Electronic Supporting Information

Cleaving bonds in $CH_3OSO_2CF_3$ with $[1,2,4\text{-}(Me_3C)_3C_5H_2]_2CeH$; An experimental and computational study.

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1. $Cp'_2CeOSO_2CF_3$

1. Cp'$_2$CeOSO$_2$CF$_3$

Light yellow block-like crystals of Cp'$_2$CeOSO$_2$CF$_3$ were obtained *via* two different methods. Crystallization from hexane solution resulted in crystals containing half a molecule of hexane per cerium complex. Sublimation under static vacuum in a sealed glass ampoule yielded solvent-free crystals. Single crystal studies were performed on both types of crystal, and while the cell dimensions and space group differ, the geometry of the organometallic complex is essentially identical in both cases. The structure obtained on a crystal from sublimation is described here (CCDC 901437). The CIF from a crystal obtained from hexane has also been deposited with the Cambridge Crystallographic Data Centre, CCDC 889315.

A crystal obtained *via* sublimation having approximate dimensions of 0.16 x 0.12 x 0.06 mm was mounted on a Kapton Loop using Paratone N hydrocarbon oil. All measurements were made on a Bruker APEX[1] CCD area detector with graphite monochromated Mo-Kα radiation.

Cell constants and an orientation matrix, obtained from a least-squares refinement using the measured positions of 9738 centered reflections with I > 10σ(I) in the range 4.94 < 2θ < 50.70° corresponded to a primitive monoclinic cell with dimensions:

a = 10.5673(12) Å
b = 21.532(2) Å ® = 98.267(2)°
c = 16.3041(18) Å
V = 3671.2(7) Å^3

For Z = 4 and F.W. = 755.99, the calculated density is 1.29 g/cm^3. The systematic absences of:

h0l: h+l ≠ 2n
0k0: k ≠ 2n

uniquely determine the space group to be:

P2$_1$/n (#14)

The data were collected at a temperature of -173 ± 1°C. Frames corresponding to an arbitrary hemisphere of data were collected using ω and φ scans of 0.3° counted for a total of 10.0 seconds per frame.

Data were integrated by the program SAINT[2] to a maximum 2θ value of 50.7°.The data were corrected for

Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP[3]. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS[4]. (Tmax = 0.92, Tmin = 0.81).

The structure was solved by direct methods[5] and expanded using Fourier techniques[6]. Non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated based on the expected geometry at each carbon. The final cycle of full-matrix least-squares refinement[7] was based on 6719 observed reflections and 406 variable parameters and converged (largest parameter shift was 0.004 times its esd) with unweighted and weighted agreement factors of R = 0.0224, Rw = 0.0499, and GOF = 1.067. The weighting scheme was based on counting statistics and included a factor (p = 0.019) to downweight the intense reflections. Plots of © w (|Fo| - |Fc|)^2 versus |Fo|, reflection order in data collection, sin \/L and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.045 and -0.533 e$^-$/Å^3, respectively. All calculations were performed using the WinGX[9] crystallographic software package.

Crystal data and structure refinement

Empirical formula	C35 H58 Ce F3 O3 S	
Formula weight	755.99	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.5673(12) Å	⟨= 90°.
	b = 21.532(2) Å	®= 98.267(2)°.
	c = 16.3041(18) Å	© = 90°.
Volume	3671.2(7) Å^3	
Z	4	
Density (calculated)	1.368 Mg/m^3	
Absorption coefficient	1.343 mm^{-1}	
F(000)	1572	
Crystal size	0.16 x 0.12 x 0.06 mm^3	
Theta range for data collection	1.58 to 25.36°.	
Index ranges	-12<=h<=12, -25<=k<=25, -19<=l<=19	
Reflections collected	46441	
Independent reflections	6719 [R(int) = 0.0313]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9238 and 0.8139	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6719 / 0 / 406	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0224, wR2 = 0.0499	
R indices (all data)	R1 = 0.0258, wR2 = 0.0522	

Largest diff. peak and hole 1.045 and -0.533 e.Å^{-3}

1.1 Atomic coordinates for $Cp'_2CeOSO_2CF_3$

.U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	499(2)	615(1)	6389(1)	17(1)
C(2)	-688(2)	922(1)	6304(1)	19(1)
C(3)	-1501(2)	658(1)	6831(1)	20(1)
C(4)	-754(2)	182(1)	7306(1)	19(1)
C(5)	459(2)	173(1)	7021(1)	16(1)
C(6)	1580(2)	732(1)	5886(1)	18(1)
C(7)	1048(2)	888(1)	4990(1)	37(1)
C(8)	2428(2)	155(1)	5885(2)	36(1)
C(9)	2410(3)	1271(1)	6263(2)	34(1)
C(10)	-2950(2)	811(1)	6708(1)	25(1)
C(11)	-3739(2)	220(1)	6459(2)	31(1)
C(12)	-3271(2)	1266(1)	5976(2)	36(1)
C(13)	-3420(2)	1115(1)	7458(2)	34(1)
C(14)	-1086(2)	-357(1)	7868(1)	22(1)
C(15)	-1522(2)	-916(1)	7304(1)	25(1)
C(16)	108(2)	-576(1)	8451(2)	30(1)
C(17)	-2094(2)	-216(1)	8429(1)	29(1)
C(18)	-159(2)	2223(1)	8824(1)	19(1)
C(19)	-609(2)	2406(1)	8009(1)	19(1)
C(20)	422(2)	2623(1)	7604(1)	18(1)
C(21)	1569(2)	2551(1)	8195(1)	17(1)
C(22)	1177(2)	2290(1)	8921(1)	19(1)
C(23)	-966(2)	2012(1)	9477(1)	24(1)
C(24)	-1165(2)	1309(1)	9425(1)	26(1)
C(25)	-2280(3)	2331(1)	9321(2)	41(1)
C(26)	-293(3)	2176(1)	10341(2)	41(1)
C(27)	79(2)	3009(1)	6807(1)	20(1)
C(28)	-1124(2)	2747(1)	6275(1)	28(1)
C(29)	1095(2)	3054(1)	6226(1)	28(1)
C(30)	-255(2)	3669(1)	7068(1)	25(1)

C(31)	2946(2)	2798(1)	8213(1)	21(1)
C(32)	3668(2)	2530(1)	7542(1)	24(1)
C(33)	3768(2)	2647(1)	9048(1)	27(1)
C(34)	2902(2)	3512(1)	8168(2)	28(1)
C(35)	3643(2)	40(1)	8942(1)	24(1)
O(1)	3055(1)	1124(1)	8294(1)	22(1)
O(2)	1624(1)	707(1)	9142(1)	23(1)
O(3)	3741(2)	1052(1)	9799(1)	31(1)
F(1)	3122(1)	-206(1)	8223(1)	31(1)
F(2)	4891(1)	85(1)	8942(1)	35(1)
F(3)	3419(1)	-336(1)	9543(1)	37(1)
S(1)	2976(1)	812(1)	9081(1)	20(1)
Ce(1)	626(1)	1306(1)	7829(1)	16(1)

1.2 Anisotropic thermal parameters for $Cp'_2CeOSO_2CF_3$

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}
C(1)	18(1)	17(1)	15(1)	-2(1)	1(1)	-2(1)
C(2)	19(1)	20(1)	18(1)	2(1)	-1(1)	-1(1)
C(3)	13(1)	24(1)	24(1)	-5(1)	2(1)	-3(1)
C(4)	18(1)	18(1)	18(1)	1(1)	0(1)	-4(1)
C(5)	15(1)	15(1)	18(1)	-1(1)	1(1)	-1(1)
C(6)	18(1)	20(1)	18(1)	0(1)	4(1)	-2(1)
C(7)	26(1)	66(2)	20(1)	9(1)	5(1)	-4(1)
C(8)	30(1)	35(1)	48(2)	6(1)	22(1)	6(1)
C(9)	35(1)	37(1)	33(1)	-11(1)	16(1)	-17(1)
C(10)	14(1)	29(1)	31(1)	0(1)	0(1)	1(1)
C(11)	16(1)	37(1)	37(1)	-6(1)	0(1)	-3(1)
C(12)	19(1)	40(1)	45(2)	9(1)	-2(1)	5(1)
C(13)	20(1)	35(1)	45(2)	-7(1)	4(1)	3(1)
C(14)	22(1)	22(1)	23(1)	3(1)	4(1)	-5(1)
C(15)	23(1)	24(1)	28(1)	1(1)	7(1)	-4(1)
C(16)	33(1)	29(1)	28(1)	11(1)	-1(1)	-9(1)
C(17)	35(1)	27(1)	26(1)	-1(1)	12(1)	-9(1)
C(18)	27(1)	14(1)	20(1)	-2(1)	10(1)	1(1)

C(19)	21(1)	17(1)	21(1)	1(1)	7(1)	3(1)
C(20)	21(1)	14(1)	19(1)	1(1)	7(1)	3(1)
C(21)	21(1)	14(1)	19(1)	-1(1)	6(1)	1(1)
C(22)	28(1)	15(1)	15(1)	-1(1)	4(1)	1(1)
C(23)	34(1)	21(1)	22(1)	1(1)	16(1)	2(1)
C(24)	30(1)	24(1)	24(1)	2(1)	8(1)	-5(1)
C(25)	45(2)	42(2)	44(2)	12(1)	32(1)	13(1)
C(26)	67(2)	37(1)	22(1)	-7(1)	20(1)	-18(1)
C(27)	21(1)	19(1)	21(1)	7(1)	6(1)	5(1)
C(28)	33(1)	26(1)	23(1)	8(1)	-1(1)	-1(1)
C(29)	31(1)	34(1)	22(1)	11(1)	12(1)	9(1)
C(30)	24(1)	19(1)	32(1)	7(1)	10(1)	4(1)
C(31)	21(1)	16(1)	24(1)	0(1)	4(1)	-1(1)
C(32)	19(1)	25(1)	29(1)	2(1)	5(1)	-1(1)
C(33)	26(1)	23(1)	31(1)	-2(1)	-2(1)	-4(1)
C(34)	25(1)	20(1)	39(1)	0(1)	5(1)	-3(1)
C(35)	23(1)	20(1)	25(1)	-2(1)	-6(1)	4(1)
O(1)	20(1)	21(1)	26(1)	3(1)	1(1)	1(1)
O(2)	24(1)	24(1)	22(1)	3(1)	5(1)	3(1)
O(3)	37(1)	24(1)	28(1)	-7(1)	-10(1)	4(1)
F(1)	30(1)	27(1)	31(1)	-12(1)	-9(1)	7(1)
F(2)	21(1)	32(1)	50(1)	-9(1)	-5(1)	6(1)
F(3)	48(1)	23(1)	37(1)	8(1)	-3(1)	6(1)
S(1)	23(1)	16(1)	19(1)	-1(1)	-2(1)	3(1)
Ce(1)	16(1)	15(1)	16(1)	0(1)	2(1)	1(1)

1.3 Bond lengths involving non-hydrogen atoms of $Cp'_2CeOSO_2CF_3$

C(1)-C(5)	1.407(3)
C(1)-C(2)	1.407(3)
C(1)-C(6)	1.521(3)
C(1)-Ce(1)	2.7661(19)
C(2)-C(3)	1.419(3)
C(2)-Ce(1)	2.794(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.448(3)
C(3)-C(10)	1.551(3)

C(3)-Ce(1)	2.931(2)
C(4)-C(5)	1.425(3)
C(4)-C(14)	1.550(3)
C(4)-Ce(1)	2.890(2)
C(5)-Ce(1)	2.7658(19)
C(5)-H(5)	0.9500
C(6)-C(7)	1.525(3)
C(6)-C(9)	1.528(3)
C(6)-C(8)	1.533(3)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(13)	1.531(3)
C(10)-C(12)	1.543(3)
C(10)-C(11)	1.544(3)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(17)	1.531(3)
C(14)-C(16)	1.540(3)
C(14)-C(15)	1.545(3)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800

C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.401(3)
C(18)-C(22)	1.406(3)
C(18)-C(23)	1.527(3)
C(18)-Ce(1)	2.758(2)
C(19)-C(20)	1.431(3)
C(19)-Ce(1)	2.741(2)
C(19)-H(19)	0.9500
C(20)-C(21)	1.444(3)
C(20)-C(27)	1.542(3)
C(20)-Ce(1)	2.864(2)
C(21)-C(22)	1.423(3)
C(21)-C(31)	1.546(3)
C(21)-Ce(1)	2.893(2)
C(22)-Ce(1)	2.775(2)
C(22)-H(22)	0.9500
C(23)-C(26)	1.525(3)
C(23)-C(24)	1.529(3)
C(23)-C(25)	1.537(3)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(29)	1.533(3)
C(27)-C(30)	1.539(3)
C(27)-C(28)	1.539(3)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800

C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32)	1.534(3)
C(31)-C(34)	1.539(3)
C(31)-C(33)	1.540(3)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-F(3)	1.320(3)
C(35)-F(2)	1.321(3)
C(35)-F(1)	1.331(2)
C(35)-S(1)	1.832(2)
O(1)-S(1)	1.4622(16)
O(1)-Ce(1)	2.5992(15)
O(2)-S(1)	1.4635(16)
O(2)-Ce(1)	2.5899(14)
O(3)-S(1)	1.4207(16)
S(1)-Ce(1)	3.1633(6)

1.4 Bond angles involving non-hydrogen atoms of $Cp'_2CeOSO_2CF_3$

C(5)-C(1)-C(2)	105.70(18)
C(5)-C(1)-C(6)	127.72(18)
C(2)-C(1)-C(6)	126.57(18)
C(5)-C(1)-Ce(1)	75.26(11)
C(2)-C(1)-Ce(1)	76.43(12)

C(6)-C(1)-Ce(1)	114.80(12)
C(1)-C(2)-C(3)	111.11(18)
C(1)-C(2)-Ce(1)	74.26(11)
C(3)-C(2)-Ce(1)	81.09(12)
C(1)-C(2)-H(2)	124.4
C(3)-C(2)-H(2)	124.4
Ce(1)-C(2)-H(2)	112.1
C(2)-C(3)-C(4)	106.04(18)
C(2)-C(3)-C(10)	120.58(19)
C(4)-C(3)-C(10)	132.22(19)
C(2)-C(3)-Ce(1)	70.33(11)
C(4)-C(3)-Ce(1)	74.04(11)
C(10)-C(3)-Ce(1)	129.40(14)
C(5)-C(4)-C(3)	106.39(18)
C(5)-C(4)-C(14)	118.26(18)
C(3)-C(4)-C(14)	133.93(19)
C(5)-C(4)-Ce(1)	70.61(11)
C(3)-C(4)-Ce(1)	77.16(11)
C(14)-C(4)-Ce(1)	126.86(13)
C(1)-C(5)-C(4)	110.65(18)
C(1)-C(5)-Ce(1)	75.28(11)
C(4)-C(5)-Ce(1)	80.32(12)
C(1)-C(5)-H(5)	124.7
C(4)-C(5)-H(5)	124.7
Ce(1)-C(5)-H(5)	111.8
C(1)-C(6)-C(7)	110.57(17)
C(1)-C(6)-C(9)	110.00(17)
C(7)-C(6)-C(9)	109.23(19)
C(1)-C(6)-C(8)	110.47(17)
C(7)-C(6)-C(8)	108.3(2)
C(9)-C(6)-C(8)	108.27(19)
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5

C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(6)-C(9)-H(9A)	109.5
C(6)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(6)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(13)-C(10)-C(12)	106.6(2)
C(13)-C(10)-C(11)	109.68(19)
C(12)-C(10)-C(11)	105.61(19)
C(13)-C(10)-C(3)	114.54(18)
C(12)-C(10)-C(3)	109.81(19)
C(11)-C(10)-C(3)	110.15(18)
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(10)-C(13)-H(13A)	109.5
C(10)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(10)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(17)-C(14)-C(16)	105.70(19)
C(17)-C(14)-C(15)	109.66(18)
C(16)-C(14)-C(15)	106.10(18)

C(17)-C(14)-C(4)	116.17(18)
C(16)-C(14)-C(4)	111.02(17)
C(15)-C(14)-C(4)	107.75(17)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(22)	106.06(18)
C(19)-C(18)-C(23)	126.7(2)
C(22)-C(18)-C(23)	127.18(19)
C(19)-C(18)-Ce(1)	74.57(11)
C(22)-C(18)-Ce(1)	75.95(12)
C(23)-C(18)-Ce(1)	116.26(13)
C(18)-C(19)-C(20)	110.60(19)
C(18)-C(19)-Ce(1)	75.90(12)
C(20)-C(19)-Ce(1)	80.00(12)
C(18)-C(19)-H(19)	124.7
C(20)-C(19)-H(19)	124.7
Ce(1)-C(19)-H(19)	111.5
C(19)-C(20)-C(21)	106.17(18)
C(19)-C(20)-C(27)	117.54(18)
C(21)-C(20)-C(27)	133.91(19)
C(19)-C(20)-Ce(1)	70.52(11)
C(21)-C(20)-Ce(1)	76.58(11)

C(27)-C(20)-Ce(1)	130.30(13)
C(22)-C(21)-C(20)	106.31(18)
C(22)-C(21)-C(31)	120.38(18)
C(20)-C(21)-C(31)	132.28(18)
C(22)-C(21)-Ce(1)	70.92(11)
C(20)-C(21)-Ce(1)	74.36(11)
C(31)-C(21)-Ce(1)	128.17(13)
C(18)-C(22)-C(21)	110.73(18)
C(18)-C(22)-Ce(1)	74.62(11)
C(21)-C(22)-Ce(1)	80.08(11)
C(18)-C(22)-H(22)	124.6
C(21)-C(22)-H(22)	124.6
Ce(1)-C(22)-H(22)	112.6
C(26)-C(23)-C(18)	110.05(19)
C(26)-C(23)-C(24)	108.83(19)
C(18)-C(23)-C(24)	110.02(17)
C(26)-C(23)-C(25)	109.9(2)
C(18)-C(23)-C(25)	109.43(18)
C(24)-C(23)-C(25)	108.6(2)
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(23)-C(26)-H(26A)	109.5
C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(29)-C(27)-C(30)	108.81(18)

C(29)-C(27)-C(28)	105.66(18)
C(30)-C(27)-C(28)	106.92(18)
C(29)-C(27)-C(20)	116.96(17)
C(30)-C(27)-C(20)	107.48(17)
C(28)-C(27)-C(20)	110.60(17)
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(27)-C(30)-H(30A)	109.5
C(27)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(27)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(34)	110.88(18)
C(32)-C(31)-C(33)	106.01(18)
C(34)-C(31)-C(33)	105.24(18)
C(32)-C(31)-C(21)	114.89(17)
C(34)-C(31)-C(21)	108.68(17)
C(33)-C(31)-C(21)	110.70(18)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5

C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(31)-C(34)-H(34A)	109.5
C(31)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(31)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
F(3)-C(35)-F(2)	109.29(17)
F(3)-C(35)-F(1)	108.29(18)
F(2)-C(35)-F(1)	108.43(19)
F(3)-C(35)-S(1)	110.60(16)
F(2)-C(35)-S(1)	109.59(15)
F(1)-C(35)-S(1)	110.59(14)
S(1)-O(1)-Ce(1)	98.42(7)
S(1)-O(2)-Ce(1)	98.78(7)
O(3)-S(1)-O(1)	117.27(10)
O(3)-S(1)-O(2)	116.44(10)
O(1)-S(1)-O(2)	108.06(9)
O(3)-S(1)-C(35)	104.39(9)
O(1)-S(1)-C(35)	103.71(10)
O(2)-S(1)-C(35)	105.40(10)
O(3)-S(1)-Ce(1)	135.24(7)
O(1)-S(1)-Ce(1)	54.37(6)
O(2)-S(1)-Ce(1)	54.01(6)
C(35)-S(1)-Ce(1)	120.37(7)
O(2)-Ce(1)-O(1)	54.30(5)
O(2)-Ce(1)-C(19)	119.04(5)
O(1)-Ce(1)-C(19)	124.35(6)
O(2)-Ce(1)-C(18)	89.53(5)
O(1)-Ce(1)-C(18)	107.72(6)
C(19)-Ce(1)-C(18)	29.52(6)
O(2)-Ce(1)-C(5)	86.86(5)
O(1)-Ce(1)-C(5)	89.95(5)
C(19)-Ce(1)-C(5)	144.54(6)
C(18)-Ce(1)-C(5)	155.18(6)
O(2)-Ce(1)-C(1)	113.44(5)

O(1)-Ce(1)-C(1)	95.28(5)
C(19)-Ce(1)-C(1)	126.16(6)
C(18)-Ce(1)-C(1)	154.45(6)
C(5)-Ce(1)-C(1)	29.46(6)
O(2)-Ce(1)-C(22)	80.03(5)
O(1)-Ce(1)-C(22)	79.66(6)
C(19)-Ce(1)-C(22)	47.97(6)
C(18)-Ce(1)-C(22)	29.43(6)
C(5)-Ce(1)-C(22)	166.45(6)
C(1)-Ce(1)-C(22)	159.29(6)
O(2)-Ce(1)-C(2)	132.83(5)
O(1)-Ce(1)-C(2)	123.96(5)
C(19)-Ce(1)-C(2)	99.65(6)
C(18)-Ce(1)-C(2)	125.61(6)
C(5)-Ce(1)-C(2)	47.58(6)
C(1)-Ce(1)-C(2)	29.31(6)
C(22)-Ce(1)-C(2)	145.97(6)
O(2)-Ce(1)-C(20)	127.81(5)
O(1)-Ce(1)-C(20)	103.85(5)
C(19)-Ce(1)-C(20)	29.47(6)
C(18)-Ce(1)-C(20)	48.89(6)
C(5)-Ce(1)-C(20)	144.48(6)
C(1)-Ce(1)-C(20)	115.51(6)
C(22)-Ce(1)-C(20)	48.00(6)
C(2)-Ce(1)-C(20)	99.23(6)
O(2)-Ce(1)-C(4)	87.44(5)
O(1)-Ce(1)-C(4)	113.28(5)
C(19)-Ce(1)-C(4)	121.84(6)
C(18)-Ce(1)-C(4)	126.26(6)
C(5)-Ce(1)-C(4)	29.07(6)
C(1)-Ce(1)-C(4)	48.55(6)
C(22)-Ce(1)-C(4)	151.54(6)
C(2)-Ce(1)-C(4)	47.49(6)
C(20)-Ce(1)-C(4)	139.99(6)
O(2)-Ce(1)-C(21)	101.74(5)
O(1)-Ce(1)-C(21)	77.46(5)
C(19)-Ce(1)-C(21)	48.07(6)
C(18)-Ce(1)-C(21)	48.58(6)

C(5)-Ce(1)-C(21)	155.85(6)
C(1)-Ce(1)-C(21)	130.35(6)
C(22)-Ce(1)-C(21)	28.99(6)
C(2)-Ce(1)-C(21)	124.79(6)
C(20)-Ce(1)-C(21)	29.06(6)
C(4)-Ce(1)-C(21)	168.89(6)
O(2)-Ce(1)-C(3)	114.24(6)
O(1)-Ce(1)-C(3)	137.44(5)
C(19)-Ce(1)-C(3)	97.57(6)
C(18)-Ce(1)-C(3)	113.29(6)
C(5)-Ce(1)-C(3)	47.52(6)
C(1)-Ce(1)-C(3)	48.18(6)
C(22)-Ce(1)-C(3)	142.44(6)
C(2)-Ce(1)-C(3)	28.57(6)
C(20)-Ce(1)-C(3)	111.25(6)
C(4)-Ce(1)-C(3)	28.80(6)
C(21)-Ce(1)-C(3)	140.31(6)

1.5 Torsion angles involving non-hydrogen atoms of $Cp'_2CeOSO_2CF_3$

C(5)-C(1)-C(2)-C(3)	-3.5(2)
C(6)-C(1)-C(2)-C(3)	175.34(18)
Ce(1)-C(1)-C(2)-C(3)	-73.67(15)
C(5)-C(1)-C(2)-Ce(1)	70.13(13)
C(6)-C(1)-C(2)-Ce(1)	-111.00(19)
C(1)-C(2)-C(3)-C(4)	3.2(2)
Ce(1)-C(2)-C(3)-C(4)	-66.01(14)
C(1)-C(2)-C(3)-C(10)	-165.91(18)
Ce(1)-C(2)-C(3)-C(10)	124.87(18)
C(1)-C(2)-C(3)-Ce(1)	69.22(15)
C(2)-C(3)-C(4)-C(5)	-1.6(2)
C(10)-C(3)-C(4)-C(5)	165.8(2)
Ce(1)-C(3)-C(4)-C(5)	-65.04(13)
C(2)-C(3)-C(4)-C(14)	-167.1(2)
C(10)-C(3)-C(4)-C(14)	0.2(4)
Ce(1)-C(3)-C(4)-C(14)	129.4(2)

C(2)-C(3)-C(4)-Ce(1)	63.48(14)
C(10)-C(3)-C(4)-Ce(1)	-129.2(2)
C(2)-C(1)-C(5)-C(4)	2.5(2)
C(6)-C(1)-C(5)-C(4)	-176.37(18)
Ce(1)-C(1)-C(5)-C(4)	73.46(14)
C(2)-C(1)-C(5)-Ce(1)	-70.97(14)
C(6)-C(1)-C(5)-Ce(1)	110.2(2)
C(3)-C(4)-C(5)-C(1)	-0.6(2)
C(14)-C(4)-C(5)-C(1)	167.67(17)
Ce(1)-C(4)-C(5)-C(1)	-70.14(14)
C(3)-C(4)-C(5)-Ce(1)	69.56(14)
C(14)-C(4)-C(5)-Ce(1)	-122.19(16)
C(5)-C(1)-C(6)-C(7)	142.7(2)
C(2)-C(1)-C(6)-C(7)	-35.9(3)
Ce(1)-C(1)-C(6)-C(7)	-127.13(17)
C(5)-C(1)-C(6)-C(9)	-96.6(2)
C(2)-C(1)-C(6)-C(9)	84.8(3)
Ce(1)-C(1)-C(6)-C(9)	-6.4(2)
C(5)-C(1)-C(6)-C(8)	22.9(3)
C(2)-C(1)-C(6)-C(8)	-155.7(2)
Ce(1)-C(1)-C(6)-C(8)	113.06(17)
C(2)-C(3)-C(10)-C(13)	-120.5(2)
C(4)-C(3)-C(10)-C(13)	73.7(3)
Ce(1)-C(3)-C(10)-C(13)	-31.6(3)
C(2)-C(3)-C(10)-C(12)	-0.5(3)
C(4)-C(3)-C(10)-C(12)	-166.4(2)
Ce(1)-C(3)-C(10)-C(12)	88.3(2)
C(2)-C(3)-C(10)-C(11)	115.4(2)
C(4)-C(3)-C(10)-C(11)	-50.5(3)
Ce(1)-C(3)-C(10)-C(11)	-155.82(15)
C(5)-C(4)-C(14)-C(17)	156.41(19)
C(3)-C(4)-C(14)-C(17)	-39.3(3)
Ce(1)-C(4)-C(14)-C(17)	70.3(2)
C(5)-C(4)-C(14)-C(16)	35.6(3)
C(3)-C(4)-C(14)-C(16)	-160.1(2)
Ce(1)-C(4)-C(14)-C(16)	-50.5(2)
C(5)-C(4)-C(14)-C(15)	-80.2(2)
C(3)-C(4)-C(14)-C(15)	84.1(3)

