)	1.539(5)	C(1)-C(6)-C(5)	119.8(3)
C(14)-C(15)	1.512(6)	C(1)-C(6)-N(2)	114.1(3)
C(14)-C(16)	1.527(6)	C(5)-C(6)-N(2)	126.0(3)
C(14)-C(17)	1.526(5)	N(1)-C(7)-C(8)	126.8(3)
C(18)-C(19)	1.517(5)	C(9)-C(8)-C(13)	120.9(3)
C(18)-C(20)	1.530(5)	C(9)-C(8)-C(7)	116.2(3)
C(18)-C(21)	1.539(5)	C(13)-C(8)-C(7)	122.9(3)
C(22)-C(23)	1.423(5)	C(10)-C(9)-C(8)	122.3(3)
C(23)-C(24)	1.423(5)	C(9)-C(10)-C(11)	115.6(3)
C(23)-C(28)	1.416(4)	C(9)-C(10)-C(14)	122.7(3)
C(24)-C(25)	1.367(5)	C(11)-C(10)-C(14)	121.6(3)
C(25)-C(26)	1.430(5)	C(12)-C(11)-C(10)	125.6(3)
C(25)-C(29)	1.524(5)	C(11)-C(12)-C(13)	118.4(3)
C(26)-C(27)	1.371(5)	C(11)-C(12)-C(18)	120.8(3)
C(27)-C(28)	1.447(4)	C(13)-C(12)-C(18)	120.8(3)
C(27)-C(33)	1.531(4)	O(1)-C(13)-C(8)	122.6(3)
C(29)-C(31)	1.526(5)	O(1)-C(13)-C(12)	120.5(3)
C(29)-C(32)	1.536(6)	C(8)-C(13)-C(12)	116.9(3)
C(29)-C(30)	1.541(5)	C(15)-C(14)-C(16)	109.7(5)
C(33)-C(36)	1.523(6)	C(15)-C(14)-C(10)	109.0(4)
C(33)-C(34)	1.532(5)	C(16)-C(14)-C(10)	110.8(3)
C(33)-C(35)	1.550(5)	C(15)-C(14)-C(17)	108.2(4)
O(1S)-C(1S)	1.378(5)	C(16)-C(14)-C(17)	106.4(4)
		C(10)-C(14)-C(17)	112.8(3)
O(3)-Co(1)-N(1)	90.84(12)	C(19)-C(18)-C(20)	110.0(4)
O(3)-Co(1)-N(2)	85.40(12)	C(19)-C(18)-C(12)	110.7(3)
N(1)-Co(1)-N(2)	84.33(11)	C(20)-C(18)-C(12)	110.1(3)
O(3)-Co(1)-O(1)	93.94(10)	C(19)-C(18)-C(21)	107.7(3)

C(20)-C(18)-C(21)	106.7(3)	O(2)-C(28)-C(27)	119.7(3)
C(12)-C(18)-C(21)	111.5(3)	C(23)-C(28)-C(27)	117.4(3)
N(2)-C(22)-C(23)	126.0(3)	C(31)-C(29)-C(25)	109.4(3)
C(24)-C(23)-C(28)	120.7(3)	C(31)-C(29)-C(32)	110.0(3)
C(24)-C(23)-C(22)	115.3(3)	C(25)-C(29)-C(32)	110.2(3)
C(28)-C(23)-C(22)	124.0(3)	C(31)-C(29)-C(30)	108.0(3)
C(25)-C(24)-C(23)	122.8(3)	C(25)-C(29)-C(30)	111.8(3)
C(24)-C(25)-C(26)	114.9(3)	C(32)-C(29)-C(30)	107.4(3)
C(24)-C(25)-C(29)	124.1(3)	C(36)-C(33)-C(27)	110.2(3)
C(26)-C(25)-C(29)	121.0(3)	C(36)-C(33)-C(34)	107.1(3)
C(27)-C(26)-C(25)	125.8(3)	C(27)-C(33)-C(34)	112.0(3)
C(26)-C(27)-C(28)	117.9(3)	C(36)-C(33)-C(35)	110.6(3)
C(26)-C(27)-C(33)	121.1(3)	C(27)-C(33)-C(35)	109.7(3)
C(28)-C(27)-C(33)	121.0(3)	C(34)-C(33)-C(35)	107.2(3)
O(2)-C(28)-C(23)	122.9(3)		