Ce(1)-C(4)-C(14)-C(15)	-166.25(14)
C(22)-C(18)-C(19)-C(20)	-3.4(2)
C(23)-C(18)-C(19)-C(20)	175.08(19)
Ce(1)-C(18)-C(19)-C(20)	-73.41(15)
C(22)-C(18)-C(19)-Ce(1)	70.03(14)
C(23)-C(18)-C(19)-Ce(1)	-111.5(2)
C(18)-C(19)-C(20)-C(21)	1.7(2)
Ce(1)-C(19)-C(20)-C(21)	-68.97(13)
C(18)-C(19)-C(20)-C(27)	-163.19(18)
Ce(1)-C(19)-C(20)-C(27)	126.10(17)
C(18)-C(19)-C(20)-Ce(1)	70.70(14)
C(19)-C(20)-C(21)-C(22)	0.6(2)
C(27)-C(20)-C(21)-C(22)	161.9(2)
Ce(1)-C(20)-C(21)-C(22)	-64.18(13)
C(19)-C(20)-C(21)-C(31)	-167.4(2)
C(27)-C(20)-C(21)-C(31)	-6.1(4)
Ce(1)-C(20)-C(21)-C(31)	127.8(2)
C(19)-C(20)-C(21)-Ce(1)	64.78(13)
C(27)-C(20)-C(21)-Ce(1)	-133.9(2)
C(19)-C(18)-C(22)-C(21)	3.8(2)
C(23)-C(18)-C(22)-C(21)	-174.67(19)
Ce(1)-C(18)-C(22)-C(21)	72.84(15)
C(19)-C(18)-C(22)-Ce(1)	-69.06(14)
C(23)-C(18)-C(22)-Ce(1)	112.5(2)
C(20)-C(21)-C(22)-C(18)	-2.7(2)
C(31)-C(21)-C(22)-C(18)	167.00(17)
Ce(1)-C(21)-C(22)-C(18)	-69.26(14)
C(20)-C(21)-C(22)-Ce(1)	66.52(13)
C(31)-C(21)-C(22)-Ce(1)	-123.73(17)
C(19)-C(18)-C(23)-C(26)	-150.4(2)
C(22)-C(18)-C(23)-C(26)	27.7(3)
Ce(1)-C(18)-C(23)-C(26)	119.69(18)
C(19)-C(18)-C(23)-C(24)	89.7(3)
C(22)-C(18)-C(23)-C(24)	-92.2(3)
Ce(1)-C(18)-C(23)-C(24)	-0.2(2)
C(19)-C(18)-C(23)-C(25)	-29.6(3)
C(22)-C(18)-C(23)-C(25)	148.5(2)
Ce(1)-C(18)-C(23)-C(25)	-119.50(18)

C(19)-C(20)-C(27)-C(29)	-160.05(19)
C(21)-C(20)-C(27)-C(29)	40.2(3)
Ce(1)-C(20)-C(27)-C(29)	-73.0(2)
C(19)-C(20)-C(27)-C(30)	77.3(2)
C(21)-C(20)-C(27)-C(30)	-82.4(3)
Ce(1)-C(20)-C(27)-C(30)	164.39(14)
C(19)-C(20)-C(27)-C(28)	-39.1(3)
C(21)-C(20)-C(27)-C(28)	161.2(2)
Ce(1)-C(20)-C(27)-C(28)	48.0(2)
C(22)-C(21)-C(31)-C(32)	126.5(2)
C(20)-C(21)-C(31)-C(32)	-66.9(3)
Ce(1)-C(21)-C(31)-C(32)	37.7(2)
C(22)-C(21)-C(31)-C(34)	-108.7(2)
C(20)-C(21)-C(31)-C(34)	58.0(3)
Ce(1)-C(21)-C(31)-C(34)	162.55(14)
C(22)-C(21)-C(31)-C(33)	6.5(3)
C(20)-C(21)-C(31)-C(33)	173.1(2)
Ce(1)-C(21)-C(31)-C(33)	-82.3(2)
Ce(1)-O(1)-S(1)-O(3)	-127.83(9)
Ce(1)-O(1)-S(1)-O(2)	6.20(9)
Ce(1)-O(1)-S(1)-C(35)	117.74(8)
Ce(1)-O(2)-S(1)-O(3)	128.24(8)
Ce(1)-O(2)-S(1)-O(1)	-6.23(9)
Ce(1)-O(2)-S(1)-C(35)	-116.62(8)
F(3)-C(35)-S(1)-O(3)	68.36(17)
F(2)-C(35)-S(1)-O(3)	-52.20(18)
F(1)-C(35)-S(1)-O(3)	-171.69(16)
F(3)-C(35)-S(1)-O(1)	-168.31(14)
F(2)-C(35)-S(1)-O(1)	71.14(16)
F(1)-C(35)-S(1)-O(1)	-48.35(18)
F(3)-C(35)-S(1)-O(2)	-54.84(16)
F(2)-C(35)-S(1)-O(2)	-175.40(14)
F(1)-C(35)-S(1)-O(2)	65.12(18)
F(3)-C(35)-S(1)-Ce(1)	-111.81(13)
F(2)-C(35)-S(1)-Ce(1)	127.63(12)
F(1)-C(35)-S(1)-Ce(1)	8.1(2)
S(1)-O(2)-Ce(1)-O(1)	4.10(6)
S(1)-O(2)-Ce(1)-C(19)	-109.22(8)

S(1)-O(2)-Ce(1)-C(18)	-108.28(8)
S(1)-O(2)-Ce(1)-C(5)	96.29(8)
S(1)-O(2)-Ce(1)-C(1)	83.25(8)
S(1)-O(2)-Ce(1)-C(22)	-80.27(8)
S(1)-O(2)-Ce(1)-C(2)	109.88(9)
S(1)-O(2)-Ce(1)-C(20)	-75.27(9)
S(1)-O(2)-Ce(1)-C(4)	125.39(8)
S(1)-O(2)-Ce(1)-C(21)	-60.92(8)
S(1)-O(2)-Ce(1)-C(3)	136.26(7)
S(1)-O(1)-Ce(1)-O(2)	-4.10(6)
S(1)-O(1)-Ce(1)-C(19)	99.37(8)
S(1)-O(1)-Ce(1)-C(18)	72.00(8)
S(1)-O(1)-Ce(1)-C(5)	-90.27(8)
S(1)-O(1)-Ce(1)-C(1)	-119.28(8)
S(1)-O(1)-Ce(1)-C(22)	81.00(8)
S(1)-O(1)-Ce(1)-C(2)	-125.78(8)
S(1)-O(1)-Ce(1)-C(20)	122.79(8)
S(1)-O(1)-Ce(1)-C(4)	-72.44(9)
S(1)-O(1)-Ce(1)-C(21)	110.51(8)
S(1)-O(1)-Ce(1)-C(3)	-92.08(10)
C(18)-C(19)-Ce(1)-O(2)	1.91(14)
C(20)-C(19)-Ce(1)-O(2)	116.28(12)
C(18)-C(19)-Ce(1)-O(1)	-62.69(14)
C(20)-C(19)-Ce(1)-O(1)	51.68(14)
C(20)-C(19)-Ce(1)-C(18)	114.37(18)
C(18)-C(19)-Ce(1)-C(5)	134.08(13)
C(20)-C(19)-Ce(1)-C(5)	-111.55(14)
C(18)-C(19)-Ce(1)-C(1)	167.70(11)
C(20)-C(19)-Ce(1)-C(1)	-77.93(14)
C(18)-C(19)-Ce(1)-C(22)	-38.02(12)
C(20)-C(19)-Ce(1)-C(22)	76.35(13)
C(18)-C(19)-Ce(1)-C(2)	153.93(12)
C(20)-C(19)-Ce(1)-C(2)	-91.71(13)
C(18)-C(19)-Ce(1)-C(20)	-114.37(18)
C(18)-C(19)-Ce(1)-C(4)	108.45(13)
C(20)-C(19)-Ce(1)-C(4)	-137.19(12)
C(18)-C(19)-Ce(1)-C(21)	-77.38(13)
C(20)-C(19)-Ce(1)-C(21)	36.99(11)

C(18)-C(19)-Ce(1)-C(3)	125.10(13)
C(20)-C(19)-Ce(1)-C(3)	-120.54(12)
C(19)-C(18)-Ce(1)-O(2)	-178.33(13)
C(22)-C(18)-Ce(1)-O(2)	70.27(12)
C(23)-C(18)-Ce(1)-O(2)	-54.56(15)
C(19)-C(18)-Ce(1)-O(1)	129.64(12)
C(22)-C(18)-Ce(1)-O(1)	18.24(13)
C(23)-C(18)-Ce(1)-O(1)	-106.59(15)
C(22)-C(18)-Ce(1)-C(19)	-111.40(18)
C(23)-C(18)-Ce(1)-C(19)	123.8(2)
C(19)-C(18)-Ce(1)-C(5)	-96.86(17)
C(22)-C(18)-Ce(1)-C(5)	151.74(14)
C(23)-C(18)-Ce(1)-C(5)	26.9(2)
C(19)-C(18)-Ce(1)-C(1)	-23.5(2)
C(22)-C(18)-Ce(1)-C(1)	-134.90(15)
C(23)-C(18)-Ce(1)-C(1)	100.27(19)
C(19)-C(18)-Ce(1)-C(22)	111.40(18)
C(23)-C(18)-Ce(1)-C(22)	-124.8(2)
C(19)-C(18)-Ce(1)-C(2)	-32.21(15)
C(22)-C(18)-Ce(1)-C(2)	-143.60(11)
C(23)-C(18)-Ce(1)-C(2)	91.56(16)
C(19)-C(18)-Ce(1)-C(20)	36.50(12)
C(22)-C(18)-Ce(1)-C(20)	-74.90(13)
C(23)-C(18)-Ce(1)-C(20)	160.27(19)
C(19)-C(18)-Ce(1)-C(4)	-91.85(13)
C(22)-C(18)-Ce(1)-C(4)	156.75(11)
C(23)-C(18)-Ce(1)-C(4)	31.91(18)
C(19)-C(18)-Ce(1)-C(21)	75.49(13)
C(22)-C(18)-Ce(1)-C(21)	-35.90(11)
C(23)-C(18)-Ce(1)-C(21)	-160.74(19)
C(19)-C(18)-Ce(1)-C(3)	-62.01(14)
C(22)-C(18)-Ce(1)-C(3)	-173.41(11)
C(23)-C(18)-Ce(1)-C(3)	61.76(17)
C(1)-C(5)-Ce(1)-O(2)	-155.12(12)
C(4)-C(5)-Ce(1)-O(2)	90.38(12)
C(1)-C(5)-Ce(1)-O(1)	-100.88(12)
C(4)-C(5)-Ce(1)-O(1)	144.62(12)
C(1)-C(5)-Ce(1)-C(19)	65.34(16)

C(4)-C(5)-Ce(1)-C(19)	-49.16(16)
C(1)-C(5)-Ce(1)-C(18)	122.83(16)
C(4)-C(5)-Ce(1)-C(18)	8.3(2)
C(4)-C(5)-Ce(1)-C(1)	-114.50(17)
C(1)-C(5)-Ce(1)-C(22)	-140.5(2)
C(4)-C(5)-Ce(1)-C(22)	105.0(3)
C(1)-C(5)-Ce(1)-C(2)	38.38(11)
C(4)-C(5)-Ce(1)-C(2)	-76.12(13)
C(1)-C(5)-Ce(1)-C(20)	13.37(17)
C(4)-C(5)-Ce(1)-C(20)	-101.13(14)
C(1)-C(5)-Ce(1)-C(4)	114.50(17)
C(1)-C(5)-Ce(1)-C(21)	-43.1(2)
C(4)-C(5)-Ce(1)-C(21)	-157.56(13)
C(1)-C(5)-Ce(1)-C(3)	77.46(13)
C(4)-C(5)-Ce(1)-C(3)	-37.04(11)
C(5)-C(1)-Ce(1)-O(2)	27.25(13)
C(2)-C(1)-Ce(1)-O(2)	137.83(11)
C(6)-C(1)-Ce(1)-O(2)	-97.86(14)
C(5)-C(1)-Ce(1)-O(1)	80.47(12)
C(2)-C(1)-Ce(1)-O(1)	-168.95(12)
C(6)-C(1)-Ce(1)-O(1)	-44.64(14)
C(5)-C(1)-Ce(1)-C(19)	-139.22(12)
C(2)-C(1)-Ce(1)-C(19)	-28.65(15)
C(6)-C(1)-Ce(1)-C(19)	95.66(15)
C(5)-C(1)-Ce(1)-C(18)	-125.14(15)
C(2)-C(1)-Ce(1)-C(18)	-14.6(2)
C(6)-C(1)-Ce(1)-C(18)	109.75(17)
C(2)-C(1)-Ce(1)-C(5)	110.57(17)
C(6)-C(1)-Ce(1)-C(5)	-125.1(2)
C(5)-C(1)-Ce(1)-C(22)	155.09(16)
C(2)-C(1)-Ce(1)-C(22)	-94.3(2)
C(6)-C(1)-Ce(1)-C(22)	30.0(3)
C(5)-C(1)-Ce(1)-C(2)	-110.57(17)
C(6)-C(1)-Ce(1)-C(2)	124.3(2)
C(5)-C(1)-Ce(1)-C(20)	-171.44(11)
C(2)-C(1)-Ce(1)-C(20)	-60.86(13)
C(6)-C(1)-Ce(1)-C(20)	63.45(15)
C(5)-C(1)-Ce(1)-C(4)	-36.14(11)

C(2)-C(1)-Ce(1)-C(4)	74.43(13)
C(6)-C(1)-Ce(1)-C(4)	-161.26(17)
C(5)-C(1)-Ce(1)-C(21)	158.50(11)
C(2)-C(1)-Ce(1)-C(21)	-90.93(13)
C(6)-C(1)-Ce(1)-C(21)	33.38(17)
C(5)-C(1)-Ce(1)-C(3)	-75.01(13)
C(2)-C(1)-Ce(1)-C(3)	35.56(12)
C(6)-C(1)-Ce(1)-C(3)	159.87(17)
C(18)-C(22)-Ce(1)-O(2)	-107.12(12)
C(21)-C(22)-Ce(1)-O(2)	138.00(13)
C(18)-C(22)-Ce(1)-O(1)	-162.35(12)
C(21)-C(22)-Ce(1)-O(1)	82.76(12)
C(18)-C(22)-Ce(1)-C(19)	38.15(12)
C(21)-C(22)-Ce(1)-C(19)	-76.73(13)
C(21)-C(22)-Ce(1)-C(18)	-114.88(18)
C(18)-C(22)-Ce(1)-C(5)	-121.9(3)
C(21)-C(22)-Ce(1)-C(5)	123.2(2)
C(18)-C(22)-Ce(1)-C(1)	120.24(18)
C(21)-C(22)-Ce(1)-C(1)	5.4(2)
C(18)-C(22)-Ce(1)-C(2)	59.53(17)
C(21)-C(22)-Ce(1)-C(2)	-55.35(18)
C(18)-C(22)-Ce(1)-C(20)	78.19(13)
C(21)-C(22)-Ce(1)-C(20)	-36.69(11)
C(18)-C(22)-Ce(1)-C(4)	-41.91(19)
C(21)-C(22)-Ce(1)-C(4)	-156.79(12)
C(18)-C(22)-Ce(1)-C(21)	114.88(18)
C(18)-C(22)-Ce(1)-C(3)	9.96(17)
C(21)-C(22)-Ce(1)-C(3)	-104.92(14)
C(1)-C(2)-Ce(1)-O(2)	-57.12(14)
C(3)-C(2)-Ce(1)-O(2)	57.89(14)
C(1)-C(2)-Ce(1)-O(1)	13.30(14)
C(3)-C(2)-Ce(1)-O(1)	128.32(12)
C(1)-C(2)-Ce(1)-C(19)	156.88(12)
C(3)-C(2)-Ce(1)-C(19)	-88.10(13)
C(1)-C(2)-Ce(1)-C(18)	172.33(11)
C(3)-C(2)-Ce(1)-C(18)	-72.65(14)
C(1)-C(2)-Ce(1)-C(5)	-38.59(11)
C(3)-C(2)-Ce(1)-C(5)	76.42(13)

C(3)-C(2)-Ce(1)-C(1)	115.01(18)
C(1)-C(2)-Ce(1)-C(22)	140.94(13)
C(3)-C(2)-Ce(1)-C(22)	-104.05(15)
C(1)-C(2)-Ce(1)-C(20)	127.00(12)
C(3)-C(2)-Ce(1)-C(20)	-117.99(12)
C(1)-C(2)-Ce(1)-C(4)	-78.37(13)
C(3)-C(2)-Ce(1)-C(4)	36.65(12)
C(1)-C(2)-Ce(1)-C(21)	111.89(12)
C(3)-C(2)-Ce(1)-C(21)	-133.10(12)
C(1)-C(2)-Ce(1)-C(3)	-115.01(18)
C(19)-C(20)-Ce(1)-O(2)	-82.87(13)
C(21)-C(20)-Ce(1)-O(2)	29.97(14)
C(27)-C(20)-Ce(1)-O(2)	167.07(16)
C(19)-C(20)-Ce(1)-O(1)	-138.15(12)
C(21)-C(20)-Ce(1)-O(1)	-25.32(12)
C(27)-C(20)-Ce(1)-O(1)	111.78(17)
C(21)-C(20)-Ce(1)-C(19)	112.84(18)
C(27)-C(20)-Ce(1)-C(19)	-110.1(2)
C(19)-C(20)-Ce(1)-C(18)	-36.57(12)
C(21)-C(20)-Ce(1)-C(18)	76.27(13)
C(27)-C(20)-Ce(1)-C(18)	-146.6(2)
C(19)-C(20)-Ce(1)-C(5)	111.74(14)
C(21)-C(20)-Ce(1)-C(5)	-135.42(12)
C(27)-C(20)-Ce(1)-C(5)	1.7(2)
C(19)-C(20)-Ce(1)-C(1)	118.98(12)
C(21)-C(20)-Ce(1)-C(1)	-128.18(12)
C(27)-C(20)-Ce(1)-C(1)	8.91(19)
C(19)-C(20)-Ce(1)-C(22)	-76.24(13)
C(21)-C(20)-Ce(1)-C(22)	36.60(11)
C(27)-C(20)-Ce(1)-C(22)	173.7(2)
C(19)-C(20)-Ce(1)-C(2)	93.31(13)
C(21)-C(20)-Ce(1)-C(2)	-153.85(12)
C(27)-C(20)-Ce(1)-C(2)	-16.76(18)
C(19)-C(20)-Ce(1)-C(4)	63.89(15)
C(21)-C(20)-Ce(1)-C(4)	176.73(11)
C(27)-C(20)-Ce(1)-C(4)	-46.2(2)
C(19)-C(20)-Ce(1)-C(21)	-112.84(18)
C(27)-C(20)-Ce(1)-C(21)	137.1(2)

C(19)-C(20)-Ce(1)-C(3)	66.36(13)
C(21)-C(20)-Ce(1)-C(3)	179.20(11)
C(27)-C(20)-Ce(1)-C(3)	-43.71(19)
C(5)-C(4)-Ce(1)-O(2)	-88.14(12)
C(3)-C(4)-Ce(1)-O(2)	159.09(12)
C(14)-C(4)-Ce(1)-O(2)	23.18(17)
C(5)-C(4)-Ce(1)-O(1)	-39.07(13)
C(3)-C(4)-Ce(1)-O(1)	-151.84(11)
C(14)-C(4)-Ce(1)-O(1)	72.24(17)
C(5)-C(4)-Ce(1)-C(19)	148.89(11)
C(3)-C(4)-Ce(1)-C(19)	36.12(14)
C(14)-C(4)-Ce(1)-C(19)	-99.79(17)
C(5)-C(4)-Ce(1)-C(18)	-175.67(11)
C(3)-C(4)-Ce(1)-C(18)	71.56(14)
C(14)-C(4)-Ce(1)-C(18)	-64.36(18)
C(3)-C(4)-Ce(1)-C(5)	-112.77(17)
C(14)-C(4)-Ce(1)-C(5)	111.3(2)
C(5)-C(4)-Ce(1)-C(1)	36.66(11)
C(3)-C(4)-Ce(1)-C(1)	-76.11(13)
C(14)-C(4)-Ce(1)-C(1)	148.0(2)
C(5)-C(4)-Ce(1)-C(22)	-151.65(13)
C(3)-C(4)-Ce(1)-C(22)	95.58(16)
C(14)-C(4)-Ce(1)-C(22)	-40.3(2)
C(5)-C(4)-Ce(1)-C(2)	76.43(13)
C(3)-C(4)-Ce(1)-C(2)	-36.34(12)
C(14)-C(4)-Ce(1)-C(2)	-172.3(2)
C(5)-C(4)-Ce(1)-C(20)	117.55(12)
C(3)-C(4)-Ce(1)-C(20)	4.79(17)
C(14)-C(4)-Ce(1)-C(20)	-131.13(16)
C(5)-C(4)-Ce(1)-C(21)	125.8(3)
C(3)-C(4)-Ce(1)-C(21)	13.1(4)
C(14)-C(4)-Ce(1)-C(21)	-122.9(3)
C(5)-C(4)-Ce(1)-C(3)	112.77(17)
C(14)-C(4)-Ce(1)-C(3)	-135.9(2)
C(22)-C(21)-Ce(1)-O(2)	-42.31(13)
C(20)-C(21)-Ce(1)-O(2)	-156.23(11)
C(31)-C(21)-Ce(1)-O(2)	71.82(17)
C(22)-C(21)-Ce(1)-O(1)	-91.26(12)

C(20)-C(21)-Ce(1)-O(1)	154.83(12)
C(31)-C(21)-Ce(1)-O(1)	22.88(16)
C(22)-C(21)-Ce(1)-C(19)	76.36(13)
C(20)-C(21)-Ce(1)-C(19)	-37.55(11)
C(31)-C(21)-Ce(1)-C(19)	-169.5(2)
C(22)-C(21)-Ce(1)-C(18)	36.47(12)
C(20)-C(21)-Ce(1)-C(18)	-77.44(13)
C(31)-C(21)-Ce(1)-C(18)	150.6(2)
C(22)-C(21)-Ce(1)-C(5)	-151.37(14)
C(20)-C(21)-Ce(1)-C(5)	94.71(17)
C(31)-C(21)-Ce(1)-C(5)	-37.2(3)
C(22)-C(21)-Ce(1)-C(1)	-177.52(11)
C(20)-C(21)-Ce(1)-C(1)	68.57(14)
C(31)-C(21)-Ce(1)-C(1)	-63.38(19)
C(20)-C(21)-Ce(1)-C(22)	-113.92(18)
C(31)-C(21)-Ce(1)-C(22)	114.1(2)
C(22)-C(21)-Ce(1)-C(2)	145.90(12)
C(20)-C(21)-Ce(1)-C(2)	31.98(14)
C(31)-C(21)-Ce(1)-C(2)	-99.97(17)
C(22)-C(21)-Ce(1)-C(20)	113.92(18)
C(31)-C(21)-Ce(1)-C(20)	-132.0(2)
C(22)-C(21)-Ce(1)-C(4)	102.9(3)
C(20)-C(21)-Ce(1)-C(4)	-11.0(4)
C(31)-C(21)-Ce(1)-C(4)	-142.9(3)
C(22)-C(21)-Ce(1)-C(3)	112.75(13)
C(20)-C(21)-Ce(1)-C(3)	-1.17(16)
C(31)-C(21)-Ce(1)-C(3)	-133.12(16)
C(2)-C(3)-Ce(1)-O(2)	-137.05(12)
C(4)-C(3)-Ce(1)-O(2)	-23.01(13)
C(10)-C(3)-Ce(1)-O(2)	109.02(18)
C(2)-C(3)-Ce(1)-O(1)	-74.18(14)
C(4)-C(3)-Ce(1)-O(1)	39.86(15)
C(10)-C(3)-Ce(1)-O(1)	171.90(15)
C(2)-C(3)-Ce(1)-C(19)	96.31(13)
C(4)-C(3)-Ce(1)-C(19)	-149.65(12)
C(10)-C(3)-Ce(1)-C(19)	-17.62(19)
C(2)-C(3)-Ce(1)-C(18)	122.34(12)
C(4)-C(3)-Ce(1)-C(18)	-123.62(12)

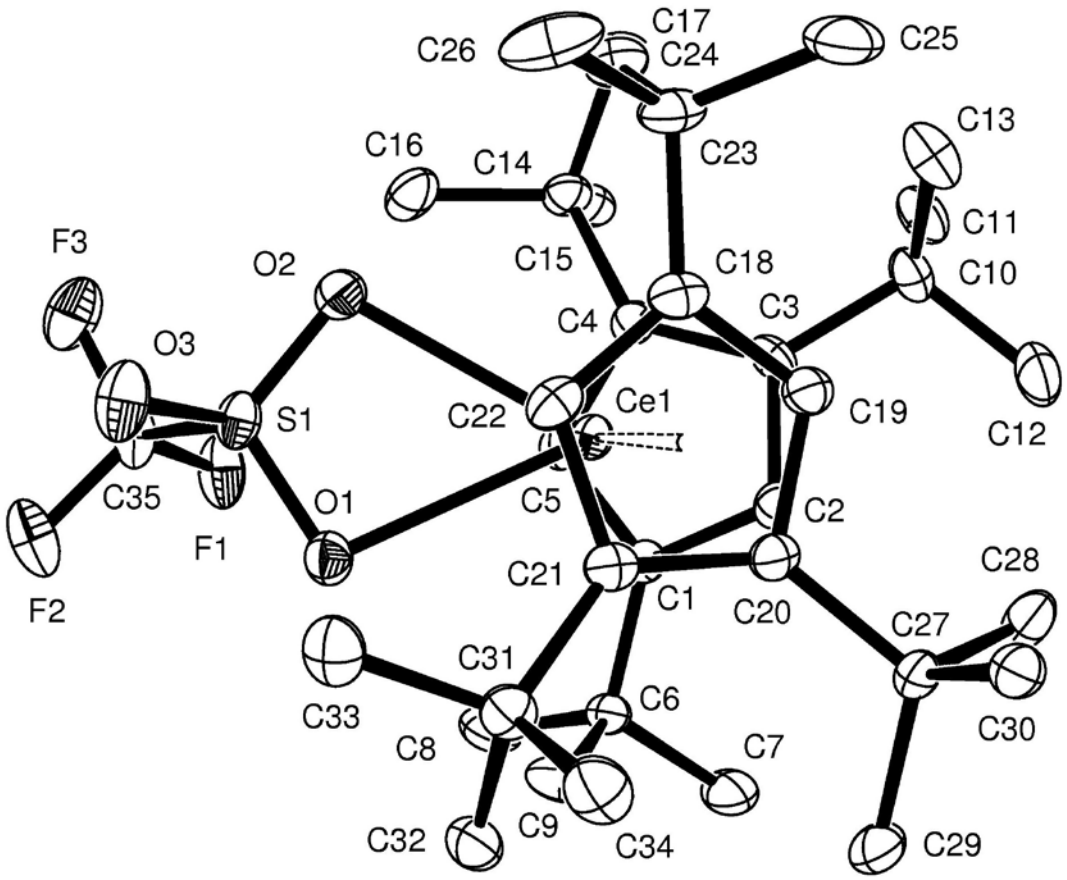
C(10)-C(3)-Ce(1)-C(18)	8.4(2)
C(2)-C(3)-Ce(1)-C(5)	-76.64(13)
C(4)-C(3)-Ce(1)-C(5)	37.40(12)
C(10)-C(3)-Ce(1)-C(5)	169.4(2)
C(2)-C(3)-Ce(1)-C(1)	-36.53(12)
C(4)-C(3)-Ce(1)-C(1)	77.51(13)
C(10)-C(3)-Ce(1)-C(1)	-150.5(2)
C(2)-C(3)-Ce(1)-C(22)	117.03(13)
C(4)-C(3)-Ce(1)-C(22)	-128.92(13)
C(10)-C(3)-Ce(1)-C(22)	3.1(2)
C(4)-C(3)-Ce(1)-C(2)	114.04(18)
C(10)-C(3)-Ce(1)-C(2)	-113.9(2)
C(2)-C(3)-Ce(1)-C(20)	69.26(13)
C(4)-C(3)-Ce(1)-C(20)	-176.70(12)
C(10)-C(3)-Ce(1)-C(20)	-44.66(19)
C(2)-C(3)-Ce(1)-C(4)	-114.04(18)
C(10)-C(3)-Ce(1)-C(4)	132.0(2)
C(2)-C(3)-Ce(1)-C(21)	69.87(15)
C(4)-C(3)-Ce(1)-C(21)	-176.09(11)
C(10)-C(3)-Ce(1)-C(21)	-44.1(2)

1.6 Least Squares Planes for $Cp'_2CeOSO_2CF_3$

```
(* indicates atom used to define plane)

2.6569 (0.0104) x + 14.4388 (0.0166) y + 10.6715 (0.0126) z = 7.8555 (0.0081)

 *    -0.0173 (0.0012)  C1
 *     0.0195 (0.0013)  C2
 *    -0.0138 (0.0013)  C3
 *     0.0030 (0.0012)  C4
 *     0.0085 (0.0012)  C5
      -0.0973 (0.0035)  C6
      -0.3090 (0.0037)  C10
      -0.2632 (0.0036)  C14

 Rms deviation of fitted atoms =   0.0138


 - 1.7172 (0.0106) x + 19.9473 (0.0085) y + 5.8614 (0.0155) z = 9.6133 (0.0111)

 Angle to previous plane (with approximate esd) = 35.17 ( 0.09 )

 *     0.0206 (0.0012)  C18
 *    -0.0145 (0.0013)  C19
 *     0.0031 (0.0012)  C20
```

```
*    0.0096 (0.0012)  C21
*   -0.0187 (0.0013)  C22
     0.1208 (0.0036)  C23
     0.3659 (0.0036)  C27
     0.2763 (0.0036)  C31

Rms deviation of fitted atoms =   0.0147


- 0.2676 (0.0075) x + 18.3020 (0.0084) y + 8.5493 (0.0106) z = 9.0662 (0.0070)

Angle to previous plane (with approximate esd) = 14.00 ( 0.09 )

*    0.0000 (0.0000)  Ce1
*    0.0000 (0.0000)  O1
*    0.0000 (0.0000)  O2
     0.1033 (0.0015)  S1

Rms deviation of fitted atoms =   0.0000


- 1.1435 (0.0119) x + 19.1157 (0.0107) y + 7.4717 (0.0161) z = 7.9964 (0.0151)

Angle to previous plane (with approximate esd) =  6.91 ( 0.11 )

*    0.0000 (0.0000)  S1
*    0.0000 (0.0000)  O1
*    0.0000 (0.0000)  O2
     0.2776 (0.0041)  Ce1

Rms deviation of fitted atoms =   0.0000


- 7.5815 (0.0118) x - 8.5268 (0.0253) y + 10.9288 (0.0161) z = 6.9759 (0.0176)

Angle to previous plane (with approximate esd) = 88.99 ( 0.09 )

*    0.0000 (0.0000)  S1
*    0.0000 (0.0000)  O3
*    0.0000 (0.0000)  C35

Rms deviation of fitted atoms =   0.0000
```

1.7 ORTEP diagram (50% ellipsoids) showing atom labeling scheme for $Cp'_2CeOSO_2CF_3$



2. $Cp'_2Ce(\mu_3\text{-}OSO_2)CeCp'_2$

A yellow, block like crystal of $Cp'_2Ce(\mu_3\text{-}OSO_2)CeCp'_2$ having approximate dimensions of 0.10 x 0.08 x 0.03 mm was mounted on a Kapton loop using Paratone N hydrocarbon oil. All measurements were made on a Bruker APEX[1] defractometer with a CCD area detector using graphite monochromated Mo-Kα radiation. Cell constants and an orientation matrix obtained from a least-squares refinement using the measured positions of 9193 reflections with I > 10σ, in the range 4.46 < 2θ < 50.66^o corresponded to a primitive monoclinic cell with dimensions:

a = 20.6275(8) Å
b = 10.5366(4) Å ® = 99.5900(10)^o
c = 30.6641(12) Å
V = 6571.5(4) Å^3

For Z = 4 and F.W. = 1293.91, the calculated density is 1.398 g/cm^3. The systematic absences of:

h0l: l ± 2n
0k0: k ± 2n

uniquely determine the space group to be $P2_1/c$ (#14). The data were collected at a temperature of -173 ± 1^{o}C using 10 second ω and ϕ scans to a maximum 2θ value of 50.74^o. Frame data were integrated using SAINT[2]. Of the 123246 reflections which were collected, 12055 were unique (R_{int} = 0.0804); equivalent reflections were merged. No decay correction was applied. An empirical absorption correction was applied using SADABS[4]. Maximum and minimum effective transmissions were 0.9580 and 0.8693 respectively. The data were also corrected for Lorentz-polarization effects. The structure was solved by direct methods[5] and expanded using Fourier techniques.[6] Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in calculated positions but not refined. The final cycle of full-matrix least-squares refinement was based on 9588 observed reflections (I > 3.00σ(I)) and 703 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of R = 0.0379, R_w = 0.0792, and GOF = 1.053. The weighting scheme was based on counting statistics and included a factor (p = 0.0328) to downweight the intense reflections. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.62 and -0.84 e$^-$/Å^3, respectively. All calculations were performed using the WinGX[7]

crystallographic software package.

Crystal data and structure refinement

Identification code	shelxl	
Empirical formula	C68 H116 Ce2 O3 S	
Formula weight	1293.91	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 20.6275(8) Å	⟨= 90°.
	b = 10.5366(4) Å	®= 99.5900(10)°.
	c = 30.6641(12) Å	© = 90°.
Volume	6571.5(4) $Å^3$	
Z	4	
Density (calculated)	1.308 Mg/m^3	
Absorption coefficient	1.442 mm^{-1}	
F(000)	2720	
Crystal size	0.10 x 0.08 x 0.03 mm^3	
Theta range for data collection	1.35 to 25.37°.	
Index ranges	-24<=h<=24, -12<=k<=12, -36<=l<=36	
Reflections collected	123246	
Independent reflections	12055 [R(int) = 0.0804]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9580 and 0.8693	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12055 / 0 / 703	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0379, wR2 = 0.0792	
R indices (all data)	R1 = 0.0558, wR2 = 0.0880	
Largest diff. peak and hole	1.618 and -0.836 $e.Å^{-3}$	

2.1 Atomic coordinates for $Cp'_2Ce(\eta_3\text{-}OSO_2)CeCp'_2$

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7544(2)	2989(4)	7499(1)	21(1)

C(2)	7266(2)	2525(4)	7854(1)	21(1)
C(3)	6594(2)	2180(4)	7709(1)	21(1)
C(4)	6456(2)	2413(4)	7241(1)	20(1)
C(5)	7052(2)	2904(4)	7127(1)	22(1)
C(6)	8234(2)	3530(4)	7527(2)	26(1)
C(7)	8324(2)	4625(4)	7864(2)	32(1)
C(8)	8730(2)	2502(5)	7693(2)	46(1)
C(9)	8353(2)	4030(5)	7079(2)	39(1)
C(10)	6160(2)	1986(4)	8067(1)	22(1)
C(11)	5959(2)	3317(4)	8216(2)	29(1)
C(12)	6554(2)	1331(5)	8477(2)	34(1)
C(13)	5536(2)	1192(4)	7939(2)	28(1)
C(14)	5813(2)	2413(4)	6895(1)	22(1)
C(15)	5316(2)	3353(4)	7031(2)	29(1)
C(16)	5953(2)	2886(5)	6449(1)	30(1)
C(17)	5495(2)	1101(4)	6809(1)	25(1)
C(18)	7349(2)	-2097(4)	7612(1)	20(1)
C(19)	7679(2)	-1481(4)	7992(1)	20(1)
C(20)	8339(2)	-1182(4)	7943(1)	20(1)
C(21)	8412(2)	-1592(4)	7509(1)	19(1)
C(22)	7796(2)	-2130(4)	7312(1)	21(1)
C(23)	6650(2)	-2617(4)	7539(1)	22(1)
C(24)	6200(2)	-1617(4)	7282(2)	26(1)
C(25)	6608(2)	-3832(4)	7266(2)	34(1)
C(26)	6423(2)	-2881(5)	7979(2)	35(1)
C(27)	8815(2)	-865(4)	8372(1)	26(1)
C(28)	8491(2)	41(5)	8665(2)	33(1)
C(29)	8950(2)	-2137(5)	8627(2)	34(1)
C(30)	9480(2)	-280(5)	8328(2)	33(1)
C(31)	9022(2)	-1738(4)	7276(1)	24(1)
C(32)	8808(2)	-2231(4)	6800(2)	31(1)
C(33)	9394(2)	-500(4)	7228(2)	28(1)
C(34)	9478(2)	-2750(4)	7517(2)	32(1)
C(35)	8781(2)	-1870(4)	5205(1)	18(1)
C(36)	8519(2)	-1308(4)	4800(1)	20(1)
C(37)	8513(2)	45(4)	4842(1)	20(1)
C(38)	8786(2)	320(4)	5297(1)	19(1)
C(39)	8925(2)	-866(4)	5510(1)	18(1)

C(40)	8859(2)	-3267(4)	5321(1)	21(1)
C(41)	8812(2)	-4086(4)	4903(1)	26(1)
C(42)	9522(2)	-3528(4)	5612(1)	26(1)
C(43)	8309(2)	-3636(4)	5579(1)	25(1)
C(44)	8383(2)	838(4)	4412(1)	22(1)
C(45)	9012(2)	762(4)	4197(2)	30(1)
C(46)	7816(2)	241(4)	4085(1)	27(1)
C(47)	8201(2)	2234(4)	4451(2)	29(1)
C(48)	9014(2)	1555(4)	5548(1)	22(1)
C(49)	9564(2)	2164(4)	5339(2)	28(1)
C(50)	8462(2)	2524(4)	5571(1)	26(1)
C(51)	9309(2)	1268(4)	6032(1)	26(1)
C(52)	6271(2)	-279(4)	5025(1)	20(1)
C(53)	6236(2)	-1002(4)	5406(1)	19(1)
C(54)	6339(2)	-2307(4)	5325(1)	19(1)
C(55)	6477(2)	-2390(4)	4879(1)	19(1)
C(56)	6433(2)	-1134(4)	4708(1)	19(1)
C(57)	6180(2)	1156(4)	4980(1)	22(1)
C(58)	6000(2)	1538(4)	4495(1)	30(1)
C(59)	6822(2)	1795(4)	5184(2)	32(1)
C(60)	5626(2)	1588(4)	5228(2)	34(1)
C(61)	6210(2)	-3317(4)	5666(1)	23(1)
C(62)	6818(2)	-4120(4)	5850(2)	30(1)
C(63)	5632(2)	-4174(4)	5473(2)	29(1)
C(64)	6001(2)	-2653(4)	6071(1)	30(1)
C(65)	6497(2)	-3488(4)	4547(1)	22(1)
C(66)	6765(2)	-4760(4)	4740(2)	28(1)
C(67)	5788(2)	-3681(4)	4300(2)	30(1)
C(68)	6924(2)	-3121(4)	4199(1)	26(1)
O(1)	8014(1)	841(3)	6732(1)	27(1)
O(2)	6927(1)	29(3)	6572(1)	26(1)
O(3)	7667(1)	-306(3)	6045(1)	31(1)
S(1)	7441(1)	698(1)	6350(1)	25(1)
Ce(1)	7434(1)	392(1)	7337(1)	17(1)
Ce(2)	7566(1)	-970(1)	5334(1)	17(1)
H(2)	7487	2453	8144	26
H(5)	7105	3135	6843	27

H(7A)	8045	5320	7752	48
H(7B)	8775	4898	7912	48
H(7C)	8210	4339	8139	48
H(8A)	8640	2173	7969	69
H(8B)	9166	2853	7736	69
H(8C)	8699	1829	7480	69
H(9A)	8300	3350	6867	59
H(9B)	8792	4362	7107	59
H(9C)	8043	4691	6980	59
H(11A)	5714	3756	7967	43
H(11B)	6347	3794	8329	43
H(11C)	5693	3224	8442	43
H(12A)	6272	1189	8692	51
H(12B)	6915	1863	8603	51
H(12C)	6720	532	8392	51
H(13A)	5266	1565	7686	42
H(13B)	5297	1170	8182	42
H(13C)	5653	344	7869	42
H(15A)	5519	4170	7086	43
H(15B)	5172	3057	7295	43
H(15C)	4944	3422	6798	43
H(16A)	6278	2351	6351	45
H(16B)	6114	3741	6479	45
H(16C)	5556	2862	6236	45
H(17A)	5082	1185	6614	37
H(17B)	5423	737	7084	37
H(17C)	5781	559	6676	37
H(19)	7493	-1295	8241	24
H(22)	7705	-2455	7026	25
H(24A)	6228	-842	7449	40
H(24B)	5755	-1918	7234	40
H(24C)	6336	-1465	7002	40
H(25A)	6762	-3669	6993	51
H(25B)	6160	-4118	7206	51
H(25C)	6877	-4475	7429	51
H(26A)	6729	-3445	8152	53
H(26B)	5996	-3266	7925	53
H(26C)	6403	-2098	8136	53

H(28A)	8802	257	8924	49
H(28B)	8117	-366	8753	49
H(28C)	8353	799	8503	49
H(29A)	9150	-2727	8451	52
H(29B)	8542	-2483	8686	52
H(29C)	9239	-1990	8902	52
H(30A)	9412	530	8185	50
H(30B)	9708	-831	8155	50
H(30C)	9738	-173	8617	50
H(32A)	9188	-2325	6659	46
H(32B)	8509	-1638	6636	46
H(32C)	8595	-3038	6808	46
H(33A)	9529	-129	7515	42
H(33B)	9112	80	7044	42
H(33C)	9775	-677	7096	42
H(34A)	9819	-2940	7350	48
H(34B)	9230	-3505	7549	48
H(34C)	9670	-2440	7804	48
H(36)	8369	-1752	4541	24
H(39)	9089	-968	5809	22
H(41A)	8388	-3970	4723	40
H(41B)	8868	-4963	4986	40
H(41C)	9149	-3838	4739	40
H(42A)	9871	-3284	5457	39
H(42B)	9558	-4417	5681	39
H(42C)	9554	-3048	5881	39
H(43A)	8348	-3139	5844	37
H(43B)	8345	-4520	5654	37
H(43C)	7889	-3478	5399	37
H(45A)	8949	1250	3929	45
H(45B)	9097	-107	4131	45
H(45C)	9379	1095	4398	45
H(46A)	7425	222	4217	40
H(46B)	7932	-609	4015	40
H(46C)	7736	738	3819	40
H(47A)	7802	2296	4573	44
H(47B)	8138	2620	4163	44
H(47C)	8549	2664	4641	44

H(49A)	9396	2403	5040	42
H(49B)	9916	1566	5342	42
H(49C)	9726	2903	5506	42
H(50A)	8645	3272	5723	39
H(50B)	8142	2158	5728	39
H(50C)	8256	2746	5277	39
H(51A)	9684	723	6041	40
H(51B)	8985	856	6174	40
H(51C)	9442	2048	6183	40
H(53)	6156	-672	5673	23
H(56)	6502	-909	4426	23
H(58A)	5925	2437	4475	44
H(58B)	5608	1099	4364	44
H(58C)	6353	1318	4342	44
H(59A)	6922	1588	5492	49
H(59B)	6778	2698	5150	49
H(59C)	7170	1502	5037	49
H(60A)	5725	1320	5531	50
H(60B)	5217	1217	5091	50
H(60C)	5590	2496	5216	50
H(62A)	6700	-4739	6053	45
H(62B)	7156	-3578	6001	45
H(62C)	6975	-4543	5611	45
H(63A)	5742	-4638	5226	43
H(63B)	5250	-3662	5377	43
H(63C)	5542	-4758	5696	43
H(64A)	5602	-2187	5977	45
H(64B)	6341	-2080	6200	45
H(64C)	5930	-3278	6285	45
H(66A)	6770	-5359	4505	42
H(66B)	6490	-5073	4940	42
H(66C)	7205	-4645	4897	42
H(67A)	5784	-4348	4086	45
H(67B)	5634	-2909	4152	45
H(67C)	5507	-3907	4507	45
H(68A)	7361	-2920	4345	39
H(68B)	6736	-2396	4036	39
H(68C)	6942	-3820	4001	39

2.2 Anisotropic thermal parameters for $Cp'_2Ce(\mu_3\text{-}OSO_2)CeCp'_2$

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}
C(1)	22(2)	13(2)	29(2)	2(2)	4(2)	1(2)
C(2)	23(2)	18(2)	23(2)	-2(2)	1(2)	1(2)
C(3)	19(2)	15(2)	28(2)	-1(2)	3(2)	2(2)
C(4)	20(2)	14(2)	26(2)	4(2)	2(2)	2(2)
C(5)	25(2)	14(2)	29(3)	3(2)	11(2)	0(2)
C(6)	20(2)	21(2)	37(3)	5(2)	9(2)	-3(2)
C(7)	29(3)	32(3)	34(3)	-1(2)	3(2)	-10(2)
C(8)	30(3)	32(3)	79(4)	6(3)	12(3)	3(2)
C(9)	39(3)	41(3)	42(3)	-14(2)	20(2)	-21(2)
C(10)	21(2)	19(2)	27(2)	0(2)	8(2)	2(2)
C(11)	26(2)	29(3)	32(3)	-4(2)	8(2)	1(2)
C(12)	39(3)	35(3)	31(3)	1(2)	12(2)	4(2)
C(13)	28(2)	24(2)	35(3)	-1(2)	15(2)	-2(2)
C(14)	17(2)	24(2)	25(2)	4(2)	3(2)	5(2)
C(15)	21(2)	23(2)	42(3)	3(2)	1(2)	2(2)
C(16)	25(2)	37(3)	26(3)	7(2)	-1(2)	-1(2)
C(17)	22(2)	24(2)	27(3)	3(2)	-1(2)	2(2)
C(18)	20(2)	14(2)	25(2)	6(2)	3(2)	4(2)
C(19)	24(2)	15(2)	22(2)	0(2)	4(2)	2(2)
C(20)	19(2)	18(2)	21(2)	3(2)	-4(2)	1(2)
C(21)	19(2)	14(2)	24(2)	3(2)	1(2)	0(2)
C(22)	26(2)	11(2)	24(2)	-1(2)	4(2)	0(2)
C(23)	17(2)	17(2)	30(3)	2(2)	2(2)	-3(2)
C(24)	19(2)	26(2)	35(3)	3(2)	5(2)	-3(2)
C(25)	24(2)	23(3)	53(3)	-9(2)	1(2)	-6(2)
C(26)	23(2)	46(3)	37(3)	13(2)	7(2)	-5(2)
C(27)	22(2)	28(2)	24(2)	0(2)	-3(2)	-1(2)
C(28)	39(3)	33(3)	23(3)	-5(2)	-4(2)	-1(2)
C(29)	31(3)	40(3)	30(3)	3(2)	-4(2)	4(2)
C(30)	24(2)	35(3)	37(3)	-4(2)	-5(2)	-4(2)
C(31)	21(2)	21(2)	32(3)	0(2)	8(2)	0(2)

C(32)	30(3)	31(3)	35(3)	-3(2)	16(2)	0(2)
C(33)	21(2)	21(2)	42(3)	5(2)	6(2)	3(2)
C(34)	23(2)	28(3)	47(3)	8(2)	12(2)	3(2)
C(35)	12(2)	20(2)	20(2)	0(2)	1(2)	0(2)
C(36)	16(2)	26(2)	19(2)	-3(2)	3(2)	-5(2)
C(37)	18(2)	22(2)	21(2)	2(2)	1(2)	1(2)
C(38)	17(2)	19(2)	22(2)	2(2)	6(2)	-2(2)
C(39)	16(2)	21(2)	16(2)	2(2)	0(2)	-2(2)
C(40)	23(2)	19(2)	20(2)	1(2)	2(2)	-2(2)
C(41)	31(2)	20(2)	27(3)	-2(2)	2(2)	0(2)
C(42)	30(2)	20(2)	28(3)	2(2)	3(2)	3(2)
C(43)	26(2)	20(2)	30(3)	2(2)	6(2)	1(2)
C(44)	21(2)	24(2)	21(2)	5(2)	4(2)	-3(2)
C(45)	28(2)	36(3)	27(3)	7(2)	7(2)	-5(2)
C(46)	26(2)	32(3)	21(2)	8(2)	1(2)	-1(2)
C(47)	37(3)	27(3)	25(3)	7(2)	4(2)	1(2)
C(48)	21(2)	20(2)	26(2)	1(2)	4(2)	-6(2)
C(49)	23(2)	26(3)	35(3)	0(2)	4(2)	-11(2)
C(50)	25(2)	23(2)	30(3)	-1(2)	4(2)	-4(2)
C(51)	25(2)	28(3)	26(3)	-4(2)	3(2)	-4(2)
C(52)	13(2)	22(2)	22(2)	2(2)	-1(2)	-2(2)
C(53)	19(2)	21(2)	18(2)	-1(2)	3(2)	-2(2)
C(54)	16(2)	20(2)	21(2)	2(2)	1(2)	-2(2)
C(55)	18(2)	16(2)	23(2)	1(2)	3(2)	-1(2)
C(56)	17(2)	25(2)	15(2)	3(2)	1(2)	-2(2)
C(57)	19(2)	22(2)	25(2)	2(2)	0(2)	3(2)
C(58)	36(3)	25(3)	27(3)	5(2)	2(2)	6(2)
C(59)	30(3)	21(2)	43(3)	9(2)	-4(2)	-5(2)
C(60)	38(3)	25(3)	39(3)	0(2)	10(2)	8(2)
C(61)	25(2)	20(2)	24(2)	4(2)	4(2)	-6(2)
C(62)	28(2)	32(3)	29(3)	17(2)	4(2)	-2(2)
C(63)	26(2)	28(3)	32(3)	1(2)	4(2)	-8(2)
C(64)	35(3)	33(3)	23(3)	5(2)	7(2)	-9(2)
C(65)	22(2)	20(2)	24(2)	-4(2)	2(2)	-5(2)
C(66)	31(3)	25(3)	29(3)	-3(2)	5(2)	0(2)
C(67)	29(3)	31(3)	29(3)	-8(2)	-2(2)	-3(2)
C(68)	29(2)	24(2)	25(2)	-7(2)	4(2)	-3(2)
O(1)	23(2)	31(2)	27(2)	-3(1)	4(1)	-4(1)

O(2)	27(2)	27(2)	24(2)	-1(1)	6(1)	-4(1)
O(3)	25(2)	34(2)	35(2)	-5(1)	10(1)	1(1)
S(1)	24(1)	28(1)	23(1)	0(1)	6(1)	1(1)
Ce(1)	16(1)	16(1)	20(1)	0(1)	3(1)	1(1)
Ce(2)	16(1)	17(1)	19(1)	1(1)	2(1)	-2(1)

2.3 Bond lengths involving non-hydrogen atoms of $Cp'_2Ce(\mu_3\text{-}OSO_2)CeCp'_2$

C(1)-C(5)	1.397(6)
C(1)-C(2)	1.401(6)
C(1)-C(6)	1.522(6)
C(1)-Ce(1)	2.784(4)
C(2)-C(3)	1.430(6)
C(2)-Ce(1)	2.807(4)
C(3)-C(4)	1.436(6)
C(3)-C(10)	1.541(5)
C(3)-Ce(1)	2.918(4)
C(4)-C(5)	1.430(5)
C(4)-C(14)	1.553(5)
C(4)-Ce(1)	2.915(4)
C(5)-Ce(1)	2.805(4)
C(6)-C(8)	1.520(6)
C(6)-C(9)	1.532(6)
C(6)-C(7)	1.538(6)
C(10)-C(13)	1.530(6)
C(10)-C(12)	1.543(6)
C(10)-C(11)	1.553(6)
C(14)-C(16)	1.529(6)
C(14)-C(15)	1.534(6)
C(14)-C(17)	1.534(6)
C(18)-C(19)	1.408(6)
C(18)-C(22)	1.407(5)
C(18)-C(23)	1.525(5)
C(18)-Ce(1)	2.769(4)
C(19)-C(20)	1.429(5)
C(19)-Ce(1)	2.803(4)

C(20)-C(21)	1.431(6)
C(20)-C(27)	1.543(6)
C(20)-Ce(1)	2.921(4)
C(21)-C(22)	1.429(6)
C(21)-C(31)	1.556(5)
C(21)-Ce(1)	2.892(4)
C(22)-Ce(1)	2.765(4)
C(23)-C(26)	1.523(6)
C(23)-C(25)	1.524(6)
C(23)-C(24)	1.532(6)
C(27)-C(30)	1.530(6)
C(27)-C(28)	1.537(6)
C(27)-C(29)	1.554(6)
C(31)-C(34)	1.529(6)
C(31)-C(33)	1.533(6)
C(31)-C(32)	1.542(6)
C(35)-C(36)	1.399(5)
C(35)-C(39)	1.411(5)
C(35)-C(40)	1.517(6)
C(35)-Ce(2)	2.770(4)
C(36)-C(37)	1.432(6)
C(36)-Ce(2)	2.783(4)
C(37)-C(38)	1.444(6)
C(37)-C(44)	1.547(5)
C(37)-Ce(2)	2.868(4)
C(38)-C(39)	1.416(5)
C(38)-C(48)	1.544(6)
C(38)-Ce(2)	2.880(4)
C(39)-Ce(2)	2.769(4)
C(40)-C(42)	1.530(6)
C(40)-C(41)	1.534(6)
C(40)-C(43)	1.537(5)
C(44)-C(47)	1.528(6)
C(44)-C(46)	1.543(6)
C(44)-C(45)	1.552(5)
C(48)-C(49)	1.533(5)
C(48)-C(51)	1.538(6)
C(48)-C(50)	1.540(6)