Table S5. Anisotropic displacement parameters ($Å^2$ x 10^3) for **10**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + \ldots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	17(1)	13(1)	23(1)	0(1)	-4(1)	0(1)
O(1)	19(1)	13(1)	26(2)	-3(1)	-8(1)	2(1)
O(2)	18(1)	14(1)	26(2)	-2(1)	-4(1)	-1(1)
O(3)	24(1)	13(1)	38(2)	1(1)	-2(1)	1(1)
O(4)	53(2)	19(1)	26(2)	2(1)	7(1)	3(1)
N(1)	22(2)	13(1)	27(2)	3(1)	-7(2)	1(1)
N(2)	26(2)	13(1)	26(2)	-4(1)	0(2)	-1(1)
C(1)	27(2)	14(2)	21(3)	-2(1)	-1(2)	3(2)
C(2)	32(2)	20(2)	42(3)	-2(2)	-15(2)	0(2)
C(3)	33(2)	13(2)	53(4)	-3(2)	-10(2)	-5(2)
C(4)	40(2)	14(2)	44(3)	-1(2)	-8(3)	5(2)
C(5)	31(2)	17(2)	30(3)	-2(2)	-10(2)	3(2)
C(6)	26(2)	16(2)	26(3)	-6(2)	-4(2)	1(1)
C(7)	27(2)	18(2)	27(3)	-3(2)	-8(2)	-1(2)
C(8)	18(2)	18(2)	26(3)	0(2)	-5(2)	3(2)
C(9)	20(2)	16(2)	29(3)	-9(2)	-3(2)	0(2)
C(10)	14(2)	25(2)	22(3)	-1(2)	0(2)	3(2)
C(11)	22(2)	15(2)	23(3)	-2(2)	-1(2)	10(2)
C(12)	21(2)	19(2)	20(2)	1(2)	-1(2)	5(2)
C(13)	22(2)	19(2)	15(2)	-1(2)	-3(2)	0(2)
C(14)	17(2)	25(2)	35(3)	-4(2)	-10(2)	6(2)
C(15)	17(2)	127(5)	71(5)	-51(4)	-14(3)	9(3)
C(16)	110(5)	74(4)	114(6)	56(4)	-93(5)	-45(3)
C(17)	41(3)	57(3)	57(4)	-28(3)	-33(3)	17(2)
C(18)	26(2)	11(2)	27(3)	-2(2)	-2(2)	1(2)
C(19)	28(2)	19(2)	36(3)	-3(2)	5(2)	1(2)
C(20)	34(2)	28(2)	24(3)	-3(2)	-2(2)	3(2)
C(21)	33(2)	19(2)	40(3)	-8(2)	-10(2)	6(2)
C(22)	16(2)	16(2)	27(3)	3(2)	-7(2)	3(2)
C(23)	14(2)	19(2)	21(2)	3(2)	0(2)	-1(2)
C(24)	17(2)	19(2)	23(3)	1(2)	-1(2)	1(2)
C(25)	10(2)	25(2)	20(2)	3(2)	0(2)	-5(2)
C(26)	17(2)	16(2)	24(3)	-2(2)	2(2)	-3(2)
C(27)	15(2)	17(2)	17(2)	-3(2)	4(2)	-1(1)
C(28)	11(2)	20(2)	13(2)	-1(2)	0(2)	0(1)
C(29)	24(2)	25(2)	22(3)	2(2)	-7(2)	-1(2)
C(30)	41(2)	35(2)	42(3)	8(2)	-21(2)	-7(2)
C(31)	28(2)	37(2)	47(3)	5(2)	-10(2)	-6(2)
C(32)	54(3)	60(3)	27(3)	-3(2)	-14(2)	8(2)
C(33)	20(2)	14(2)	23(3)	-2(2)	0(2)	-1(2)
C(34)	29(2)	16(2)	35(3)	0(2)	3(2)	-8(2)
C(35)	22(2)	23(2)	41(3)	-6(2)	4(2)	4(2)
C(36)	41(2)	20(2)	19(2)	0(2)	-6(3)	-1(2)
C(37)	49(3)	38(3)	33(3)	6(2)	11(3)	3(2)
C(38)	41(2)	29(2)	27(3)	0(2)	5(2)	-1(2)
O(1S)	42(2)	32(2)	67(3)	29(2)	-6(2)	-10(2)
C(1S)	31(3)	59(3)	131(6)	48(4)	0(3)	-3(2)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **10**.