C(52)-C(56)	1.406(6)
C(52)-C(53)	1.406(5)
C(52)-C(57)	1.526(6)
C(52)-Ce(2)	2.778(4)
C(53)-C(54)	1.420(6)
C(53)-Ce(2)	2.788(4)
C(54)-C(55)	1.444(6)
C(54)-C(61)	1.547(5)
C(54)-Ce(2)	2.891(4)
C(55)-C(56)	1.421(6)
C(55)-C(65)	1.546(6)
C(55)-Ce(2)	2.861(4)
C(56)-Ce(2)	2.772(4)
C(57)-C(59)	1.523(6)
C(57)-C(58)	1.524(6)
C(57)-C(60)	1.543(6)
C(61)-C(63)	1.532(6)
C(61)-C(62)	1.539(6)
C(61)-C(64)	1.547(6)
C(65)-C(66)	1.531(6)
C(65)-C(68)	1.542(5)
C(65)-C(67)	1.544(6)
O(1)-S(1)	1.527(3)
O(1)-Ce(1)	2.415(3)
O(2)-S(1)	1.524(3)
O(2)-Ce(1)	2.432(3)
O(3)-S(1)	1.537(3)
O(3)-Ce(2)	2.264(3)
S(1)-Ce(1)	3.0433(11)

2.4 Bond angles involving non-hydrogen atoms of $Cp'_2Ce(\mu_3\text{-}OSO_2)CeCp'_2$

C(5)-C(1)-C(2)	106.1(4)
C(5)-C(1)-C(6)	128.0(4)
C(2)-C(1)-C(6)	125.8(4)
C(5)-C(1)-Ce(1)	76.4(2)

C(2)-C(1)-Ce(1)	76.4(2)
C(6)-C(1)-Ce(1)	115.2(3)
C(1)-C(2)-C(3)	110.3(4)
C(1)-C(2)-Ce(1)	74.6(2)
C(3)-C(2)-Ce(1)	79.9(2)
C(2)-C(3)-C(4)	106.8(3)
C(2)-C(3)-C(10)	117.4(4)
C(4)-C(3)-C(10)	133.7(4)
C(2)-C(3)-Ce(1)	71.3(2)
C(4)-C(3)-Ce(1)	75.6(2)
C(10)-C(3)-Ce(1)	130.2(3)
C(5)-C(4)-C(3)	105.7(4)
C(5)-C(4)-C(14)	120.2(4)
C(3)-C(4)-C(14)	133.4(3)
C(5)-C(4)-Ce(1)	71.3(2)
C(3)-C(4)-Ce(1)	75.9(2)
C(14)-C(4)-Ce(1)	124.4(3)
C(1)-C(5)-C(4)	111.1(4)
C(1)-C(5)-Ce(1)	74.7(2)
C(4)-C(5)-Ce(1)	79.8(2)
C(8)-C(6)-C(1)	108.9(4)
C(8)-C(6)-C(9)	110.2(4)
C(1)-C(6)-C(9)	111.5(4)
C(8)-C(6)-C(7)	108.1(4)
C(1)-C(6)-C(7)	109.1(3)
C(9)-C(6)-C(7)	109.0(4)
C(13)-C(10)-C(3)	117.0(3)
C(13)-C(10)-C(12)	105.7(3)
C(3)-C(10)-C(12)	110.5(3)
C(13)-C(10)-C(11)	108.4(3)
C(3)-C(10)-C(11)	107.7(3)
C(12)-C(10)-C(11)	107.1(4)
C(16)-C(14)-C(15)	105.5(3)
C(16)-C(14)-C(17)	106.2(3)
C(15)-C(14)-C(17)	110.0(3)
C(16)-C(14)-C(4)	110.1(3)
C(15)-C(14)-C(4)	110.4(3)
C(17)-C(14)-C(4)	114.2(3)

C(19)-C(18)-C(22)	105.9(3)
C(19)-C(18)-C(23)	127.0(4)
C(22)-C(18)-C(23)	127.1(4)
C(19)-C(18)-Ce(1)	76.7(2)
C(22)-C(18)-Ce(1)	75.1(2)
C(23)-C(18)-Ce(1)	113.7(2)
C(18)-C(19)-C(20)	110.5(3)
C(18)-C(19)-Ce(1)	74.1(2)
C(20)-C(19)-Ce(1)	80.2(2)
C(19)-C(20)-C(21)	106.3(3)
C(19)-C(20)-C(27)	116.1(4)
C(21)-C(20)-C(27)	135.1(4)
C(19)-C(20)-Ce(1)	71.0(2)
C(21)-C(20)-Ce(1)	74.6(2)
C(27)-C(20)-Ce(1)	132.0(3)
C(22)-C(21)-C(20)	106.9(3)
C(22)-C(21)-C(31)	119.7(4)
C(20)-C(21)-C(31)	132.6(4)
C(22)-C(21)-Ce(1)	70.5(2)
C(20)-C(21)-Ce(1)	76.9(2)
C(31)-C(21)-Ce(1)	125.4(3)
C(18)-C(22)-C(21)	110.3(4)
C(18)-C(22)-Ce(1)	75.5(2)
C(21)-C(22)-Ce(1)	80.4(2)
C(26)-C(23)-C(25)	109.6(4)
C(26)-C(23)-C(18)	111.0(3)
C(25)-C(23)-C(18)	110.3(3)
C(26)-C(23)-C(24)	109.4(3)
C(25)-C(23)-C(24)	108.8(4)
C(18)-C(23)-C(24)	107.7(3)
C(30)-C(27)-C(28)	106.6(4)
C(30)-C(27)-C(20)	117.7(4)
C(28)-C(27)-C(20)	110.9(3)
C(30)-C(27)-C(29)	107.7(4)
C(28)-C(27)-C(29)	107.5(4)
C(20)-C(27)-C(29)	106.1(3)
C(34)-C(31)-C(33)	111.2(3)
C(34)-C(31)-C(32)	106.2(4)

C(33)-C(31)-C(32)	105.4(3)
C(34)-C(31)-C(21)	109.0(3)
C(33)-C(31)-C(21)	114.6(3)
C(32)-C(31)-C(21)	110.1(3)
C(36)-C(35)-C(39)	106.2(4)
C(36)-C(35)-C(40)	128.9(4)
C(39)-C(35)-C(40)	124.8(4)
C(36)-C(35)-Ce(2)	75.9(2)
C(39)-C(35)-Ce(2)	75.2(2)
C(40)-C(35)-Ce(2)	111.2(2)
C(35)-C(36)-C(37)	110.4(4)
C(35)-C(36)-Ce(2)	74.9(2)
C(37)-C(36)-Ce(2)	78.6(2)
C(36)-C(37)-C(38)	106.2(3)
C(36)-C(37)-C(44)	117.7(4)
C(38)-C(37)-C(44)	134.4(4)
C(36)-C(37)-Ce(2)	72.1(2)
C(38)-C(37)-Ce(2)	75.9(2)
C(44)-C(37)-Ce(2)	127.8(2)
C(39)-C(38)-C(37)	106.5(3)
C(39)-C(38)-C(48)	119.5(3)
C(37)-C(38)-C(48)	133.4(4)
C(39)-C(38)-Ce(2)	71.2(2)
C(37)-C(38)-Ce(2)	75.0(2)
C(48)-C(38)-Ce(2)	125.0(2)
C(35)-C(39)-C(38)	110.6(3)
C(35)-C(39)-Ce(2)	75.3(2)
C(38)-C(39)-Ce(2)	79.9(2)
C(35)-C(40)-C(42)	111.1(3)
C(35)-C(40)-C(41)	111.2(3)
C(42)-C(40)-C(41)	108.2(3)
C(35)-C(40)-C(43)	107.9(3)
C(42)-C(40)-C(43)	108.6(3)
C(41)-C(40)-C(43)	109.7(3)
C(47)-C(44)-C(46)	105.9(3)
C(47)-C(44)-C(37)	117.6(3)
C(46)-C(44)-C(37)	109.8(3)
C(47)-C(44)-C(45)	108.5(3)

C(46)-C(44)-C(45)	107.5(3)
C(37)-C(44)-C(45)	107.2(3)
C(49)-C(48)-C(51)	106.5(3)
C(49)-C(48)-C(50)	110.3(3)
C(51)-C(48)-C(50)	105.2(3)
C(49)-C(48)-C(38)	109.3(3)
C(51)-C(48)-C(38)	110.7(3)
C(50)-C(48)-C(38)	114.6(3)
C(56)-C(52)-C(53)	106.1(4)
C(56)-C(52)-C(57)	127.7(4)
C(53)-C(52)-C(57)	126.1(4)
C(56)-C(52)-Ce(2)	75.1(2)
C(53)-C(52)-Ce(2)	75.7(2)
C(57)-C(52)-Ce(2)	112.8(2)
C(52)-C(53)-C(54)	110.5(4)
C(52)-C(53)-Ce(2)	75.0(2)
C(54)-C(53)-Ce(2)	79.6(2)
C(53)-C(54)-C(55)	106.4(3)
C(53)-C(54)-C(61)	120.0(3)
C(55)-C(54)-C(61)	133.0(4)
C(53)-C(54)-Ce(2)	71.5(2)
C(55)-C(54)-Ce(2)	74.3(2)
C(61)-C(54)-Ce(2)	125.3(3)
C(56)-C(55)-C(54)	106.4(3)
C(56)-C(55)-C(65)	117.5(3)
C(54)-C(55)-C(65)	134.3(4)
C(56)-C(55)-Ce(2)	71.9(2)
C(54)-C(55)-Ce(2)	76.6(2)
C(65)-C(55)-Ce(2)	127.4(2)
C(52)-C(56)-C(55)	110.4(3)
C(52)-C(56)-Ce(2)	75.6(2)
C(55)-C(56)-Ce(2)	78.9(2)
C(59)-C(57)-C(58)	109.7(4)
C(59)-C(57)-C(52)	108.4(3)
C(58)-C(57)-C(52)	110.9(3)
C(59)-C(57)-C(60)	109.4(4)
C(58)-C(57)-C(60)	108.8(3)
C(52)-C(57)-C(60)	109.7(3)

C(63)-C(61)-C(62)	110.6(4)
C(63)-C(61)-C(54)	110.8(3)
C(62)-C(61)-C(54)	113.9(3)
C(63)-C(61)-C(64)	105.9(3)
C(62)-C(61)-C(64)	105.9(3)
C(54)-C(61)-C(64)	109.5(3)
C(66)-C(65)-C(68)	106.0(3)
C(66)-C(65)-C(67)	109.1(3)
C(68)-C(65)-C(67)	107.2(3)
C(66)-C(65)-C(55)	116.7(3)
C(68)-C(65)-C(55)	110.4(3)
C(67)-C(65)-C(55)	107.2(3)
S(1)-O(1)-Ce(1)	98.56(14)
S(1)-O(2)-Ce(1)	97.94(14)
S(1)-O(3)-Ce(2)	144.20(19)
O(2)-S(1)-O(1)	102.19(16)
O(2)-S(1)-O(3)	104.93(17)
O(1)-S(1)-O(3)	105.10(17)
O(2)-S(1)-Ce(1)	52.33(11)
O(1)-S(1)-Ce(1)	51.69(11)
O(3)-S(1)-Ce(1)	125.83(13)
O(1)-Ce(1)-O(2)	58.65(9)
O(1)-Ce(1)-C(22)	89.77(11)
O(2)-Ce(1)-C(22)	84.11(11)
O(1)-Ce(1)-C(18)	118.92(11)
O(2)-Ce(1)-C(18)	96.08(11)
C(22)-Ce(1)-C(18)	29.46(11)
O(1)-Ce(1)-C(1)	84.77(11)
O(2)-Ce(1)-C(1)	109.63(11)
C(22)-Ce(1)-C(1)	159.26(12)
C(18)-Ce(1)-C(1)	152.10(12)
O(1)-Ce(1)-C(19)	129.44(11)
O(2)-Ce(1)-C(19)	125.31(11)
C(22)-Ce(1)-C(19)	47.60(12)
C(18)-Ce(1)-C(19)	29.26(11)
C(1)-Ce(1)-C(19)	124.35(12)
O(1)-Ce(1)-C(5)	78.23(11)
O(2)-Ce(1)-C(5)	82.45(11)

C(22)-Ce(1)-C(5)	165.33(12)
C(18)-Ce(1)-C(5)	159.01(11)
C(1)-Ce(1)-C(5)	28.94(12)
C(19)-Ce(1)-C(5)	147.00(12)
O(1)-Ce(1)-C(2)	113.65(11)
O(2)-Ce(1)-C(2)	126.69(11)
C(22)-Ce(1)-C(2)	147.63(12)
C(18)-Ce(1)-C(2)	124.48(12)
C(1)-Ce(1)-C(2)	29.03(11)
C(19)-Ce(1)-C(2)	100.51(12)
C(5)-Ce(1)-C(2)	46.96(12)
O(1)-Ce(1)-C(21)	82.07(10)
O(2)-Ce(1)-C(21)	103.73(11)
C(22)-Ce(1)-C(21)	29.14(11)
C(18)-Ce(1)-C(21)	48.47(11)
C(1)-Ce(1)-C(21)	130.12(12)
C(19)-Ce(1)-C(21)	47.37(11)
C(5)-Ce(1)-C(21)	152.22(11)
C(2)-Ce(1)-C(21)	128.57(12)
O(1)-Ce(1)-C(4)	101.75(11)
O(2)-Ce(1)-C(4)	80.76(11)
C(22)-Ce(1)-C(4)	152.31(12)
C(18)-Ce(1)-C(4)	130.15(11)
C(1)-Ce(1)-C(4)	48.23(11)
C(19)-Ce(1)-C(4)	128.71(11)
C(5)-Ce(1)-C(4)	28.87(11)
C(2)-Ce(1)-C(4)	47.37(12)
C(21)-Ce(1)-C(4)	175.27(11)
O(1)-Ce(1)-C(3)	125.21(11)
O(2)-Ce(1)-C(3)	106.91(11)
C(22)-Ce(1)-C(3)	144.32(11)
C(18)-Ce(1)-C(3)	114.88(11)
C(1)-Ce(1)-C(3)	48.02(11)
C(19)-Ce(1)-C(3)	102.81(11)
C(5)-Ce(1)-C(3)	46.99(11)
C(2)-Ce(1)-C(3)	28.85(11)
C(21)-Ce(1)-C(3)	146.78(11)
C(4)-Ce(1)-C(3)	28.50(11)

O(1)-Ce(1)-C(20)	104.69(11)
O(2)-Ce(1)-C(20)	130.59(11)
C(22)-Ce(1)-C(20)	47.54(12)
C(18)-Ce(1)-C(20)	48.29(11)
C(1)-Ce(1)-C(20)	114.81(12)
C(19)-Ce(1)-C(20)	28.83(11)
C(5)-Ce(1)-C(20)	143.75(12)
C(2)-Ce(1)-C(20)	102.72(12)
C(21)-Ce(1)-C(20)	28.49(11)
C(4)-Ce(1)-C(20)	146.78(11)
C(3)-Ce(1)-C(20)	118.38(11)
O(3)-Ce(2)-C(39)	82.69(11)
O(3)-Ce(2)-C(35)	107.64(11)
C(39)-Ce(2)-C(35)	29.50(11)
O(3)-Ce(2)-C(56)	128.17(11)
C(39)-Ce(2)-C(56)	147.86(11)
C(35)-Ce(2)-C(56)	123.91(11)
O(3)-Ce(2)-C(52)	100.18(11)
C(39)-Ce(2)-C(52)	160.22(12)
C(35)-Ce(2)-C(52)	151.92(11)
C(56)-Ce(2)-C(52)	29.36(11)
O(3)-Ce(2)-C(36)	130.14(11)
C(39)-Ce(2)-C(36)	47.74(12)
C(35)-Ce(2)-C(36)	29.19(11)
C(56)-Ce(2)-C(36)	100.41(12)
C(52)-Ce(2)-C(36)	124.45(12)
O(3)-Ce(2)-C(53)	82.08(11)
C(39)-Ce(2)-C(53)	164.42(12)
C(35)-Ce(2)-C(53)	158.90(12)
C(56)-Ce(2)-C(53)	47.71(11)
C(52)-Ce(2)-C(53)	29.27(11)
C(36)-Ce(2)-C(53)	147.71(12)
O(3)-Ce(2)-C(55)	124.76(11)
C(39)-Ce(2)-C(55)	143.42(11)
C(35)-Ce(2)-C(55)	114.00(11)
C(56)-Ce(2)-C(55)	29.16(11)
C(52)-Ce(2)-C(55)	48.61(12)
C(36)-Ce(2)-C(55)	102.70(11)

C(53)-Ce(2)-C(55)	47.90(11)
O(3)-Ce(2)-C(37)	115.44(11)
C(39)-Ce(2)-C(37)	47.96(11)
C(35)-Ce(2)-C(37)	48.67(11)
C(56)-Ce(2)-C(37)	103.19(11)
C(52)-Ce(2)-C(37)	115.04(11)
C(36)-Ce(2)-C(37)	29.30(12)
C(53)-Ce(2)-C(37)	144.25(11)
C(55)-Ce(2)-C(37)	119.11(11)
O(3)-Ce(2)-C(38)	87.21(11)
C(39)-Ce(2)-C(38)	28.96(11)
C(35)-Ce(2)-C(38)	48.53(11)
C(56)-Ce(2)-C(38)	130.04(11)
C(52)-Ce(2)-C(38)	131.27(12)
C(36)-Ce(2)-C(38)	47.88(11)
C(53)-Ce(2)-C(38)	152.47(12)
C(55)-Ce(2)-C(38)	147.96(11)
C(37)-Ce(2)-C(38)	29.10(11)
O(3)-Ce(2)-C(54)	95.77(11)
C(39)-Ce(2)-C(54)	151.35(11)
C(35)-Ce(2)-C(54)	130.01(12)
C(56)-Ce(2)-C(54)	47.75(11)
C(52)-Ce(2)-C(54)	48.30(11)
C(36)-Ce(2)-C(54)	129.35(12)
C(53)-Ce(2)-C(54)	28.89(11)
C(55)-Ce(2)-C(54)	29.07(11)
C(37)-Ce(2)-C(54)	148.01(11)
C(38)-Ce(2)-C(54)	177.02(11)

2.5 Least Squares Planes for $Cp'_2Ce(\mu_3\text{-}OSO_2)CeCp'_2$

(* indicates atom used to define plane)

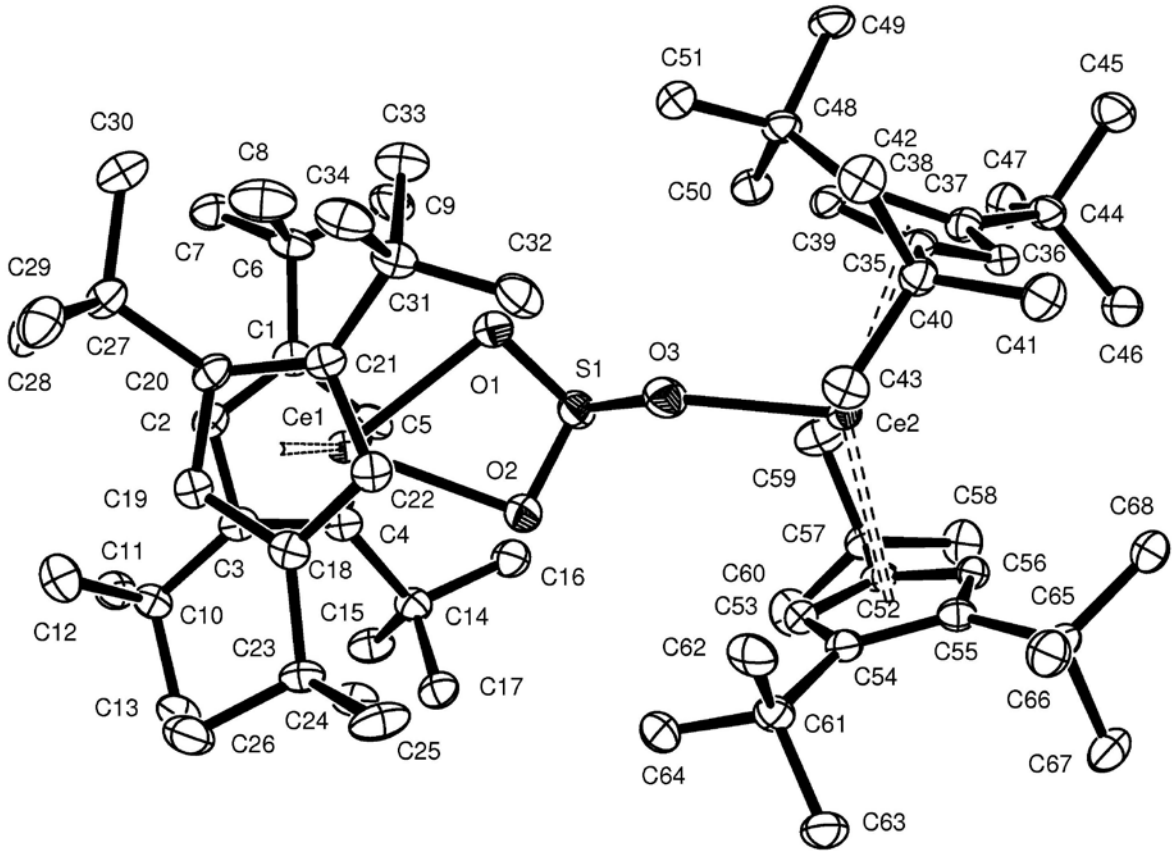
- 6.7557 (0.0398) x + 9.7797 (0.0080) y + 7.0175 (0.0622) z = 3.0815 (0.0520)

*	0.0079 (0.0025)	C1
*	-0.0084 (0.0025)	C2
*	0.0057 (0.0025)	C3
*	-0.0009 (0.0025)	C4
*	-0.0043 (0.0025)	C5

```
      0.0911 (0.0073)  C6
      0.3598 (0.0071)  C10
      0.1897 (0.0073)  C14

Rms deviation of fitted atoms =   0.0061


 5.3078 (0.0399) x - 9.4075 (0.0096) y + 9.8612 (0.0597) z = 13.3641 (0.0463)

Angle to previous plane (with approximate esd) = 32.04 ( 0.14 )

*     0.0157 (0.0024)  C18
*    -0.0136 (0.0025)  C19
*     0.0062 (0.0025)  C20
*     0.0035 (0.0025)  C21
*    -0.0119 (0.0025)  C22
      0.0619 (0.0070)  C23
      0.3845 (0.0073)  C27
      0.2338 (0.0073)  C31

Rms deviation of fitted atoms =   0.0112


 20.0538 (0.0094) x + 0.4556 (0.0200) y - 11.9261 (0.0546) z = 11.3039 (0.0362)

Angle to previous plane (with approximate esd) = 82.73 ( 0.15 )

*     0.0129 (0.0023)  C35
*    -0.0051 (0.0024)  C36
*    -0.0044 (0.0023)  C37
*     0.0124 (0.0023)  C38
*    -0.0158 (0.0023)  C39
     -0.0330 (0.0067)  C40
      0.2839 (0.0068)  C44
      0.2276 (0.0068)  C48

Rms deviation of fitted atoms =   0.0111


 19.2458 (0.0148) x + 1.4231 (0.0205) y + 5.3181 (0.0601) z = 14.7165 (0.0227)

Angle to previous plane (with approximate esd) = 33.27 ( 0.10 )

*    -0.0149 (0.0024)  C52
*     0.0174 (0.0025)  C53
*    -0.0129 (0.0024)  C54
*     0.0036 (0.0024)  C55
*     0.0068 (0.0024)  C56
     -0.0096 (0.0070)  C57
     -0.2238 (0.0071)  C61
     -0.2907 (0.0070)  C65

Rms deviation of fitted atoms =   0.0123


 7.3657 (0.0336) x - 9.8260 (0.0067) y - 0.2169 (0.0307) z = 4.9313 (0.0326)

Angle to previous plane (with approximate esd) = 77.00 ( 0.14 )

*     0.0000 (0.0000)  Ce1
*     0.0000 (0.0000)  O1
```

```
*    0.0000 (0.0000)  O2
    -0.2744 (0.0032)  S1

Rms deviation of fitted atoms =   0.0000


- 8.2929 (0.0331) x + 9.3409 (0.0099) y + 8.9791 (0.0716) z = 0.1837 (0.0497)

Angle to previous plane (with approximate esd) = 16.64 ( 0.17 )

*    0.0000 (0.0000)  S1
*    0.0000 (0.0000)  O1
*    0.0000 (0.0000)  O2
     0.6051 (0.0068)  Ce1

Rms deviation of fitted atoms =   0.0000


 16.4866 (0.0624) x + 6.1747 (0.0368) y - 8.1130 (0.0660) z = 7.5463 (0.0858)

Angle to previous plane (with approximate esd) = 80.35 ( 0.21 )

*   -0.0001 (0.0000)  S1
*    0.0001 (0.0000)  O3
*    0.0000 (0.0000)  Ce2

Rms deviation of fitted atoms =   0.0001
```

2.6 ORTEP diagram (50% ellipsoids) showing atom labeling scheme $Cp'_2Ce(\mu_3\text{-}OSO_3)CeCp'_2$



3. References

(1) SMART: Area-Detector Software Package,
Bruker Analytical X-ray Systems, Inc.: Madison, WI, (2001-03)

(2) SAINT: SAX Area-Dectector Integration Program, V6.40;
Bruker Analytical X-ray Systems Inc.: Madison, WI, (2003)

(3) XPREP:(v 6.12) Part of the SHELXTL Crystal Structure Determination Package,
Bruker Analytical X-ray Systems, Inc.: Madison, WI, (2001)

(4) SADABS: Bruker-Nonius Area Detector Scaling and Absorption v. 2.05
Bruker Analytical X-ray Systems, Inc.: Madison, WI (2003).

(5) SIR92: Altomare, A., Cascarano, M., Giacovazzo, C., Guagliardi, A. (1993). J. Appl. Cryst., 26, 343.

(6) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(7) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(8) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

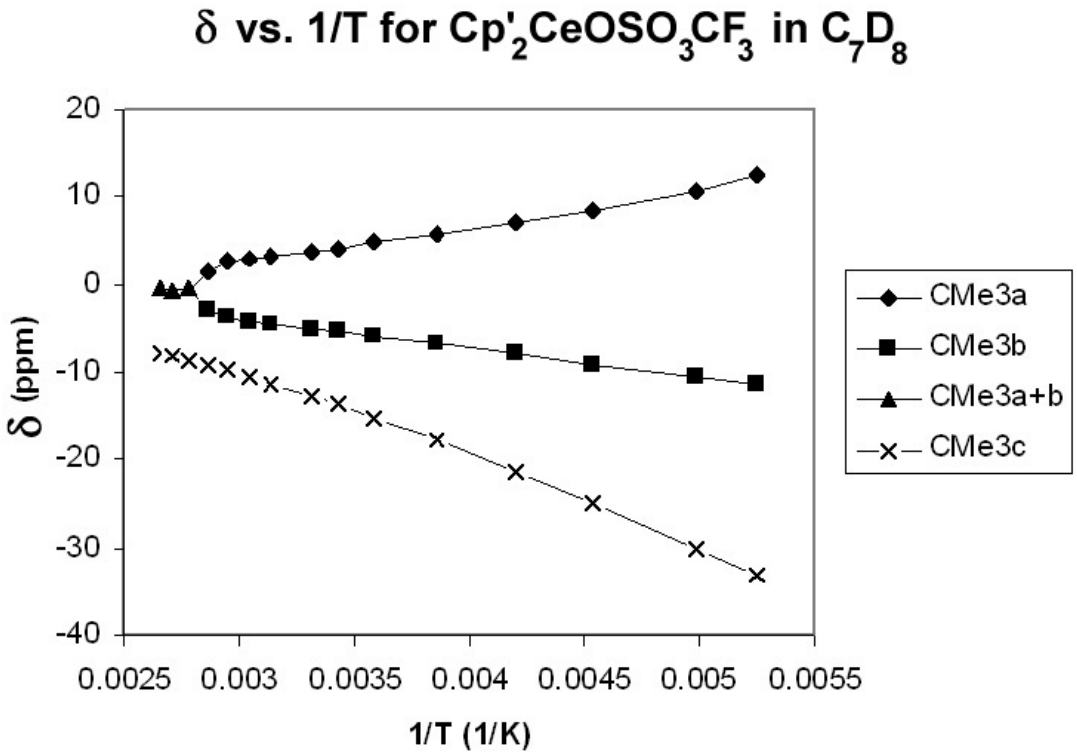
(9) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(10) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

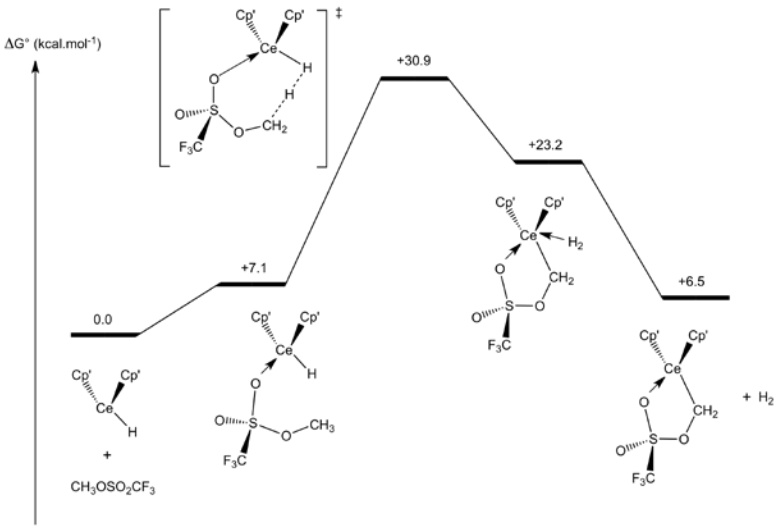
(11) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

(12) XL: Program for the Refinement of X-ray Crystal Structures, Part of the SHELXTL Crystal Structure Determination Package, Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

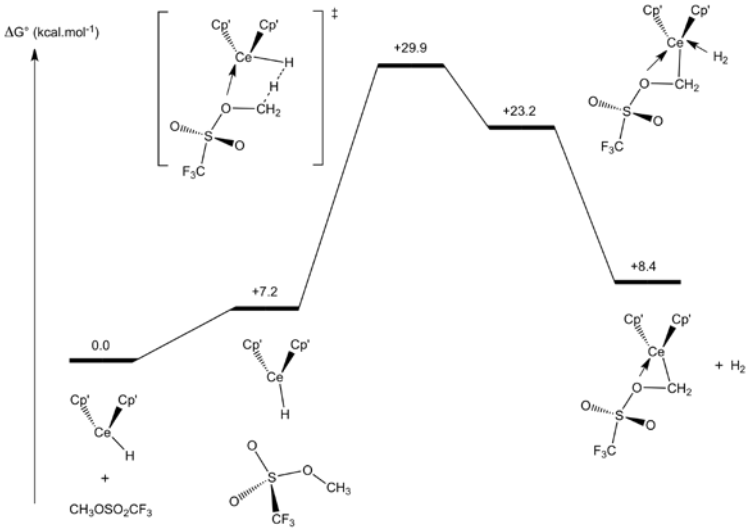
(13) WinGX: L.J. Farrugia, *J. Appl. Cryst.* (1999), 32, 837-838.



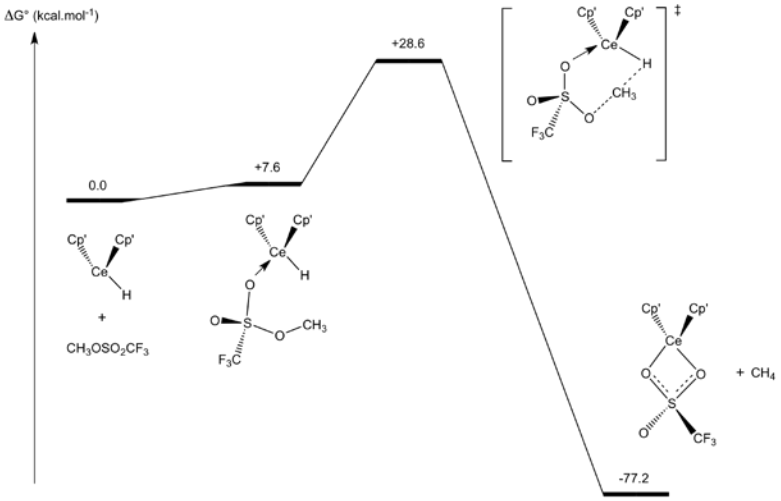
^{1}H NMR chemical shit, δ, vs. 1/T plot of CMe_3 resonances in $Cp'_2Ce(OSO_2CF_3)$ in C_7D_8.



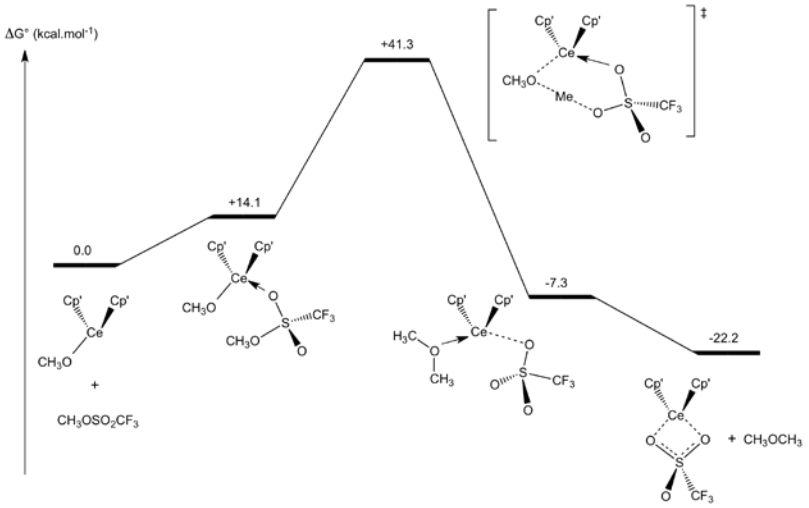
CH Bond activation coordination by OMe



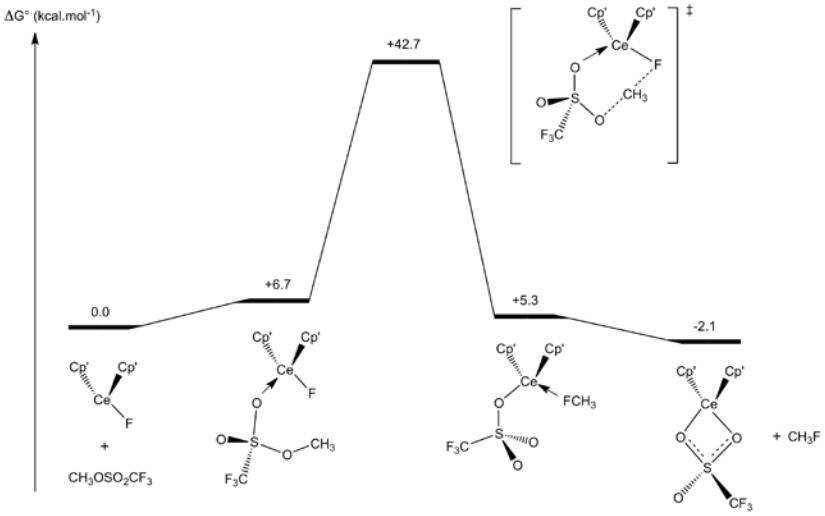
Me Transfer



OMe /OSO2CF3 exchange

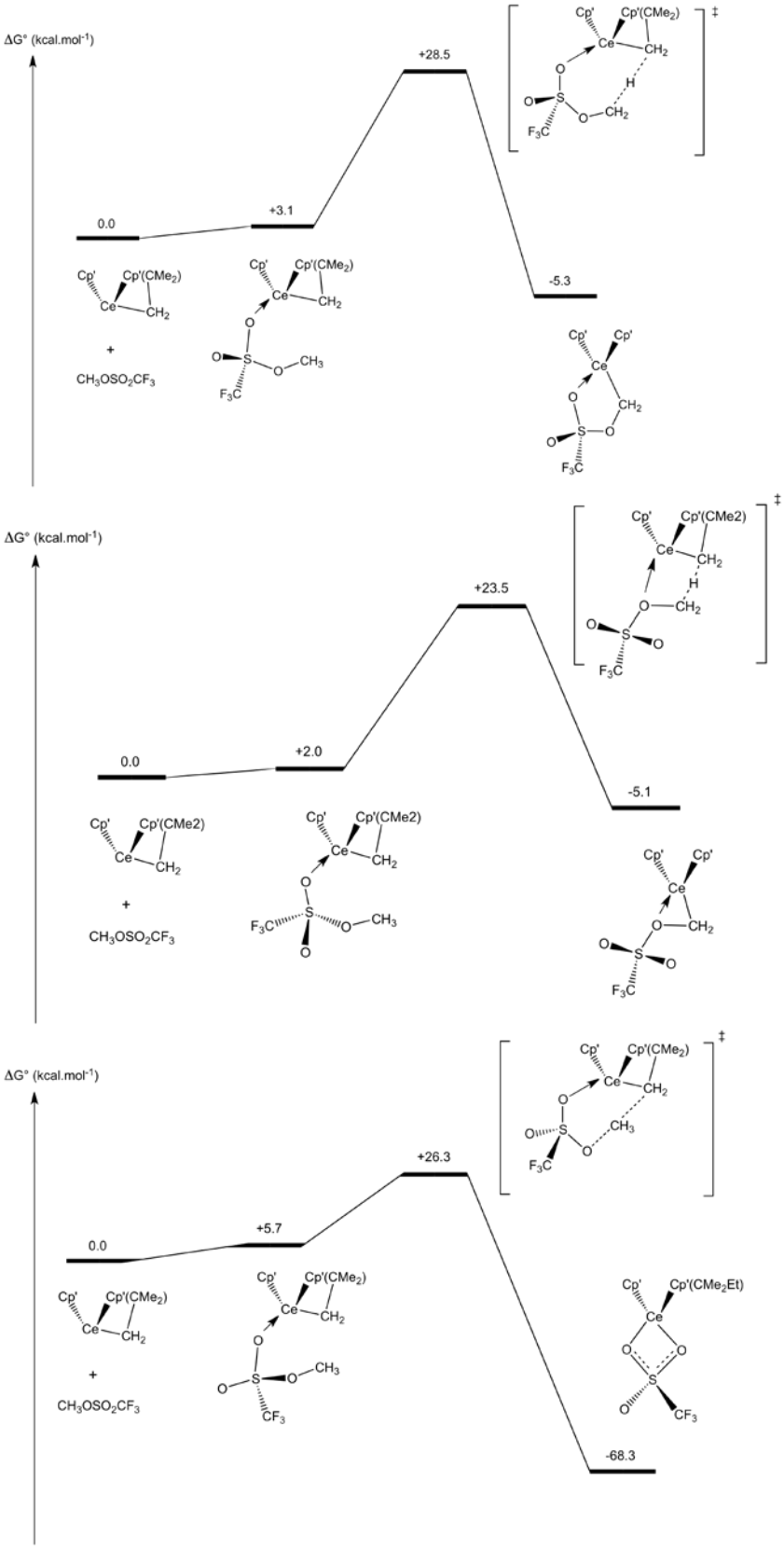


F/OSO2CF3 exchange



Reactions with the metallacycle

CH Activation



Cartesian coordinates, E and G in a.u for all extrema

$MeOSO_2CF_3$ (trans)

E = -386.631695
G = -386.600105

C	-0.825045	1.610620	-0.456301
S	-0.113311	-0.083451	0.001449
O	1.359795	0.249871	-0.668878
C	2.325467	-0.814989	-0.525671
O	-0.821865	-1.113167	-0.784796
O	-0.008294	-0.162418	1.472443
F	-2.069411	1.643700	-0.016830
F	-0.122034	2.563929	0.120189
F	-0.808294	1.765177	-1.764437
H	3.228539	-0.435888	-1.003019
H	2.515936	-1.017944	0.531002
H	1.979726	-1.715548	-1.039177

$MeOSO_2CF_3$ (gauche)

E = -386.633271
G = -386.602588

C	-0.642998	1.493352	-0.267637
F	-0.641398	1.934203	-1.509060
S	-0.258258	-0.358867	-0.239466
O	-0.137040	-0.741258	1.181710
F	-1.828120	1.688016	0.277079
F	0.278334	2.138866	0.432850
O	1.221958	-0.321565	-0.966594
C	2.381607	-0.238596	-0.106920
O	-1.176234	-1.000267	-1.190739
H	3.205155	-0.606870	-0.719046
H	2.563858	0.797714	0.186086
H	2.255717	-0.868194	0.774727

H_2

E = -1.177516
G = -1.178848

H	0.000000	0.000000	0.003369
H	0.000000	0.000000	0.746631

CH_4

E = -40.508109
G = -40.482693

C	-0.000004	0.000000	0.000009
H	-0.000001	0.000000	1.091768
H	1.029319	0.000000	-0.363923
H	-0.514658	-0.891417	-0.363925
H	-0.514658	0.891417	-0.363925

CH_3F

E = -64.207280
G = -64.190236

F	-0.000015	-0.000044	-0.036580
C	-0.000002	0.000002	1.345159
H	1.034836	0.000016	1.700156
H	-0.517407	0.896206	1.700176
H	-0.517411	-0.896180	1.700086

CH_3OCH_3

E = -154.971201
G = -154.916451

O	0.020261	0.000000	0.014435
C	-0.011059	0.000000	1.418022
C	1.333178	0.000000	-0.482997
H	1.271186	0.000000	-1.574162
H	1.896193	0.891643	-0.160785
H	1.896193	-0.891643	-0.160785
H	-1.060521	0.000000	1.723202
H	0.480514	-0.891649	1.841213
H	0.480514	0.891649	1.841213

Hydride

E = -1363.065034
G = -1362.291033

C	-2.078844	-3.228817	1.608546
C	-2.155631	-3.546306	0.232958
C	-1.189093	-4.538808	-0.124577
C	-0.458995	-4.834339	1.094220
C	-1.011111	-4.006969	2.118863
Ce	0.340579	-2.197921	0.413248
C	1.525483	0.147443	-0.574192
C	0.340073	0.612299	0.036252
C	0.525619	0.434230	1.428584
C	1.821472	-0.107046	1.697563
C	2.462255	-0.293792	0.408598
H	0.812519	-2.639038	-1.610180
H	-2.901840	-3.152602	-0.444232
C	-3.111930	-2.477360	2.439263
H	-0.717495	-4.034976	3.160549
C	0.697545	-5.805200	1.404445
C	-1.289314	-5.225388	-1.504315
H	-0.181438	0.740928	2.186581
C	-0.829906	1.268858	-0.687827
H	1.713722	0.157888	-1.638300
C	3.898399	-0.650904	-0.032101
C	2.291466	-0.341314	3.148317
C	4.537901	-1.825435	0.727110
C	3.922154	-1.051616	-1.523841
C	4.792596	0.600883	0.104717
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H	4.653410	-1.641987	1.795646
H	3.958633	-2.748086	0.598309
H	4.927114	-1.396295	-1.790909
H	3.209199	-1.852881	-1.746793
H	3.692215	-0.206028	-2.178260
H	5.802316	0.390054	-0.268662
H	4.378752	1.425078	-0.484708
H	4.878464	0.943809	1.137224
C	-1.534420	0.246975	-1.600681
C	-1.846226	1.839753	0.309007
C	-0.298709	2.425356	-1.556630
H	-2.682530	2.303725	-0.225034
H	-2.260881	1.061111	0.958091
H	-1.389230	2.603054	0.947204
H	-1.123724	2.929179	-2.074304
H	0.222081	3.165432	-0.940626
H	0.403729	2.066884	-2.315055
H	-2.327010	0.722432	-2.191013
H	-0.830345	-0.222983	-2.295771
H	-2.015277	-0.548855	-1.013575
C	2.374935	-1.846653	3.477642
C	3.638744	0.339900	3.448755
C	1.286424	0.263881	4.148583

H	2.733822	-2.007576	4.501764
H	1.377882	-2.306387	3.421790
H	3.046832	-2.389526	2.808688
H	3.884592	0.231690	4.511663
H	4.467361	-0.081011	2.879647
H	3.584824	1.409744	3.223486
H	1.651089	0.107164	5.169556
H	1.167956	1.341230	3.997230
H	0.300027	-0.204482	4.081207
C	-4.037985	-1.632400	1.554582
C	-3.972577	-3.524941	3.178573
C	-2.447220	-1.566386	3.482419
H	-3.201482	-1.098271	4.125466
H	-1.763840	-2.126156	4.129732
H	-1.876828	-0.765465	2.999411
H	-4.765511	-1.094655	2.172290
H	-3.480464	-0.889432	0.974541
H	-4.599302	-2.256003	0.851711
H	-4.755145	-3.036094	3.771573
H	-4.455315	-4.202982	2.467723
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C	-2.220332	-6.451237	-1.361982
C	-1.941945	-4.277853	-2.532785
C	0.042271	-5.654823	-2.141623
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H	-3.203787	-6.144859	-0.990345
C	1.004446	-5.827631	2.914948
C	0.354043	-7.258734	1.031303
C	1.992938	-5.353180	0.700157
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H	0.197304	-7.402077	-0.036865
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H	0.139967	-6.161275	3.497216

Metallacycle

E = -1361.851823
G = -1361.092321

C	3.155034	-0.142706	-2.721582
C	2.343263	-0.880410	-1.773235
C	1.320091	-1.517686	-2.541316
C	1.477306	-1.244187	-3.919736
C	2.591163	-0.382007	-4.014966
Ce	0.569062	1.198054	-2.771019
C	-0.051026	1.798872	-0.387492
C	-0.292207	3.326463	-0.480037
C	0.889097	4.075628	0.146591
C	2.519829	-1.288555	-0.294943
C	1.158375	-1.675602	0.321983
C	0.665165	-1.863625	-5.049244
C	1.086291	-1.298822	-6.411797
C	4.450857	0.679451	-2.569488
C	4.974891	1.133771	-3.946189
C	-1.395313	3.124978	-2.829908
C	-1.017969	3.221991	-4.209672
C	0.327279	3.752913	-4.221612
C	0.697667	3.944983	-2.847389
C	-0.366035	3.591734	-1.984344
C	1.257895	4.226848	-5.356591
C	0.587491	5.318609	-6.214053
C	-2.107571	3.024526	-5.283633
C	-2.834756	4.371362	-5.497747
C	-1.583252	3.778743	0.218498
C	0.895006	-3.387848	-5.054881
C	-0.835341	-1.591609	-4.839161
C	4.227015	1.965162	-1.749463
C	5.585095	-0.162987	-1.953652
C	3.415532	-2.547218	-0.246629
C	3.106962	-0.214542	0.633443
C	2.530499	4.876144	-4.777002
C	1.737169	3.069186	-6.253758
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H	0.578667	-2.191826	-2.128993
H	-2.359935	2.779860	-2.477334
H	1.641132	4.358673	-2.516052
H	0.451504	1.515336	0.543647
H	-1.035243	1.282405	-0.382925
H	0.911870	3.897727	1.227254
H	1.847205	3.732437	-0.259235
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H	-1.741260	4.860139	0.115437
H	-2.461260	3.272509	-0.196833
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H	-2.738685	1.044781	-4.547460
H	-3.721966	2.380182	-3.921744
H	-3.659872	4.254401	-6.211185
H	-3.249340	4.734412	-4.552248
H	-2.162739	5.141901	-5.881155
H	-2.480888	2.334083	-7.300151
H	-0.949479	3.181383	-7.151672
H	-1.107147	1.530640	-6.533310
H	2.407733	3.442482	-7.037413
H	2.297742	2.335297	-5.663122
H	0.917426	2.542858	-6.741614
H	0.241797	6.143862	-5.583181
H	1.304622	5.723992	-6.937762
H	-0.268856	4.948492	-6.778910
H	3.174431	5.207352	-5.598657
H	2.296867	5.751098	-4.162931
H	3.114833	4.177018	-4.169911
H	0.485444	-1.744416	-7.212012
H	0.954564	-0.212081	-6.459335
H	2.137705	-1.518391	-6.622915
H	-1.441544	-2.067434	-5.618845
H	-1.183735	-1.971102	-3.872150
H	-1.053603	-0.514524	-4.891864
H	0.331268	-3.865506	-5.865475
H	1.956143	-3.616237	-5.194644
H	0.578850	-3.839799	-4.109549
H	5.167584	2.515425	-1.623431
H	3.534756	2.637129	-2.275142
H	3.815575	1.771800	-0.759545
H	6.517781	0.413374	-1.940285
H	5.378721	-0.473284	-0.929512
H	5.755114	-1.066163	-2.548781
H	5.892459	1.715925	-3.809349
H	5.213303	0.283413	-4.592520
H	4.260320	1.775649	-4.471690
H	3.135786	-0.599569	1.659202
H	4.127640	0.067214	0.374156
H	2.485935	0.685366	0.632612
H	3.523802	-2.901488	0.785804
H	2.974051	-3.355156	-0.839089
H	4.414947	-2.354359	-0.643813
H	1.290246	-1.903700	1.385182
H	0.439480	-0.854116	0.240486
H	0.726562	-2.567960	-0.140327

Cp'_2CeOMe

E = -1477.618681
G = -1476.812507

C	-1.249988	-2.122438	-0.442057
C	-2.143745	-1.442301	0.434506
C	-1.858625	-1.938952	1.772973
C	-0.819321	-2.905639	1.628130
C	-0.422770	-3.015620	0.272295
C	-2.977600	-0.267764	-0.122310
C	-2.137169	1.025844	-0.037084
C	-2.346317	-1.513870	3.173435
C	-1.525048	-2.220166	4.270434
Ce	-3.028158	-4.203265	0.270579
C	0.780427	-3.757366	-0.298866
C	1.426719	-4.669157	0.751182
C	-5.311430	-5.712237	0.968772
C	-4.569522	-5.687842	2.178768
C	-3.428048	-6.539459	2.086677
C	-3.421013	-7.065103	0.730990
C	-4.592381	-6.547001	0.095589
C	-6.655072	-5.037470	0.717298
C	-7.208748	-5.416480	-0.662357
C	-2.618436	-6.897789	3.350140
C	-3.203360	-6.187886	4.587479
C	-2.630148	-8.173411	0.001390
C	-1.155710	-8.320903	0.404309
O	-3.605644	-4.044190	-1.803147
C	-3.955921	-4.103651	-3.145608
C	-7.657744	-5.486061	1.796540
C	-6.505366	-3.506016	0.779330
C	-2.723787	-8.406875	3.648652
C	-1.139334	-6.479001	3.275373
C	-3.347421	-9.523777	0.225086
C	-2.621339	-7.914942	-1.521972
C	0.373633	-4.603936	-1.517387
C	1.826517	-2.717280	-0.749702
C	-2.139305	-0.004963	3.410027
C	-3.817590	-1.892862	3.429736
C	-3.298040	-0.497064	-1.615970
C	-4.331775	-0.035966	0.564904
H	-4.887298	-5.182335	3.081523
H	-4.891120	-6.772013	-0.918502
H	-0.337560	-3.417495	2.448871
H	-1.199993	-1.960925	-1.510482
H	-4.320476	-3.130003	-3.510933
H	-3.096781	-4.383641	-3.775151
H	-4.751919	-4.843367	-3.331428
H	1.248084	-5.086701	-1.969401
H	-0.322092	-5.406051	-1.235487
H	-0.111342	-3.996869	-2.287906
H	2.720962	-3.211904	-1.148010
H	1.423325	-2.063830	-1.529414
H	2.130125	-2.085672	0.091194
H	2.279593	-5.203099	0.318001
H	1.795307	-4.093662	1.606499
H	0.721635	-5.416350	1.129633
H	-2.683059	1.866590	-0.482884
H	-1.888740	1.292449	0.992319
H	-1.196699	0.903224	-0.583249
H	-3.963227	0.296883	-1.973101
H	-2.400996	-0.464920	-2.240570
H	-3.786641	-1.462254	-1.781642
H	-4.858993	0.785490	0.066678
H	-4.973948	-0.920789	0.495432
H	-4.240183	0.236420	1.616387
H	-2.388683	0.251238	4.446616
H	-1.093862	0.270376	3.237313
H	-2.758913	0.617014	2.763762
H	-4.131417	-1.577189	4.432372
H	-4.502672	-1.439830	2.712458
H	-3.940717	-2.981570	3.378272
H	-1.882212	-1.897946	5.254567
H	-1.627654	-3.308742	4.229177
H	-0.461180	-1.972288	4.204300
H	-2.612549	-6.454480	5.470386
H	-3.173568	-5.097878	4.493357
H	-4.238288	-6.488530	4.777680
H	-2.240333	-8.636365	4.605779
H	-3.772793	-8.712652	3.717644
H	-2.246080	-9.023241	2.886215
H	-0.617252	-6.751516	4.200527
H	-0.608848	-6.948073	2.448019
H	-1.053770	-5.394407	3.154248
H	-0.679119	-9.077814	-0.228726
H	-0.602902	-7.385384	0.263852
H	-1.022737	-8.642359	1.437583
H	-2.839605	-10.325982	-0.324701
H	-3.373244	-9.802070	1.281386
H	-4.381775	-9.469723	-0.128119
H	-2.028965	-8.689387	-2.021753
H	-3.621200	-7.943966	-1.960934
H	-2.177119	-6.945009	-1.772699
H	-7.474067	-3.003847	0.669901
H	-6.075402	-3.183342	1.734206
H	-5.875326	-3.140938	-0.045104
H	-8.176920	-4.931165	-0.829073
H	-6.532056	-5.100838	-1.463059
H	-7.356938	-6.497994	-0.745382
H	-8.640730	-5.030994	1.625459
H	-7.777204	-6.574044	1.783733
H	-7.324469	-5.198956	2.798846