	x	y	z	U(eq)
H(4O)	1993(15)	2038(16)	3530(40)	51(12)
H(2)	3328(15)	3217(12)	2570(30)	24(10)
H(3)	2913(16)	3946(13)	2160(30)	37(11)
H(4)	2021(14)	3957(13)	1230(30)	30(10)
H(5)	1556(15)	3260(11)	740(40)	23(10)
H(7)	3530(15)	2435(14)	3150(40)	47(13)
H(9)	4179(12)	1980(12)	3900(30)	7(8)
H(11)	4302(13)	539(12)	3690(30)	14(9)
H(15A)	5354	928	3445	108
H(15B)	5711	1226	4388	108
H(15C)	5390	1533	3405	108
H(16A)	4930	513	5100	149
H(16B)	4493	812	5890	149
H(16C)	5151	881	6090	149
H(17A)	5241	1731	5879	78
H(17B)	4575	1790	5860	78
H(17C)	4946	2046	4877	78
H(19A)	2875	126	3605	42
H(19B)	2772	-214	2490	42
H(19C)	2617	375	2472	42
H(20A)	3360	-91	755	43
H(20B)	3863	309	772	43
H(20C)	3229	503	739	43
H(21A)	3735	-504	2418	46
H(21B)	3846	-204	3588	46
H(21C)	4240	-108	2502	46
H(22)	1294(11)	2539(10)	260(30)	4(8)
H(24)	673(11)	2149(11)	-850(30)	3(8)
H(26)	595(13)	658(12)	-1250(30)	22(10)
H(30A)	-84	2212	-1909	59
H(30B)	-253	2021	-3165	59
H(30C)	387	2142	-2871	59
H(31A)	-389	906	-1469	56
H(31B)	-718	1274	-2326	56
H(31C)	-552	1467	-1072	56
H(32A)	676	1242	-3473	71
H(32B)	37	1227	-3883	71
H(32C)	278	787	-3077	71
H(34A)	1048	-430	42	40
H(34B)	988	-86	-1080	40
H(34C)	555	-21	-44	40
H(35A)	2194	413	303	43
H(35B)	1968	219	-910	43
H(35C)	2024	-168	139	43
H(36C)	1383(11)	-106(12)	1800(30)	18(8)
H(36B)	1484(14)	477(12)	2000(30)	18(9)
H(36A)	862(19)	284(14)	1840(50)	71(16)
H(37C)	3035(13)	1531(13)	-1320(40)	35(11)
H(37B)	2664(16)	1085(15)	-490(40)	43(12)
H(37A)	3360(20)	1328(16)	10(40)	65(15)
H(38A)	1922	952	3306	49
H(38B)	1725	1294	4364	49
H(38C)	2377	1211	4123	49

H(1OS)	3068(18)	2386(14)	-450(40)	25(15)
H(1S1)	3906	2870	-129	110
H(1S2)	3967	2375	-910	110
H(1S3)	3769	2324	395	110