Cp'_2CeF

E = -1386.889160
G = -1386.118287

C	2.438974	-0.229459	0.346764
C	1.471597	0.224545	-0.592510
C	0.284484	0.633130	0.057511
C	0.506271	0.410919	1.437828
C	1.816654	-0.115224	1.657340
Ce	0.394056	-2.209752	0.317286
C	-0.981969	-3.943665	2.123469
C	-2.046463	-3.188422	1.579375
C	-2.108378	-3.551533	0.212739
C	-1.147168	-4.567709	-0.093615
C	-0.429736	-4.822582	1.135944
C	-3.104133	-2.435599	2.377509
C	-2.475935	-1.495848	3.417383
C	-1.208812	-5.263661	-1.472242
C	0.123329	-5.803336	-2.019722
C	0.662704	-5.842315	1.518222
C	2.007812	-5.532566	0.831174
C	-0.896779	1.319403	-0.618851
C	-0.383109	2.538218	-1.410331
C	2.312438	-0.418072	3.087107
C	1.338550	0.161738	4.132242
C	3.870152	-0.550169	-0.134389
C	4.773442	0.680387	0.099396
C	-4.032089	-1.628118	1.460476
C	-3.959273	-3.485359	3.121353
C	0.935245	-5.808974	3.035621
C	0.212437	-7.283834	1.213528
C	-2.232104	-6.417337	-1.378017
C	-1.722523	-4.282592	-2.549438
C	-1.588743	0.353025	-1.599558
C	-1.917043	1.811832	0.415037
C	4.494032	-1.796265	0.516181
C	3.883675	-0.822015	-1.654926
C	2.368009	-1.938953	3.339667
C	3.681277	0.212384	3.396449
F	1.383530	-2.951685	-1.464340
H	-2.854838	-3.189719	-0.482360
H	-0.707446	-3.946584	3.170598
H	-0.190343	0.672417	2.221788
H	1.635896	0.274220	-1.660654

H	5.494141	-1.967395	0.102281
H	4.606937	-1.712689	1.597790
H	3.901652	-2.692172	0.293866
H	4.896181	-1.113704	-1.955279
H	3.196060	-1.627098	-1.930604
H	3.629705	0.073112	-2.231283
H	5.778501	0.492289	-0.297608
H	4.362484	1.551147	-0.421561
H	4.871221	0.942661	1.153664
H	-2.762615	2.296466	-0.085166
H	-2.316197	0.991191	1.019307
H	-1.466652	2.541797	1.095431
H	-1.215933	3.065479	-1.890924
H	0.131031	3.241757	-0.747920
H	0.322105	2.239575	-2.191772
H	-2.408537	0.847405	-2.134359
H	-0.885847	-0.024628	-2.350913
H	-2.027291	-0.506396	-1.072750
H	2.736639	-2.161128	4.348817
H	1.360218	-2.375539	3.276540
H	3.021992	-2.459479	2.634861
H	3.935208	0.051319	4.450705
H	4.490324	-0.209826	2.800837
H	3.656406	1.292021	3.218409
H	1.723282	-0.038197	5.138151
H	1.232404	1.245471	4.023249
H	0.343986	-0.289940	4.071053
H	-3.251808	-1.030142	4.035861
H	-1.799233	-2.034841	4.088935
H	-1.907341	-0.693579	2.935498
H	-4.775203	-1.085457	2.054918
H	-3.479917	-0.892941	0.866374
H	-4.575689	-2.279436	0.768843
H	-4.763845	-2.999914	3.687110
H	-4.413358	-4.187945	2.415463
H	-3.350120	-4.063750	3.823004
H	-1.743717	-4.790195	-3.519864
H	-2.739382	-3.930373	-2.355037
H	-1.058791	-3.417085	-2.649970
H	-0.051711	-6.239012	-3.010397
H	0.852849	-4.996637	-2.126455
H	0.553252	-6.593413	-1.403451
H	-2.341896	-6.910643	-2.351591
H	-1.927550	-7.172963	-0.649554
H	-3.214620	-6.041214	-1.073939
H	0.971295	-7.995462	1.559726
H	-0.723443	-7.507494	1.736236
H	0.051514	-7.466910	0.151931
H	2.752416	-6.299897	1.075453
H	1.932739	-5.461279	-0.252996
H	2.417375	-4.581091	1.202193
H	1.703136	-6.550693	3.280246
H	1.308441	-4.835788	3.370976
H	0.040015	-6.053245	3.615923

C-H activation / Hydride / Coordination by O / Adduct of $MeOSO_2CF_3$

E = -1749.711501
G = -1748.882303

C	-0.936638	-4.979311	1.067893
C	-1.060534	-4.290355	2.296957
C	-1.925746	-3.201306	2.034868
C	-2.391689	-3.238761	0.681770
C	-1.747491	-4.377810	0.056101
Ce	0.456257	-2.563415	0.588598
O	2.533840	-4.273473	0.508512
S	2.959708	-5.653277	0.120903
C	4.768228	-5.764625	0.680811
C	-0.635356	-4.818425	3.663086
C	-0.591637	-3.706657	4.718116
C	-3.510080	-2.282955	0.211263
C	-4.033094	-1.435170	1.387508
C	-1.964579	-5.131030	-1.274244
C	-0.726796	-5.982873	-1.623799
C	2.558431	-0.718255	0.024510
C	2.406797	-0.567745	1.436631
C	1.122611	0.070830	1.645440
C	0.564362	0.271640	0.339360
C	1.455710	-0.167673	-0.666437
C	3.555606	-0.948205	2.392995
C	3.152677	-2.049680	3.391940
C	1.387781	0.181544	-2.148651
C	1.834927	1.653407	-2.293327
C	0.488345	0.815153	2.840390
C	1.051371	2.254772	2.861569
O	2.281716	-6.861763	0.602848
O	3.148702	-5.779416	-1.487025
C	3.184289	-4.555035	-2.287384
C	-0.035129	0.039517	-2.705297
C	2.326504	-0.697989	-2.984484
C	0.687509	0.175941	4.221981
C	-1.038001	0.929534	2.662885
C	4.095402	0.287593	3.139354
C	4.756762	-1.508731	1.604678
C	0.738535	-5.503358	3.609758
C	-1.684569	-5.863970	4.101109
C	-3.025753	-1.292320	-0.862603
C	-4.740023	-3.059328	-0.300010
C	-3.141920	-6.116742	-1.094354
C	-2.204870	-4.242620	-2.504151
H	-0.372376	-5.893223	0.933749
H	0.610528	-3.011913	-1.493527
H	-0.352851	0.813263	0.146116
H	3.428865	-1.140908	-0.457937
H	-2.269117	-2.498120	2.781757
H	3.160922	-4.927154	-3.311103
H	4.112838	-4.013631	-2.100344
F	5.237155	-6.955864	0.380911
F	5.474040	-4.834113	0.062692
F	4.812903	-5.571838	1.982289
H	-1.473070	1.439640	3.529263
H	-1.322671	1.503777	1.777887
H	-1.498138	-0.060672	2.592624
H	0.174123	0.779424	4.979253
H	0.253191	-0.827885	4.257277
H	1.732146	0.109235	4.524500
H	0.591222	2.835594	3.670556
H	2.133638	2.269046	3.008680
H	0.840151	2.762156	1.915143
H	2.278347	-0.403210	-4.038959
H	3.369289	-0.597233	-2.664121
H	2.028212	-1.747622	-2.903993
H	1.819081	1.961216	-3.346057
H	1.173030	2.321931	-1.733345
H	2.851886	1.793422	-1.911995
H	-0.065623	0.350995	-3.756017
H	-0.364882	-1.002267	-2.645699
H	-0.750145	0.663071	-2.158934
H	5.550730	-1.789031	2.305917
H	4.488646	-2.401965	1.033546
H	5.171427	-0.768550	0.913337
H	4.969562	0.012056	3.741433
H	4.406043	1.056488	2.424530
H	3.364257	0.736053	3.811618
H	3.969153	-2.253656	4.095742
H	2.268595	-1.793662	3.975251
H	2.951642	-2.988440	2.861448
H	-4.837006	-0.781885	1.031324
H	-4.441758	-2.059599	2.188247
H	-3.260150	-0.790217	1.812906
H	-3.850750	-0.651929	-1.198795
H	-2.249664	-0.635304	-0.453113
H	-2.610549	-1.791544	-1.737942
H	-5.558786	-2.360442	-0.508397
H	-4.547360	-3.614052	-1.217668

H	-5.089061	-3.769164	0.457049
H	-1.435119	-6.277185	5.086317
H	-2.680281	-5.413119	4.160860
H	-1.733990	-6.690442	3.385430
H	0.993060	-5.923216	4.589747
H	0.758109	-6.320921	2.884093
H	1.530238	-4.794307	3.342230
H	-0.328598	-4.121610	5.697533
H	0.158335	-2.949631	4.467851
H	-1.559218	-3.205777	4.822430
H	-2.288772	-4.872667	-3.397536
H	-3.122311	-3.657075	-2.444108
H	-1.359951	-3.560818	-2.645028
H	-0.891845	-6.485445	-2.583502
H	0.156436	-5.344482	-1.722538
H	-0.524373	-6.764032	-0.886480
H	-3.288423	-6.704987	-2.008471
H	-2.934362	-6.811405	-0.273884
H	-4.080964	-5.608900	-0.867184
H	2.300120	-3.941638	-2.075029

C-H activation / Hydride / Coordination by O / TS

E = -1749.672896
G = -1748.844386

C	-0.891050	-5.069303	1.012910
C	-1.014207	-4.327352	2.211190
C	-1.840493	-3.222720	1.885849
C	-2.288771	-3.302575	0.530303
C	-1.672042	-4.487955	-0.034342
Ce	0.579989	-2.693487	0.488524
O	2.484007	-4.384876	1.168064
S	2.885946	-5.606343	0.387546
C	4.779434	-5.641293	0.484893
C	-0.681852	-4.807379	3.621152
C	-0.292596	-3.645114	4.543424
C	-3.389404	-2.354426	0.008683
C	-3.833257	-1.372727	1.110436
C	-1.923753	-5.316399	-1.315131
C	-0.689999	-6.171075	-1.670273
C	2.605155	-0.738703	0.034870
C	2.459196	-0.642539	1.452507
C	1.151237	-0.063257	1.689101
C	0.571726	0.152664	0.393904
C	1.476560	-0.204263	-0.632739
C	3.661628	-0.933723	2.376844
C	3.367671	-1.966150	3.481708
C	1.433330	0.260467	-2.086490
C	2.041102	1.681868	-2.112221
C	0.516271	0.667734	2.895149
C	0.958200	2.148143	2.817831
O	2.423884	-6.948316	0.767871
O	2.671043	-5.354617	-1.178799
C	2.343135	-3.955932	-1.614212
C	0.003721	0.334331	-2.636968
C	2.267663	-0.635420	-3.012461
C	0.851398	0.128505	4.292572
C	-1.020727	0.645104	2.809066
C	4.187078	0.378817	2.995369
C	4.840576	-1.509324	1.567306
C	0.450370	-5.843031	3.630796
C	-1.956591	-5.474052	4.184689
C	-2.923649	-1.487049	-1.173671
C	-4.661846	-3.140822	-0.367622
C	-3.076807	-6.303456	-1.017202
C	-2.251822	-4.524515	-2.590277
H	-0.360195	-6.008507	0.929462
H	0.202952	-2.754344	-1.708109
H	-0.370834	0.659039	0.227980
H	3.502443	-1.081752	-0.461802
H	-2.187446	-2.488072	2.600097
H	2.331630	-4.100150	-2.698925
H	3.210714	-3.330862	-1.381609
F	5.215119	-6.745572	-0.082941
F	5.275848	-4.590911	-0.143359
F	5.135891	-5.613893	1.753991
H	-1.444879	1.198146	3.654289
H	-1.404985	1.111231	1.898698
H	-1.397760	-0.380002	2.858576
H	0.312765	0.719389	5.042129
H	0.533026	-0.910914	4.409097
H	1.910563	0.195998	4.538914
H	0.518942	2.722962	3.642360
H	2.044487	2.251228	2.873828
H	0.631488	2.599054	1.875724
H	2.288639	-0.213356	-4.023463
H	3.305734	-0.720899	-2.675011
H	1.838847	-1.639161	-3.081334
H	2.041245	2.083800	-3.132762
H	1.466408	2.363086	-1.476793
H	3.073119	1.673356	-1.747212
H	0.014172	0.739824	-3.655118
H	-0.457293	-0.656763	-2.671274
H	-0.631664	0.990094	-2.032902
H	5.663456	-1.749336	2.249309
H	4.564148	-2.429345	1.046586
H	5.223256	-0.795517	0.831059
H	5.103803	0.185420	3.565124
H	4.425367	1.102809	2.209107
H	3.473645	0.847660	3.673556
H	4.243078	-2.077616	4.132827
H	2.524648	-1.689184	4.111658
H	3.160385	-2.949220	3.047519
H	-4.610954	-0.712648	0.711189
H	-4.254683	-1.892545	1.976779
H	-3.011778	-0.738548	1.451350
H	-3.751216	-0.871152	-1.546708
H	-2.127633	-0.806521	-0.852958
H	-2.538224	-2.074302	-2.005933
H	-5.468057	-2.442260	-0.620932
H	-4.523257	-3.799619	-1.224244
H	-4.999072	-3.751851	0.476139
H	-1.779637	-5.854537	5.198163
H	-2.786123	-4.760990	4.226478
H	-2.267227	-6.312974	3.553982
H	0.620680	-6.199747	4.652897
H	0.210036	-6.714943	3.015358
H	1.388299	-5.418953	3.262668
H	-0.132313	-4.004419	5.566260
H	0.637885	-3.173364	4.210940
H	-1.072688	-2.878219	4.583408
H	-2.351332	-5.222341	-3.429545
H	-3.188323	-3.970763	-2.528341
H	-1.450606	-3.820072	-2.834367
H	-0.904399	-6.760449	-2.568680
H	0.182215	-5.548099	-1.884327
H	-0.419852	-6.880127	-0.884305
H	-3.270650	-6.938272	-1.890427
H	-2.815070	-6.953244	-0.176072
H	-4.005173	-5.788848	-0.760571
H	0.993781	-3.304922	-1.663031

C-H activation / Hydride / Coordination by O / Adduct of H_2

E = -1749.686945
G = -1748.856591

C	-0.880423	-5.116001	0.986044
C	-1.020690	-4.354666	2.169675
C	-1.835461	-3.252710	1.814255
C	-2.260227	-3.347914	0.451564
C	-1.646565	-4.555052	-0.079666
Ce	0.651012	-2.727146	0.507921
O	2.502773	-4.382742	1.277197

S	2.926597	-5.559734	0.432228
C	4.820566	-5.502328	0.434700
C	-0.692346	-4.800251	3.591767
C	-0.175308	-3.632959	4.442772
C	-3.378748	-2.420414	-0.079280
C	-3.778812	-1.384290	0.989411
C	-1.923474	-5.442649	-1.315803
C	-0.704612	-6.328448	-1.645421
C	2.654065	-0.726741	0.066509
C	2.496319	-0.642453	1.484364
C	1.181249	-0.077408	1.716571
C	0.608653	0.143332	0.419466
C	1.528926	-0.191725	-0.602359
C	3.701958	-0.910784	2.412771
C	3.425828	-1.941151	3.523705
C	1.521968	0.318171	-2.043634
C	2.313211	1.647855	-2.035795
C	0.526710	0.638087	2.921892
C	0.933460	2.128800	2.846200
O	2.558716	-6.929297	0.825720
O	2.627890	-5.280153	-1.107429
C	2.085645	-3.898200	-1.457708
C	0.109762	0.622266	-2.561439
C	2.223555	-0.641194	-3.016449
C	0.873798	0.110877	4.321091
C	-1.009405	0.578661	2.831860
C	4.203375	0.414937	3.023029
C	4.890960	-1.471256	1.608105
C	0.345038	-5.930254	3.615724
C	-1.998536	-5.327702	4.224344
C	-2.984783	-1.602077	-1.322387
C	-4.661413	-3.227103	-0.369583
C	-3.080576	-6.403481	-0.951115
C	-2.279901	-4.717006	-2.621709
H	-0.344417	-6.053752	0.923525
H	-0.500168	-2.288299	-1.797107
H	-0.334355	0.648796	0.252386
H	3.554522	-1.065096	-0.427587
H	-2.184932	-2.502786	2.510942
H	1.621691	-4.142472	-2.420009
H	2.991994	-3.325930	-1.691015
F	5.283161	-6.584371	-0.157214
F	5.234204	-4.429910	-0.216252
F	5.244742	-5.457517	1.683819
H	-1.449512	1.121258	3.675741
H	-1.400910	1.036695	1.920359
H	-1.363462	-0.454827	2.878418
H	0.315849	0.687134	5.067961
H	0.588226	-0.937287	4.440607
H	1.929976	0.211933	4.569023
H	0.480791	2.692453	3.671225
H	2.017184	2.256185	2.903132
H	0.597180	2.573576	1.904518
H	2.291274	-0.186144	-4.011030
H	3.243265	-0.871297	-2.692560
H	1.683699	-1.586317	-3.124837
H	2.339333	2.087862	-3.040216
H	1.851581	2.371282	-1.356425
H	3.343888	1.487967	-1.704781
H	0.167123	1.059814	-3.564255
H	-0.510738	-0.274785	-2.632224
H	-0.407247	1.344128	-1.921283
H	5.715771	-1.695522	2.293067
H	4.629661	-2.396555	1.090415
H	5.264558	-0.754643	0.869947
H	5.121749	0.240556	3.596287
H	4.431658	1.137079	2.232094
H	3.480757	0.876907	3.696296
H	4.304757	-2.035797	4.172654
H	2.581237	-1.673414	4.155455
H	3.233617	-2.929316	3.094363
H	-4.554933	-0.727508	0.581953
H	-4.187928	-1.857987	1.887047
H	-2.936380	-0.753342	1.283820
H	-3.836690	-1.003890	-1.667273
H	-2.178250	-0.900589	-1.079371
H	-2.662397	-2.221168	-2.160117
H	-5.485395	-2.544043	-0.607990
H	-4.554610	-3.912008	-1.211057
H	-4.952413	-3.813571	0.507735
H	-1.817374	-5.682759	5.246168
H	-2.762293	-4.544642	4.264537
H	-2.402535	-6.160341	3.639918
H	0.534648	-6.239836	4.649625
H	-0.005930	-6.810989	3.069352
H	1.296031	-5.618520	3.177134
H	-0.003446	-3.952992	5.476925
H	0.776706	-3.252682	4.055911
H	-0.891457	-2.805299	4.469897
H	-2.438848	-5.458919	-3.412179
H	-3.195444	-4.129605	-2.552569
H	-1.471855	-4.059501	-2.955453
H	-0.922193	-6.929003	-2.535578
H	0.185820	-5.731230	-1.850646
H	-0.462776	-7.029787	-0.843324
H	-3.283245	-7.088476	-1.783671
H	-2.815624	-7.003293	-0.074963
H	-4.005215	-5.870641	-0.719802
H	0.160055	-2.602458	-1.972149

C-H activation / Hydride / Coordination by O / Product

E = -1748.519538
G = -1747.704451

C	-0.987747	-5.099236	0.850538
C	-1.041192	-4.349371	2.049408
C	-1.813092	-3.159857	1.875532
C	-2.323264	-3.196755	0.518654
C	-1.821260	-4.408819	-0.060377
Ce	-3.680724	-5.428765	1.875416
C	-2.615429	-7.009510	3.723600
O	-3.383630	-7.079498	5.037776
S	-4.247690	-5.798153	5.435109
O	-5.521505	-6.169998	6.071444
C	-1.785735	-2.052230	2.951449
C	-1.009373	-2.526357	4.195821
C	-2.902562	-2.128689	-0.437332
C	-3.766197	-2.786391	-1.531036
C	-0.014497	-6.240424	0.542308
C	-0.448460	-7.577930	1.166396
C	-6.234745	-6.696227	2.268868
C	-6.523039	-5.494696	1.585559
C	-6.008330	-5.666887	0.277317
C	-5.458321	-6.977938	0.117909
C	-5.610081	-7.642848	1.400657
C	-7.427766	-4.358284	2.051393
C	-8.721321	-4.402397	1.211477
C	-5.000073	-7.472217	-1.271551
C	-5.821670	-8.681658	-1.758060
C	-5.551482	-9.123513	1.838254
C	-4.344633	-9.917977	1.315371
O	-4.224900	-4.772297	4.327610
C	-3.170466	-5.055778	6.808106
F	-3.573584	-3.821595	7.045054
F	-3.298816	-5.786308	7.896391
F	-1.906102	-5.046965	6.426080
C	-6.755644	-2.992809	1.845350
C	-7.807558	-4.508477	3.530307
C	-5.208744	-6.374942	-2.333298
C	-3.502189	-7.819437	-1.302414
C	-5.521151	-9.250861	3.375113
C	-6.859201	-9.816918	1.388423
C	-3.180497	-1.636150	3.453631
C	-1.011914	-0.823613	2.429638
C	1.370776	-5.873230	1.111016
C	0.138741	-6.425453	-0.975380

C	-1.712844	-1.438181	-1.144231
C	-3.791646	-1.043700	0.187573
H	-6.527907	-6.903792	3.289049
H	-1.943250	-4.677608	-1.101729
H	-0.493011	-4.594041	2.948270
H	-6.115865	-4.946274	-0.523579
H	-2.580985	-8.075237	3.474345
H	-1.607191	-6.724365	4.047053
H	-4.162300	-2.017089	-2.202892
H	-3.204166	-3.490304	-2.149774
H	-4.617035	-3.318296	-1.093677
H	-4.160700	-0.383739	-0.605751
H	-4.665320	-1.472342	0.686039
H	-3.264513	-0.413361	0.903169
H	-2.073259	-0.691581	-1.862576
H	-1.056852	-0.932165	-0.431437
H	-1.107942	-2.169910	-1.688534
H	0.264630	-8.371880	0.913721
H	-0.493144	-7.511807	2.257160
H	-1.429885	-7.895664	0.796605
H	2.102224	-6.650957	0.861710
H	1.725534	-4.924119	0.697166
H	1.348474	-5.777089	2.200739
H	0.878379	-7.206346	-1.183784
H	-0.797509	-6.728277	-1.452688
H	0.479700	-5.501245	-1.452699
H	-1.037968	-1.741904	4.959805
H	-1.445086	-3.427879	4.632134
H	0.042513	-2.727197	3.969901
H	-0.905107	-0.080530	3.228925
H	-0.007939	-1.115218	2.103936
H	-1.502948	-0.331308	1.589663
H	-3.091396	-0.814381	4.174334
H	-3.838826	-1.300502	2.654399
H	-3.666815	-2.469005	3.970335
H	-4.862773	-6.742490	-3.305303
H	-6.264496	-6.106216	-2.438482
H	-4.641542	-5.468349	-2.105592
H	-3.205760	-8.174073	-2.297280
H	-2.905629	-6.927067	-1.082586
H	-3.232674	-8.592035	-0.582095
H	-5.565887	-8.907485	-2.799957
H	-5.632379	-9.584770	-1.177448
H	-6.894076	-8.466591	-1.714063
H	-9.415367	-3.615075	1.529856
H	-8.511088	-4.258836	0.146831
H	-9.224024	-5.367904	1.326180
H	-8.461732	-3.683363	3.833065
H	-8.349456	-5.442407	3.709580
H	-6.929809	-4.496660	4.181596
H	-7.432278	-2.176192	2.123331
H	-5.859095	-2.891909	2.469904
H	-6.470712	-2.843483	0.798901
H	-4.355467	-10.927332	1.741767
H	-4.346624	-10.032856	0.230915
H	-3.398951	-9.448300	1.607967
H	-5.441515	-10.309152	3.646658
H	-4.675850	-8.725910	3.821494
H	-6.436412	-8.875116	3.840230
H	-6.870674	-10.859458	1.729568
H	-7.724247	-9.308660	1.826036
H	-6.988354	-9.815294	0.305743

C-H activation / Hydride / Coordination by OMe / Adduct of $MeOSO_2CF_3$

E = -1749.702105
G = -1748.882217

C	-0.783525	-4.812094	1.248352
C	-1.881200	-4.201068	0.601932
C	-2.341669	-3.199819	1.491416
C	-1.586720	-3.213536	2.705535
C	-0.570875	-4.238092	2.540241
Ce	0.196504	-2.254676	0.605725
O	2.112318	-4.926899	-3.496924
S	1.881092	-5.823666	-4.850599
O	2.002673	-7.268171	-4.567714
C	-2.600599	-4.715666	-0.640679
C	-3.599659	-5.799843	-0.179356
C	-2.046392	-2.372198	3.916532
C	-2.363797	-3.273948	5.125677
C	0.451967	-4.906127	3.485291
C	1.107504	-3.971344	4.512107
C	2.195902	-0.484978	-0.271842
C	1.041183	-0.111965	-1.018007
C	0.119916	0.502860	-0.078140
C	0.775433	0.475738	1.194338
C	2.054734	-0.114539	1.086573
C	0.939551	-0.470417	-2.516395
C	-0.014427	-1.668650	-2.695726
C	-1.187242	1.301277	-0.257852
C	-2.252788	0.590995	-1.110522
C	3.167510	-0.137965	2.126835
C	3.899711	-1.490344	2.120619
C	4.179244	0.971382	1.769275
C	2.628644	0.134833	3.536655
C	-1.855415	1.569947	1.105481
C	-0.861582	2.685912	-0.858970
C	0.502245	0.703977	-3.406829
C	2.311466	-0.922378	-3.056328
C	-0.244054	-6.066097	4.231334
C	1.611784	-5.523868	2.672583
C	-3.362703	-1.636018	3.594969
C	-1.035266	-1.283868	4.323002
C	-3.392067	-3.603822	-1.344304
C	-1.623463	-5.349022	-1.642154
C	2.797838	-5.549373	-2.377066
C	3.435640	-5.331572	-5.809224
O	0.744528	-5.222585	-5.566331
H	-1.238168	2.198998	1.752887
H	-3.093641	-4.042389	4.851480
H	-0.887448	-4.627237	-2.011252
H	3.075662	-0.950619	-0.691319
H	0.380326	0.922120	2.096566
H	-0.213040	-5.636985	0.845577
H	-3.210295	-2.577861	1.318930
H	2.443085	-6.571087	-2.237012
H	3.876569	-5.537868	-2.547914
F	3.424357	-5.939499	-6.980918
F	3.459117	-4.024283	-5.985697
F	4.509711	-5.703745	-5.128805
H	2.225662	-1.143380	-4.125522
H	3.066411	-0.139392	-2.933709
H	2.663751	-1.832178	-2.562705
H	0.531042	0.399885	-4.459377
H	-0.509318	1.053005	-3.200087
H	1.184340	1.551696	-3.284852
H	-0.122351	-1.948057	-3.750149
H	0.403125	-2.563549	-2.203315
H	-1.019933	-1.463934	-2.314213
H	-3.159260	1.204626	-1.166018
H	-1.932239	0.400827	-2.134914
H	-2.541817	-0.368352	-0.662001
H	-1.773467	3.289127	-0.947888
H	-0.162460	3.222286	-0.209408
H	-0.405673	2.615603	-1.846846
H	-2.801776	2.098536	0.949341
H	-2.079310	0.641860	1.642026
H	3.445982	0.114759	4.265609
H	2.152972	1.118750	3.602186
H	1.891984	-0.615280	3.842250
H	4.721349	-1.487568	2.846114
H	3.228912	-2.316043	2.387845
H	4.321800	-1.718357	1.137480
H	4.999726	0.998719	2.496692
H	4.609262	0.806087	0.776617

H	3.693760	1.952610	1.764312
H	-2.168015	-5.738892	-2.509117
H	-1.076082	-6.184502	-1.195281
H	-3.939661	-4.012367	-2.200577
H	-4.125673	-3.142825	-0.675479
H	-2.736166	-2.813976	-1.726424
H	-4.146864	-6.213201	-1.035176
H	-3.078281	-6.621186	0.321940
H	-4.328178	-5.385314	0.524936
H	-3.674744	-1.055525	4.469539
H	-3.255210	-0.934117	2.762207
H	-4.169656	-2.334732	3.353900
H	-1.407452	-0.717253	5.185079
H	-0.061819	-1.691710	4.594843
H	-0.886065	-0.571705	3.503517
H	-2.793185	-2.674534	5.937090
H	-1.482383	-3.776360	5.524617
H	1.852689	-4.527894	5.091413
H	1.633081	-3.140235	4.027628
H	0.397933	-3.552593	5.225743
H	2.369231	-5.919279	3.358196
H	1.281989	-6.357863	2.047321
H	2.093989	-4.791869	2.014766
H	0.473581	-6.596864	4.868823
H	-1.063208	-5.716035	4.863345
H	-0.660289	-6.783554	3.517363
H	2.527649	-4.920453	-1.522564
H	1.687733	-3.535143	-0.247275

C-H activation / Hydride / Coordination by OMe / TS

E = -1749.671336
G = -1748.846033

C	-0.886051	-4.984189	0.927749
C	-1.921058	-4.154356	0.432703
C	-2.119441	-3.164437	1.426866
C	-1.282893	-3.408667	2.562034
C	-0.483860	-4.575611	2.238686
Ce	0.424636	-2.557217	0.315757
O	1.660369	-4.054422	-1.682910
S	1.631141	-5.299269	-2.826219
O	1.565577	-6.609249	-2.148562
C	-2.869272	-4.478636	-0.717219
C	-4.020995	-5.325198	-0.131097
C	-1.491585	-2.621929	3.875149
C	-1.920795	-3.560053	5.022340
C	0.384923	-5.532934	3.086584
C	1.247876	-4.877460	4.176088
C	2.143380	-0.591988	-0.761024
C	0.910347	-0.277826	-1.413064
C	0.024391	0.236556	-0.388961
C	0.772026	0.203638	0.836922
C	2.092380	-0.252095	0.611823
C	0.790079	-0.376425	-2.948039
C	-0.322233	-1.341304	-3.399236
C	-1.278170	1.066497	-0.434325
C	-2.305319	0.675587	-1.507079
C	3.290460	-0.065794	1.538601
C	4.469111	-0.967532	1.146302
C	3.738123	1.406788	1.394803
C	2.936735	-0.324876	3.008522
C	-2.038014	0.970952	0.901384
C	-0.883122	2.548981	-0.627763
C	0.584757	1.016913	-3.576201
C	2.098353	-0.916036	-3.556744
C	-0.557265	-6.580426	3.726750
C	1.381835	-6.318878	2.211797
C	-2.649637	-1.615195	3.734863
C	-0.253897	-1.803843	4.281125
C	-3.467232	-3.211110	-1.341434
C	-2.179741	-5.292483	-1.819017
C	2.567254	-4.199957	-0.547316
C	3.391913	-5.182521	-3.565229
O	0.691428	-4.876409	-3.880436
H	-1.459027	1.337961	1.752246
H	-2.815873	-4.124406	4.740674
H	-1.374148	-4.729514	-2.299264
H	3.025687	-0.961026	-1.265495
H	0.419426	0.611934	1.775497
H	-0.523065	-5.872445	0.426237
H	-2.883120	-2.398522	1.387601
H	2.600009	-5.248924	-0.247702
H	3.558319	-3.846311	-0.845742
F	3.376082	-5.815208	-4.722103
F	3.723690	-3.919511	-3.751511
F	4.261284	-5.756331	-2.756189
H	1.979426	-1.013317	-4.641130
H	2.941766	-0.242392	-3.374774
H	2.348709	-1.903001	-3.162559
H	0.609011	0.940368	-4.669589
H	-0.365025	1.476358	-3.302926
H	1.386660	1.696161	-3.268506
H	-0.415947	-1.334550	-4.491678
H	-0.080658	-2.371492	-3.115094
H	-1.295942	-1.087432	-2.982708
H	-3.188569	1.316847	-1.408826
H	-1.939529	0.795449	-2.526052
H	-2.640073	-0.358452	-1.380016
H	-1.776219	3.185751	-0.632011
H	-0.231652	2.881315	0.186522
H	-0.347752	2.710728	-1.565870
H	-2.950033	1.575596	0.850286
H	-2.336040	-0.061282	1.105203
H	3.800561	-0.111048	3.648313
H	2.114408	0.313560	3.346995
H	2.648352	-1.368598	3.165201
H	5.324124	-0.771788	1.802944
H	4.207717	-2.025499	1.242187
H	4.799376	-0.781121	0.119139
H	4.611394	1.608207	2.026885
H	4.005768	1.634537	0.358002
H	2.936666	2.090516	1.692277
H	-2.900678	-5.555272	-2.600962
H	-1.759871	-6.227348	-1.435832
H	-4.196481	-3.475788	-2.115084
H	-3.985149	-2.595815	-0.598887
H	-2.693664	-2.599115	-1.816942
H	-4.736670	-5.601144	-0.915102
H	-3.635920	-6.245082	0.319882
H	-4.559587	-4.771406	0.644586
H	-2.784824	-1.090676	4.686709
H	-2.451096	-0.856411	2.974886
H	-3.595284	-2.110927	3.493946
H	-0.436772	-1.270006	5.221715
H	0.636360	-2.417449	4.411686
H	-0.030274	-1.054600	3.514122
H	-2.162918	-2.968691	5.913175
H	-1.151081	-4.275288	5.307916
H	1.863389	-5.645491	4.658480
H	1.923277	-4.133751	3.741129
H	0.667222	-4.398306	4.963288
H	1.905463	-7.050879	2.835996
H	0.905580	-6.875168	1.400853
H	2.135962	-5.653257	1.786094
H	0.017975	-7.289642	4.334223
H	-1.314094	-6.123550	4.367086
H	-1.080695	-7.146865	2.949748
H	2.365928	-3.547128	0.734566
H	2.161485	-3.088109	1.602696

C-H activation / Hydride / Coordination by OMe / Adduct of H_2

E = -1749.683246
G = -1748.856696

C	-0.876294	-5.022027	0.903219
C	-1.903015	-4.165599	0.435101
C	-2.072845	-3.190061	1.448079
C	-1.215108	-3.459402	2.560696
C	-0.449952	-4.644998	2.212195
Ce	0.437915	-2.561158	0.287470
O	1.603973	-3.994207	-1.703755
S	1.623666	-5.279839	-2.777392
O	1.494199	-6.564185	-2.058491
C	-2.864565	-4.454619	-0.713623
C	-4.021400	-5.301283	-0.138329
C	-1.377984	-2.684338	3.885522
C	-1.923607	-3.606718	4.995357
C	0.360684	-5.673516	3.040719
C	1.183613	-5.139771	4.224715
C	2.132143	-0.551302	-0.787888
C	0.890821	-0.268058	-1.437174
C	-0.001747	0.241870	-0.414836
C	0.748423	0.230906	0.808547
C	2.078208	-0.200041	0.580414
C	0.770423	-0.379607	-2.971741
C	-0.345144	-1.343592	-3.417149
C	-1.309609	1.065494	-0.464867
C	-2.328877	0.683655	-1.548214
C	3.287296	0.050199	1.479785
C	4.451734	-0.902818	1.170073
C	3.760485	1.492809	1.183289
C	2.946411	-0.033759	2.973863
C	-2.082017	0.963617	0.863316
C	-0.914573	2.549520	-0.649092
C	0.570669	1.011303	-3.607435
C	2.076308	-0.929213	-3.577680
C	-0.651829	-6.715421	3.574729
C	1.374316	-6.439471	2.166671
C	-2.423802	-1.562445	3.743073
C	-0.079124	-1.993089	4.336462
C	-3.450844	-3.165094	-1.302390
C	-2.192707	-5.249685	-1.840071
C	2.404141	-4.074624	-0.466788
C	3.428283	-5.213874	-3.399841
O	0.761614	-4.903326	-3.914786
H	-1.505988	1.313649	1.723411
H	-2.868838	-4.060540	4.680073
H	-1.386238	-4.684529	-2.316697
H	3.017667	-0.911703	-1.292138
H	0.391149	0.642387	1.744209
H	-0.530984	-5.904433	0.379552
H	-2.817716	-2.405293	1.428390
H	2.399318	-5.110366	-0.123280
H	3.421339	-3.751258	-0.706674
F	3.489733	-5.913592	-4.518241
F	3.780187	-3.964017	-3.639803
F	4.242606	-5.740039	-2.505129
H	1.953426	-1.036898	-4.660615
H	2.921526	-0.254862	-3.406734
H	2.325638	-1.912931	-3.174749
H	0.588248	0.927846	-4.700423
H	-0.373921	1.479890	-3.331208
H	1.379337	1.686516	-3.308519
H	-0.440020	-1.340158	-4.509413
H	-0.103638	-2.373343	-3.131515
H	-1.318339	-1.085982	-3.001732
H	-3.209189	1.329607	-1.454087
H	-1.953977	0.806248	-2.563443
H	-2.671670	-0.348225	-1.428556
H	-1.808344	3.185244	-0.664335
H	-0.274321	2.881355	0.174256
H	-0.366777	2.713069	-1.579843
H	-2.984581	1.582330	0.811166
H	-2.398935	-0.065684	1.053572
H	3.817669	0.250830	3.574110
H	2.130874	0.645381	3.241881
H	2.657625	-1.044457	3.276299
H	5.314057	-0.658342	1.800289
H	4.188888	-1.948031	1.355188
H	4.775886	-0.816566	0.128344
H	4.641161	1.743042	1.787281
H	4.025182	1.606746	0.127550
H	2.971885	2.216793	1.411537
H	-2.924036	-5.489149	-2.619817
H	-1.776250	-6.195416	-1.481563
H	-4.185005	-3.399899	-2.080902
H	-3.958307	-2.562351	-0.542459
H	-2.670396	-2.551076	-1.764452
H	-4.747788	-5.548443	-0.922049
H	-3.643883	-6.237301	0.285052
H	-4.545558	-4.761006	0.656598
H	-2.513081	-1.030339	4.696347
H	-2.136935	-0.829482	2.986024
H	-3.414406	-1.953763	3.491838
H	-0.228464	-1.477657	5.292888
H	0.752615	-2.685381	4.461575
H	0.217904	-1.236308	3.601124
H	-2.115823	-3.025014	5.904645
H	-1.241618	-4.413270	5.261454
H	1.706454	-5.978545	4.697900
H	1.949794	-4.428661	3.901764
H	0.582007	-4.666495	4.999678
H	1.841312	-7.228684	2.765868
H	0.922301	-6.923488	1.298401
H	2.172508	-5.781327	1.814067
H	-0.136158	-7.482210	4.165362
H	-1.416011	-6.257453	4.207245
H	-1.163988	-7.211933	2.745009
H	2.350794	-3.236678	1.695256
H	2.055927	-2.847762	2.278163

C-H activation / Hydride / Coordination by OMe / Product

E = -1748.512888
G = -1747.701481

C	-1.112519	-5.056524	0.699090
C	-2.085068	-4.088196	0.374024
C	-2.142053	-3.068496	1.376169
C	-1.166959	-3.430247	2.384861
C	-0.586720	-4.667557	1.954732
Ce	-3.239433	-5.463369	2.556456
C	-4.640208	-6.477780	0.646650
O	-5.291272	-5.164680	0.823581
S	-6.897713	-4.960087	0.395511
O	-7.257422	-3.568069	0.731155
C	-3.090165	-1.859677	1.214922
C	-3.775545	-1.895746	-0.165105
C	-0.507089	-2.640523	3.533334
C	0.487989	-1.621243	2.933909
C	-0.613456	-6.209526	-0.163917
C	-0.897840	-7.557422	0.521030
C	-4.983051	-7.063905	4.108832
C	-4.838887	-5.870724	4.857679
C	-3.518364	-5.897852	5.365632
C	-2.861755	-7.118899	5.011984
C	-3.800704	-7.863632	4.191165
C	-5.961703	-4.938001	5.302332
C	-6.940242	-4.626176	4.161909
C	-1.531059	-7.508888	5.696624
C	-0.356474	-7.648544	4.710589
C	-3.851481	-9.334397	3.715076
C	-4.764978	-9.504204	2.484908
O	-7.706888	-6.125751	0.807268
C	-6.769470	-5.055295	-1.507824
F	-6.705974	-6.313234	-1.900063
C	-6.735302	-5.656942	6.429410
C	-5.412765	-3.618234	5.862123
C	-1.684538	-8.802843	6.523304

C	-1.120591	-6.440879	6.731886
C	-2.506254	-9.947747	3.294891
C	-4.477236	-10.181215	4.847898
C	-4.218355	-1.890673	2.264742
C	-2.357498	-0.506808	1.277919
C	-1.488536	-1.924781	4.475914
C	0.331760	-3.576188	4.423044
C	-1.288090	-6.199301	-1.542282
C	0.907298	-6.062748	-0.365176
F	-7.848131	-4.487925	-2.016035
F	-5.693437	-4.408052	-1.920327
H	1.189578	-3.997455	3.891488
H	-2.513940	-8.709352	7.231776
H	-6.472361	-4.028593	3.372394
H	-2.679610	-4.096689	-0.528162
H	0.236345	-5.164101	2.451757
H	-5.896765	-7.370046	3.614964
H	-3.103731	-5.149469	6.027023
H	-5.357780	-7.251348	0.925088
H	-4.362661	-6.577684	-0.406705
H	-4.440237	-1.030955	-0.262151
H	-3.044434	-1.849562	-0.978568
H	-4.386935	-2.790688	-0.295727
H	-3.056925	0.300852	1.033363
H	-1.943852	-0.285990	2.262069
H	-1.541051	-0.473683	0.549276
H	-4.879338	-1.022634	2.156051
H	-4.856332	-2.771814	2.118590
H	-3.840146	-1.888305	3.289043
H	-0.935168	-1.433437	5.284233
H	-2.077360	-1.154133	3.978532
H	-2.182440	-2.635331	4.940707
H	1.020909	-1.096286	3.736085
H	1.229237	-2.138149	2.316176
H	0.000018	-0.874232	2.308189
H	0.726451	-3.016093	5.277219
H	-0.267195	-4.402244	4.813255
H	-0.519020	-8.395713	-0.075889
H	-0.419703	-7.610165	1.505384
H	-1.979235	-7.709219	0.642187
H	-0.904570	-7.021754	-2.155854
H	-2.372556	-6.321637	-1.462829
H	-1.089975	-5.263074	-2.074097
H	1.290677	-6.866777	-1.004502
H	1.146053	-5.105380	-0.839185
H	1.444898	-6.107713	0.587118
H	-7.790350	-4.045368	4.536893
H	-7.341757	-5.535116	3.705076
H	-6.237438	-2.973319	6.184291
H	-4.767091	-3.783013	6.730610
H	-4.838685	-3.064654	5.110935
H	-7.546623	-5.022826	6.806784
H	-7.173911	-6.592013	6.067684
H	-6.070855	-5.898123	7.265382
H	-0.167987	-6.729601	7.188629
H	-0.979570	-5.451730	6.290877
H	-1.860605	-6.353283	7.533540
H	0.553878	-7.957448	5.238267
H	-0.550145	-8.381918	3.927402
H	-0.146059	-6.688873	4.227552
H	-0.769622	-8.982157	7.100082
H	-1.861658	-9.688797	5.915383
H	-2.673823	-10.965098	2.923784
H	-2.046881	-9.376852	2.481864
H	-1.784622	-10.021534	4.107140
H	-4.832833	-10.568292	2.233298
H	-5.785221	-9.152131	2.655247
H	-4.361090	-8.982919	1.613529
H	-4.546214	-11.232819	4.543910
H	-3.898351	-10.133279	5.771811
H	-5.488094	-9.826529	5.072504

Methyl transfer / Hydride / Adduct of $MeOSO_2CF_3$

E = -1749.710928
G = -1748.881568

C	-1.376701	-1.761962	-2.070950
C	-2.512510	-0.941955	-1.896439
C	-2.943798	-1.167290	-0.564676
C	-2.133364	-2.157808	0.068428
C	-1.119550	-2.535958	-0.897912
Ce	-0.463233	0.228248	-0.229021
O	1.934841	-0.667492	0.581506
S	3.286497	-0.372562	0.007736
O	3.807873	1.001986	-0.080806
C	-3.323515	-0.282599	-3.007625
C	-3.974501	1.030059	-2.551416
C	-2.489964	-2.690930	1.471366
C	-3.816359	-2.077983	1.962726
C	-0.117406	-3.707111	-0.985380
C	-0.872796	-4.974651	-1.445018
C	-1.439125	2.531132	1.270047
C	-0.049534	2.434326	1.673332
C	0.727867	2.721767	0.510634
C	-0.099540	3.046499	-0.586576
C	-1.425933	2.882106	-0.120818
C	-2.762364	2.655365	2.054300
C	-2.890197	1.751071	3.287903
C	0.643113	2.256562	3.043658
C	2.170182	2.419517	2.902860
C	0.331271	3.732062	-1.878032
C	-0.427433	3.186918	-3.094636
O	3.557018	-1.216635	-1.354942
C	3.629405	-0.460023	-2.604406
C	4.455083	-1.396630	1.091183
C	-2.462535	-0.013992	-4.249618
C	-4.446157	-1.267828	-3.402928
C	-2.723509	-4.214010	1.472850
C	-1.421981	-2.320233	2.517682
C	0.947975	-3.422201	-2.065056
C	0.657118	-4.015312	0.306623
C	0.209630	3.353557	4.036953
C	0.419907	0.864033	3.663274
C	-2.936348	4.130578	2.482922
C	-3.967770	2.312158	1.156200
C	0.021212	5.237552	-1.729173
C	1.835892	3.564975	-2.125492
F	4.128441	-2.669655	1.027021
F	5.690323	-1.222631	0.667971
F	4.337673	-0.962117	2.330265
H	0.883609	0.386087	-1.898708
H	4.399093	0.308943	-2.526039
H	3.907721	-1.216042	-3.337726
H	2.642234	-0.034848	-2.808973
H	-0.819002	-1.841571	-2.992514
H	-3.837669	-0.739539	-0.131886
H	1.807712	2.743463	0.482900
H	-2.311437	3.123976	-0.694129
H	0.337159	5.787254	-2.624309
H	-1.050933	5.407607	-1.586590
H	0.545407	5.660039	-0.865664
H	2.117655	4.052343	-3.065930
H	2.429737	4.021531	-1.326907
H	2.096645	2.504760	-2.189336
H	-0.146499	3.736531	-4.001049
H	-0.184122	2.129898	-3.243976
H	-1.511482	3.285147	-2.975898
H	-3.887634	4.266620	3.012312
H	-2.132187	4.466439	3.140437
H	-2.939107	4.783362	1.604424
H	-4.891926	2.381177	1.740657
H	-4.071792	2.998517	0.312185
H	-3.894342	1.295703	0.759162
H	-3.885855	1.870655	3.730189
H	-2.776583	0.696125	3.019413
H	-2.166011	1.981264	4.068787

H	0.918023	0.795737	4.638124
H	-0.633566	0.630959	3.816952
H	0.856548	0.084519	3.027480
H	0.798476	3.276857	4.958879
H	0.382229	4.346449	3.609115
H	-0.841519	3.289672	4.317780
H	2.639331	2.282816	3.883422
H	2.604776	1.683558	2.222815
H	2.440772	3.416037	2.540818
H	-4.605136	1.440600	-3.348580
H	-4.609825	0.882294	-1.672560
H	-3.220319	1.781523	-2.300590
H	-5.049105	-0.858971	-4.223177
H	-4.026183	-2.224265	-3.730240
H	-5.111723	-1.466688	-2.556759
H	-3.062961	0.473206	-5.026134
H	-1.613158	0.635508	-4.021060
H	-2.071427	-0.944228	-4.673944
H	-1.676617	-2.734312	3.501166
H	-0.426510	-2.681335	2.254425
H	-1.369355	-1.231660	2.639685
H	-3.089816	-4.532155	2.456143
H	-3.478430	-4.487407	0.728689
H	-1.821269	-4.787810	1.262838
H	-4.042488	-2.457772	2.964919
H	-3.772092	-0.987482	2.030166
H	-4.651289	-2.346089	1.307824
H	1.374489	-4.822939	0.119616
H	1.223950	-3.144029	0.648208
H	0.015588	-4.345547	1.123810
H	-0.172344	-5.808231	-1.580969
H	-1.635308	-5.288743	-0.730400
H	-1.371791	-4.791279	-2.401863
H	1.700990	-4.218078	-2.051951
H	0.519057	-3.403961	-3.070740
H	1.453995	-2.469488	-1.892996

Methyl transfer / Hydride / TS

E = -1749.680123
G = -1748.848001

C	-0.061581	-4.396260	-0.965838
C	-1.190516	-3.553458	-0.873138
C	-1.661406	-3.697776	0.455222
C	-0.884147	-4.663520	1.169169
C	0.146775	-5.113575	0.252959
Ce	0.777289	-2.277284	0.750536
O	3.198092	-3.313025	1.789603
S	4.659393	-3.148098	1.432827
O	5.470799	-2.188932	2.206338
C	-1.943216	-2.925107	-2.040609
C	-2.590063	-1.587965	-1.654863
C	-1.310467	-5.135179	2.575220
C	-2.624189	-4.449352	2.998776
C	1.092602	-6.335580	0.246422
C	0.281055	-7.569859	-0.211683
C	-0.267474	-0.026717	2.286237
C	1.132957	-0.062988	2.653937
C	1.867338	0.253560	1.466969
C	0.993141	0.561742	0.394053
C	-0.306823	0.324304	0.894878
C	-1.576467	0.070389	3.100515
C	-1.650503	-0.807316	4.356978
C	1.862947	-0.188114	4.010750
C	3.376556	0.042033	3.835428
C	1.336558	1.382067	-0.846255
C	0.345955	1.139333	-1.991152
O	4.822476	-3.001772	-0.132335
C	3.365434	-2.438014	-0.823907
C	5.460095	-4.843471	1.718669
C	-1.023326	-2.711229	-3.250984
C	-3.063624	-3.908149	-2.446818
C	-1.622089	-6.644863	2.610261
C	-0.261929	-4.786431	3.647604
C	2.220238	-6.162836	-0.791405
C	1.788592	-6.643164	1.581500
C	1.401089	0.907456	4.993313
C	1.707127	-1.578694	4.653833
C	-1.781681	1.549643	3.502789
C	-2.791604	-0.317330	2.232745
C	1.249260	2.866768	-0.423195
C	2.755348	1.112769	-1.364417
F	4.976025	-5.732488	0.874146
F	6.761778	-4.730675	1.546129
F	5.202846	-5.219231	2.958356
H	1.563618	-1.844509	-1.276627
H	3.219636	-1.553226	-0.217933
H	3.703583	-2.239115	-1.833438
H	2.783559	-3.341998	-0.712499
H	0.510260	-4.541729	-1.871741
H	-2.561937	-3.236173	0.835808
H	2.942640	0.374421	1.436388
H	-1.218142	0.528388	0.349911
H	1.473363	3.523087	-1.272759
H	0.247015	3.111440	-0.057416
H	1.962013	3.088567	0.377650
H	3.000412	1.817311	-2.166991
H	3.511208	1.239170	-0.581903
H	2.829653	0.101975	-1.773583
H	0.598852	1.771867	-2.849724
H	0.378481	0.094712	-2.313896
H	-0.681127	1.383622	-1.700669
H	-2.726235	1.668206	4.047792
H	-0.975675	1.920974	4.138112
H	-1.821408	2.184727	2.612279
H	-3.701843	-0.286502	2.841217
H	-2.944359	0.369242	1.396312
H	-2.690729	-1.327154	1.826448
H	-2.639564	-0.705105	4.817546
H	-1.510021	-1.864619	4.116167
H	-0.916965	-0.535193	5.114832
H	2.237234	-1.613656	5.613149
H	0.666720	-1.842473	4.844992
H	2.149757	-2.350414	4.014353
H	2.016900	0.872690	5.899545
H	1.519802	1.899817	4.546063
H	0.362106	0.802589	5.304716
H	3.867313	-0.051627	4.810099
H	3.842144	-0.688871	3.172091
H	3.592085	1.046061	3.456066
H	-3.192321	-1.203088	-2.485803
H	-3.252636	-1.693269	-0.789739
H	-1.832552	-0.836491	-1.416106
H	-3.620836	-3.521505	-3.308758
H	-2.647004	-4.883236	-2.718784
H	-3.770788	-4.063077	-1.625418
H	-1.573035	-2.216948	-4.059691
H	-0.157363	-2.095461	-2.989328
H	-0.652489	-3.663766	-3.644197
H	-0.567394	-5.167823	4.629535
H	0.724518	-5.193792	3.424522
H	-0.160747	-3.699483	3.744758
H	-2.043697	-6.911322	3.586494
H	-2.360861	-6.903367	1.844769
H	-0.744745	-7.272683	2.457435
H	-2.891128	-4.769982	4.011430
H	-2.539893	-3.360122	3.014462
H	-3.452450	-4.718661	2.335709
H	2.488854	-7.475412	1.447126
H	2.359594	-5.781461	1.938257
H	1.094797	-6.938456	2.368089
H	0.928485	-8.453861	-0.262082
H	-0.546567	-7.795213	0.461934
H	-0.139774	-7.399727	-1.207798
H	2.862454	-7.049851	-0.781238
H	1.843328	-6.054833	-1.811298

H	2.859661	-5.306191	-0.564599

Methyl transfer / Hydride / Product

E = -1709.326187
G = -1708.534006

C	1.849701	-2.073404	2.082341
C	1.961947	-0.846374	2.778851
C	2.164274	0.242639	1.864789
C	2.131139	-0.335387	0.535567
C	1.900407	-1.733835	0.709892
Ce	-0.586011	-0.715604	1.552590
O	-1.658732	-2.793050	0.421710
S	-1.892410	-2.179658	-0.963031
C	-0.920080	-3.314838	-2.124687
C	2.711372	1.575132	2.424604
C	2.464365	2.823860	1.566795
C	2.477150	0.226730	-0.862327
C	1.524123	1.340984	-1.333733
C	1.850493	-3.489442	2.661536
C	0.437298	-4.099661	2.688472
C	-2.216101	-0.053666	3.888273
C	-1.802570	1.175184	3.277793
C	-2.457658	1.366482	2.037837
C	-3.239926	0.203795	1.838460
C	-3.152889	-0.670034	2.964783
C	-1.796212	-0.387848	5.339013
C	-3.010447	-0.533518	6.277158
C	-2.546841	2.648763	1.214353
C	-2.102002	2.422267	-0.238894
C	-4.185409	-1.810283	3.111552
C	-5.411173	-1.256296	3.875314
O	-1.150807	-0.840786	-0.973307
O	-3.267038	-2.191158	-1.502012
C	-4.017735	3.114688	1.212158
C	-1.695827	3.763992	1.835245
C	-4.719291	-2.271227	1.740651
C	-3.661000	-3.076007	3.806981
H	-2.801830	-3.493305	3.270325
C	-0.926861	-1.654216	5.423434
C	-0.952422	0.754715	5.936391
C	2.094902	1.891246	3.800147
C	4.233142	1.405201	2.642055
C	2.748624	-4.388989	1.792144
C	2.418739	-3.481880	4.088937
C	3.941562	0.710656	-0.899300
C	2.381226	-0.877985	-1.933079
H	2.039837	-0.755970	3.854036
H	-1.173110	1.911750	3.756316
H	1.852845	-2.447924	-0.098912
H	-3.891252	0.041978	0.988827
F	-1.589235	-4.443238	-2.278573
F	-0.771781	-2.723072	-3.297541
F	0.274910	-3.589243	-1.619750
H	1.877156	1.760395	-2.283322
H	0.525792	0.931439	-1.515640
H	1.438882	2.163273	-0.624623
H	4.211925	0.994920	-1.922916
H	4.127680	1.575660	-0.262467
H	4.617973	-0.090567	-0.583493
H	2.620541	-0.447525	-2.911205
H	3.087733	-1.693917	-1.751187
H	1.372822	-1.290894	-1.997041
H	-2.237677	3.334782	-0.831111
H	-1.039538	2.158990	-0.294424
H	-2.671522	1.622339	-0.721325
H	-1.770085	4.674544	1.231268
H	-2.033484	4.006375	2.848199
H	-0.636997	3.490867	1.889898
H	-4.118331	4.059109	0.664290
H	-4.668950	2.377313	0.733487
H	-4.379726	3.270767	2.233445
H	2.836721	3.706873	2.097930
H	2.971930	2.794287	0.603462
H	1.396676	2.980557	1.383751
H	4.664542	2.322451	3.060923
H	4.431147	0.586389	3.340902
H	4.757191	1.178699	1.711313
H	2.513454	2.827563	4.184980
H	1.011215	2.017117	3.726841
H	2.303249	1.120707	4.546631
H	2.462702	-4.504103	4.480560
H	3.431370	-3.066547	4.108227
H	1.798853	-2.897308	4.775794
H	2.808394	-5.393805	2.225619
H	2.356925	-4.492464	0.775715
H	3.763292	-3.984241	1.724270
H	0.462859	-5.122000	3.084250
H	-0.231310	-3.528753	3.345067
H	-0.005753	-4.142876	1.688979
H	-5.440280	-3.080915	1.897046
H	-5.250206	-1.476991	1.209436
H	-3.927379	-2.650878	1.095326
H	-6.183182	-2.031127	3.954839
H	-5.170283	-0.916637	4.882694
H	-5.840762	-0.408072	3.332841
H	-4.443526	-3.842699	3.810651
H	-3.374341	-2.910228	4.845743
H	-0.672997	0.496470	6.963328
H	-0.026409	0.919822	5.380126
H	-1.509268	1.696204	5.972445
H	-2.664809	-0.626459	7.313330
H	-3.657364	0.347546	6.217827
H	-3.615115	-1.414005	6.060299
H	-0.649817	-1.864741	6.463503
H	-1.431527	-2.537742	5.031363
H	0.002737	-1.512240	4.860636

C-H activation / Metallacycle / Coordination by O / Adduct of $MeOSO_2CF_3$

E = -1748.499138
G = -1747.690038

C	0.781998	3.781260	-2.991768
C	-0.421039	3.703641	-2.220825
C	-1.532012	3.418047	-3.040744
C	-1.026322	3.362801	-4.361679
C	0.392349	3.546986	-4.367019
Ce	-0.851553	6.132907	-3.668557
C	1.307204	7.511119	-3.497287
C	0.892459	8.856271	-4.148926
C	1.891057	9.325580	-5.218079
C	-2.938908	3.036923	-2.597053
C	-3.140217	1.529045	-2.852928
C	1.205212	3.318151	-5.657464
C	2.169926	2.126895	-5.491677
C	2.128060	3.799103	-2.234840
C	3.327558	4.402220	-2.980478
C	-0.698128	7.765168	-5.915557
C	-2.091021	7.454217	-6.054727
C	-2.753638	8.038221	-4.911814
C	-1.731401	8.700843	-4.151959
C	-0.472595	8.570030	-4.774756
C	-2.618628	6.822927	-7.358713
C	-3.334994	5.476595	-7.142626
C	-4.225747	8.309031	-4.533521
C	-4.611569	9.703835	-5.075319
O	-1.587109	6.782818	-1.178648
S	-1.445192	7.713203	-0.023509
C	-2.551171	6.984656	1.333933
F	-2.428517	7.720509	2.417945
O	-1.716949	9.154841	-0.157352
O	-0.033314	7.431570	0.744597
C	1.006726	8.440424	0.594019

C	0.776661	9.956723	-3.089210
C	-5.262435	7.287298	-5.022090
C	-4.386783	8.348867	-2.997593
C	-1.458521	6.535490	-8.332962
C	-3.538033	7.814971	-8.101563
C	-4.001702	3.816488	-3.387057
C	-3.143522	3.306512	-1.100103
C	0.274562	2.932682	-6.824643
C	1.972141	4.571766	-6.116670
C	1.995585	4.625037	-0.937049
C	2.471259	2.348507	-1.826375
F	-3.792120	7.021795	0.896364
F	-2.190539	5.745305	1.578859
H	-3.896159	3.663705	-4.465351
H	-4.541965	9.743462	-6.165568
H	-5.335149	7.232712	-6.107944
H	1.394847	8.423663	-0.424801
H	-1.617604	3.112293	-5.232860
H	-0.461292	3.783383	-1.142466
H	-1.912148	9.272462	-3.250323
H	0.068533	7.484876	-6.625995
H	2.874774	9.497936	-4.765542
H	2.020515	8.571449	-6.001418
H	1.562914	10.255863	-5.699761
H	1.764721	10.166687	-2.662250
H	0.385301	10.888602	-3.513185
H	0.113182	9.663167	-2.268440
H	-5.434449	8.542792	-2.740946
H	-4.109676	7.390101	-2.543225
H	-3.789847	9.133056	-2.526699
H	-5.639687	9.960132	-4.790371
H	-3.943018	10.471438	-4.673732
H	-6.252759	7.574013	-4.649714
H	-5.049384	6.284053	-4.641839
H	-3.723205	5.093702	-8.094423
H	-2.631702	4.733403	-6.751161
H	-4.168139	5.543332	-6.445303
H	-3.007461	8.754209	-8.289267
H	-3.840519	7.398427	-9.069977
H	-4.447280	8.054484	-7.549436
H	-1.857509	6.077719	-9.244576
H	-0.933579	7.450652	-8.623199
H	-0.726722	5.839258	-7.911859
H	-5.012785	3.502597	-3.101183
H	-3.929118	4.894100	-3.191629
H	-4.161079	3.032302	-0.800046
H	-2.447457	2.722219	-0.489612
H	-2.996447	4.364774	-0.860396
H	-4.137841	1.207153	-2.529366
H	-3.035517	1.292270	-3.916296
H	-2.396095	0.941500	-2.305855
H	2.538254	4.360712	-7.032223
H	1.272756	5.385131	-6.343841
H	2.671433	4.939621	-5.367583
H	2.671742	1.913754	-6.443163
H	2.945029	2.305928	-4.746279
H	1.619786	1.229089	-5.191237
H	0.872311	2.786184	-7.730797
H	-0.262947	1.999857	-6.627596
H	-0.460425	3.713437	-7.042525
H	4.205058	4.380642	-2.323442
H	3.597268	3.851303	-3.881574
H	3.143259	5.444625	-3.252321
H	3.398691	2.320940	-1.240550
H	1.669293	1.919676	-1.216987
H	2.604290	1.702538	-2.698085
H	2.966385	4.674403	-0.430535
H	1.675051	5.646915	-1.164655
H	1.287981	4.188065	-0.227367
H	1.924184	7.659152	-2.598628
H	1.943635	6.959549	-4.208723
H	0.617178	9.425890	0.852553
H	1.772028	8.128914	1.303508

C-H activation / Metallacycle / Coordination by O / TS

E = -1748.460901
G = -1747.649434

C	-2.132733	7.464039	-5.892066
C	-0.708610	7.632002	-5.850262
C	-0.339938	8.530385	-4.824610
C	-1.539795	8.858833	-4.155416
C	-2.664145	8.236429	-4.791968
Ce	-0.885226	6.262290	-3.420911
O	-2.443479	6.364931	-1.234638
S	-2.111806	7.106095	0.032429
O	-2.904848	8.296350	0.386048
C	1.084497	8.814231	-4.357125
C	1.152271	10.132291	-3.574075
C	-4.084596	8.694080	-4.398447
C	-5.199478	7.665104	-4.637408
C	-2.792905	6.790809	-7.117332
C	-1.721144	6.378967	-8.146975
C	-0.442933	3.765828	-2.130248
C	-1.501927	3.496913	-3.023158
C	-0.928216	3.556981	-4.316460
C	0.486405	3.763753	-4.238230
C	0.795259	3.924072	-2.831976
C	-2.904644	2.993638	-2.687073
C	-3.996606	3.933190	-3.224756
C	1.373367	3.503706	-5.477318
C	0.505168	3.155706	-6.702710
C	2.096845	3.931500	-1.998833
C	1.909829	4.779250	-0.723179
C	1.455544	7.612961	-3.459259
C	-3.086635	2.844568	-1.171591
C	-3.089163	1.604953	-3.332177
C	2.384813	2.479391	-1.553170
C	3.353034	4.491487	-2.682206
C	2.244495	4.699428	-5.899865
C	2.253539	2.258612	-5.239080
C	2.041155	8.938052	-5.553538
C	-4.155758	9.033966	-2.895617
C	-4.408906	9.997522	-5.163269
C	-3.705687	7.782034	-7.868995
C	-3.576359	5.510743	-6.776259
O	-0.527429	7.319396	0.129359
C	0.041127	8.078590	-1.041075
C	-2.241866	5.875736	1.468180
H	-3.913458	4.062122	-4.307582
H	-4.399126	9.856989	-6.245619
H	-5.351407	7.428632	-5.690156
H	0.587949	7.601585	-2.204155
H	-1.460899	3.333805	-5.230836
H	-0.534987	3.761506	-1.052444
H	-1.615420	9.557021	-3.332268
H	-0.020917	7.211024	-6.570863
H	3.062635	9.121927	-5.201316
H	2.064213	8.022854	-6.152878
H	1.750616	9.765223	-6.212447
H	2.178683	10.316840	-3.237428
H	0.844505	10.975044	-4.202176
H	0.512002	10.134672	-2.686982
H	-5.170042	9.363948	-2.645463
H	-3.929583	8.165567	-2.272296
H	-3.482598	9.846608	-2.611284
H	-5.399987	10.370828	-4.877772
H	-3.673050	10.771655	-4.923620
H	-6.148057	8.062432	-4.259172
H	-4.999165	6.730900	-4.102720
H	-4.033697	5.094384	-7.681787
H	-2.902754	4.750503	-6.367549
H	-4.372338	5.679340	-6.051329
H	-3.158329	8.697536	-8.115796
H	-4.047716	7.331191	-8.808071
H	-4.594049	8.064153	-7.304113

H	-2.206995	5.898110	-9.002822
H	-1.165516	7.243747	-8.522450
H	-1.003641	5.663219	-7.737034
H	-4.994475	3.529017	-3.016206
H	-3.941081	4.918654	-2.747767
H	-4.084048	2.449430	-0.949354
H	-2.349682	2.155756	-0.745947
H	-2.991016	3.807763	-0.665670
H	-4.073275	1.192662	-3.079330
H	-3.017611	1.656470	-4.422909
H	-2.324060	0.906487	-2.978530
H	2.868417	4.426241	-6.759308
H	1.613446	5.540095	-6.206897
H	2.906666	5.049192	-5.109269
H	2.799331	2.005190	-6.155784
H	2.990452	2.400056	-4.448432
H	1.633062	1.398546	-4.966886
H	1.153060	2.998941	-7.571694
H	-0.069241	2.237205	-6.548580
H	-0.192427	3.958535	-6.956053
H	4.185573	4.467326	-1.969739
H	3.665948	3.913043	-3.551351
H	3.215758	5.531339	-2.988937
H	3.283978	2.440832	-0.926104
H	1.547694	2.078025	-0.973598
H	2.541097	1.817324	-2.408883
H	2.838642	4.782297	-0.141720
H	1.669467	5.817746	-0.972336
H	1.124775	4.394468	-0.068105
H	2.350183	7.816302	-2.853830
H	1.739013	6.763376	-4.101773
H	-0.584857	8.966726	-1.179457
H	0.986974	8.421671	-0.612022
F	-3.487739	5.445834	1.507238
F	-1.420995	4.864456	1.281342
F	-1.943848	6.498139	2.588287

C-H activation / Metallacycle / Coordination by O / Product

E = -1748.517368
G = -1747.703303

C	0.639875	3.689477	-2.646256
C	-0.624627	3.607170	-1.989610
C	-1.666177	3.394367	-2.916523
C	-1.048135	3.403043	-4.191438
C	0.369194	3.557965	-4.067177
Ce	-0.934549	6.117439	-3.366749
C	2.211371	8.452581	-4.252961
C	1.018696	9.370604	-4.570113
C	1.303474	10.081505	-5.911298
C	-3.113929	3.019873	-2.611082
C	-3.404619	1.636215	-3.224376
C	1.284570	3.418867	-5.305027
C	2.335458	2.303575	-5.145839
C	1.926131	3.578756	-1.799288
C	3.108275	4.416853	-2.311608
C	-0.563986	7.664198	-5.759954
C	-1.967798	7.404323	-5.846392
C	-2.582213	8.129982	-4.750706
C	-1.519262	8.822961	-4.084066
C	-0.283423	8.586520	-4.722266
C	-2.544846	6.717566	-7.105655
C	-3.330795	5.427777	-6.813145
C	-4.038169	8.528586	-4.411330
C	-4.345978	9.858700	-5.137854
O	-2.319516	6.460307	-1.206598
S	-1.755022	7.253212	-0.050714
C	-2.118045	6.227704	1.498438
F	-1.639618	6.852180	2.554801
O	-2.270568	8.613285	0.187427
O	-0.167028	7.133454	-0.024181
C	0.456006	7.282948	-1.414130
C	0.896662	10.456162	-3.491675
C	-5.124117	7.502870	-4.767664
C	-4.204527	8.795105	-2.901099
C	-1.414173	6.323707	-8.077245
C	-3.428895	7.703384	-7.898689
C	-4.093296	4.042764	-3.209117
C	-3.355909	2.941508	-1.097804
C	0.455705	3.018585	-6.541234
C	1.996278	4.739610	-5.651392
C	1.668957	4.015009	-0.340227
C	2.342853	2.092049	-1.708393
F	-3.428447	6.104357	1.603288
F	-1.565720	5.036140	1.392393
H	-3.956289	4.142968	-4.289920
H	-4.257272	9.765603	-6.222546
H	-5.211438	7.318450	-5.838163
H	2.088105	7.950415	-3.287535
H	-1.562231	3.199931	-5.121205
H	-0.756549	3.632734	-0.917257
H	-1.662003	9.508943	-3.259220
H	0.161623	7.337996	-6.492386
H	2.205743	10.699984	-5.833144
H	1.458548	9.363532	-6.722409
H	0.467587	10.729823	-6.192377
H	1.836512	11.013195	-3.411934
H	0.105281	11.169783	-3.742371
H	0.672731	10.043201	-2.504554
H	-5.231703	9.121411	-2.703387
H	-4.022953	7.896599	-2.305933
H	-3.544658	9.582100	-2.529738
H	-5.364790	10.193346	-4.907151
H	-3.651006	10.640159	-4.815181
H	-6.096633	7.877699	-4.429289
H	-4.954823	6.544718	-4.267268
H	-3.738232	5.011784	-7.742299
H	-2.672782	4.670517	-6.374852
H	-4.163589	5.585965	-6.129192
H	-2.874736	8.620633	-8.122812
H	-3.730226	7.250174	-8.850601
H	-4.339409	7.984211	-7.369648
H	-1.845189	5.811077	-8.943857
H	-0.873036	7.199630	-8.448113
H	-0.690349	5.641709	-7.622833
H	-5.133531	3.743003	-3.033913
H	-3.966177	5.027947	-2.741910
H	-4.393616	2.652141	-0.898409
H	-2.704423	2.198269	-0.626926
H	-3.180133	3.907258	-0.615743
H	-4.430269	1.321104	-2.997422
H	-3.289851	1.648486	-4.312767
H	-2.718602	0.883120	-2.823831
H	2.666732	4.607980	-6.509587
H	1.264022	5.507368	-5.924286
H	2.591174	5.121823	-4.819994
H	2.849761	2.145864	-6.101023
H	3.100274	2.542005	-4.406707
H	1.862980	1.358732	-4.859569
H	1.113934	2.946366	-7.413645
H	-0.025742	2.045177	-6.403946
H	-0.319512	3.751534	-6.778405
H	3.952717	4.335337	-1.617846
H	3.467564	4.093148	-3.289201
H	2.843001	5.476810	-2.385328
H	3.214446	1.984740	-1.050925
H	1.526107	1.498164	-1.285833
H	2.597387	1.662081	-2.676296
H	2.615466	4.006089	0.210846
H	1.244264	5.017218	-0.266466
H	0.995199	3.325284	0.176531
H	3.144197	9.026889	-4.206542
H	2.335313	7.684819	-5.023470
H	0.613860	8.362398	-1.492717
H	1.437062	6.838877	-1.222657

C-H activation / Metallacyle / Coordination by OMe / Adduct of $MeOSO_2CF_3$

E = -1748.499820
G = -1747.691780

C	0.942982	3.909496	-3.031157
C	-0.251553	3.898081	-2.234422
C	-1.379756	3.578273	-3.017693
C	-0.892650	3.432437	-4.337706
C	0.531946	3.588282	-4.378956
Ce	-0.861474	6.137131	-3.709827
C	-3.420241	7.199383	1.343057
O	-2.610272	7.743469	0.264636
S	-1.059046	7.244603	0.167631
O	-0.797645	6.083030	1.033859
C	-2.846726	3.781261	-2.634783
C	-3.732542	2.723541	-3.309261
C	1.316516	3.221726	-5.656033
C	2.272523	2.041804	-5.389675
C	2.304678	3.996405	-2.311729
C	3.459664	4.582460	-3.136077
C	-0.276997	7.743834	-6.016938
C	-1.702616	7.651347	-6.102240
C	-2.230191	8.401696	-4.981330
C	-1.094972	8.915122	-4.278570
C	0.108648	8.547796	-4.920978
C	-3.628372	8.933868	-4.596368
C	-4.823476	8.035724	-4.947391
C	-2.367043	7.007896	-7.337205
C	-3.257962	5.799068	-6.994862
C	1.495345	9.100741	-4.614491
C	1.511807	10.598015	-4.987793
C	-3.174913	5.221185	-3.110567
C	-0.192208	8.751684	0.924361
F	-0.631319	8.905849	2.161158
O	-0.692290	7.289789	-1.270065
F	1.103365	8.526351	0.929617
F	-0.467369	9.821752	0.212684
C	2.576534	8.384577	-5.433719
C	1.833027	8.967399	-3.120314
C	-3.171615	8.060686	-8.126807
C	-1.298748	6.483455	-8.317658
C	-3.822580	10.310554	-5.271583
C	-3.717629	9.151422	-3.070572
C	-3.025922	3.658559	-1.117602
C	2.091749	4.406011	-6.263017
C	0.355224	2.735367	-6.759971
C	2.196199	4.896591	-1.060826
C	2.697784	2.586589	-1.815922
H	-1.793480	6.025847	-9.181251
H	-3.560851	7.622579	-9.053826
H	2.417399	8.519718	-6.508279
H	2.830066	1.886165	-2.643644
H	3.729591	3.969101	-3.995679
H	-4.431112	7.515534	1.088695
H	0.409251	7.327974	-6.741371
H	-1.153352	9.572724	-3.419635
H	-0.275906	4.070460	-1.166109
H	-1.508970	3.170422	-5.187458
H	-4.784827	2.895041	-3.053762
H	-3.649859	2.772201	-4.400115
H	-3.459933	1.706760	-2.997710
H	-4.083934	3.779975	-0.857544
H	-2.690520	2.683322	-0.745760
H	-2.460857	4.429275	-0.581661
H	3.176583	4.974476	-0.577515
H	1.877138	5.911999	-1.323007
H	1.501013	4.504163	-0.315292
H	3.636668	2.623640	-1.249269
H	1.919413	2.181662	-1.161726
H	4.353795	4.661540	-2.506986
H	3.222498	5.589833	-3.495842
H	2.647862	4.081247	-7.151045
H	1.398777	5.193424	-6.577606
H	2.804933	4.849539	-5.569547
H	1.724761	1.191836	-4.969805
H	2.737990	1.714839	-6.327233
H	3.076572	2.294943	-4.697831
H	0.932612	2.478359	-7.654767
H	-0.199801	1.843543	-6.453433
H	-0.365733	3.506570	-7.048679
H	3.566732	8.786748	-5.192237
H	2.591496	7.308684	-5.230566
H	2.803631	9.426261	-2.897482
H	1.080082	9.457074	-2.494792
H	1.895721	7.914662	-2.816856
H	2.500685	11.036281	-4.804059
H	1.267616	10.734513	-6.045981
H	0.776271	11.157856	-4.401564
H	-3.715004	5.393720	-7.905910
H	-2.661553	4.997116	-6.543908
H	-4.058714	6.043480	-6.299143
H	-4.021375	8.452023	-7.567023
H	-2.531063	8.907261	-8.395355
H	-0.656371	7.287017	-8.690851
H	-0.663135	5.717303	-7.862505
H	-5.745766	8.514713	-4.597877
H	-4.940116	7.874279	-6.019047
H	-4.747087	7.063667	-4.453550
H	-4.783807	10.750574	-4.977754
H	-3.026226	11.001255	-4.976341
H	-3.805808	10.234299	-6.361953
H	-4.721633	9.506102	-2.809893
H	-3.538931	8.214844	-2.533132
H	-3.011351	9.902785	-2.707073
H	-3.841113	5.746680	-2.411988
H	-3.702201	5.171727	-4.074715
H	-3.115785	7.625717	2.300484
H	-3.355057	6.111873	1.358415

C-H activation / Metallacycle / Coordination by OMe / TS

E = -1748.466641
G = -1747.657383

C	-2.361040	8.399171	-4.703741
C	-1.874527	7.655926	-5.848309
C	-0.446663	7.752834	-5.813237
C	-0.024731	8.579098	-4.743275
C	-1.202702	8.932719	-4.051886
Ce	-0.875728	6.175214	-3.495026
O	-0.646006	7.335282	-1.043517
S	0.224358	7.943681	0.301944
C	-0.717241	9.569667	0.607521
C	1.395490	9.076524	-4.487142
C	2.259654	7.969245	-3.858890
C	-2.581421	7.074293	-7.092836
C	-3.386177	8.177203	-7.811950
C	-3.745670	8.934177	-4.271347
C	-3.935971	10.331708	-4.904199
C	-0.349272	3.766687	-2.240254
C	-1.449862	3.548546	-3.096798
C	-0.919023	3.548532	-4.406823
C	0.509614	3.680775	-4.376431
C	0.873802	3.838607	-2.986323
C	-2.928373	3.633879	-2.724355
C	-3.291423	5.128534	-2.869774
C	1.338514	3.413693	-5.650948
C	2.190049	4.618264	-6.089739
C	2.205531	3.777245	-2.206173
C	2.100052	4.567994	-0.884671
C	-1.823237	6.519462	-0.800197
C	2.472702	2.301337	-1.833187

C	3.440907	4.345825	-2.919316
C	-3.155809	3.159153	-1.282667
C	-3.779934	2.754139	-3.652163
C	0.414390	3.082961	-6.840332
C	2.226967	2.165485	-5.470915
C	-1.546812	6.588869	-8.127499
C	-3.484907	5.865442	-6.789457
C	1.384945	10.287349	-3.543784
C	2.033824	9.502634	-5.821891
C	-3.801778	9.114454	-2.739538
C	-4.960746	8.061618	-4.619599
O	1.568072	8.315139	-0.184765
O	-0.023152	7.091579	1.481712
H	-2.070724	6.165734	-8.991165
H	-3.793216	7.790432	-8.753757
H	2.286616	7.080822	-4.499175
H	2.582392	1.670415	-2.718370
H	3.707654	3.801765	-3.824986
H	-2.446039	5.949772	-1.868950
H	0.209888	7.353922	-6.574509
H	-1.233171	9.593063	-3.195867
H	-0.407417	3.794326	-1.160493
H	-1.499588	3.376568	-5.302728
H	-4.839200	2.840526	-3.385164
H	-3.682253	3.056405	-4.699667
H	-3.491087	1.698742	-3.577264
H	-4.220074	3.224446	-1.030309
H	-2.839380	2.118155	-1.157463
H	-2.609262	3.762150	-0.551916
H	3.047335	4.496080	-0.339474
H	1.913475	5.631954	-1.062829
H	1.322977	4.187259	-0.217862
H	3.390962	2.216352	-1.239493
H	1.645502	1.898699	-1.240468
H	4.303137	4.284737	-2.245942
H	3.305636	5.400387	-3.177318
H	2.763313	4.372279	-6.991644
H	1.543864	5.469398	-6.330235
H	2.897048	4.938077	-5.325312
H	1.620716	1.303161	-5.174991
H	2.722109	1.919929	-6.417862
H	3.006685	2.297318	-4.720681
H	1.024396	2.911255	-7.733598
H	-0.172466	2.177022	-6.660608
H	-0.276526	3.898816	-7.071278
H	3.294351	8.303799	-3.717196
H	1.888590	7.688963	-2.864194
H	2.404100	10.663961	-3.404256
H	0.774978	11.100395	-3.950470
H	0.996965	10.026181	-2.555583
H	3.040406	9.902253	-5.652561
H	2.124515	8.660523	-6.515156
H	1.435352	10.277817	-6.310727
H	-3.985097	5.526834	-7.704691
H	-2.888924	5.026046	-6.414264
H	-4.256475	6.082817	-6.051835
H	-4.224019	8.548864	-7.222374
H	-2.739740	9.028836	-8.047694
H	-0.918544	7.408166	-8.489940
H	-0.894741	5.807472	-7.726833
H	-5.867362	8.543655	-4.236495
H	-5.104223	7.927515	-5.691287
H	-4.893999	7.075299	-4.152676
H	-4.890422	10.768880	-4.586486
H	-3.132206	11.007841	-4.596313
H	-3.931088	10.288389	-5.996043
H	-4.783829	9.506667	-2.452742
H	-3.664852	8.157132	-2.227397
H	-3.055636	9.819512	-2.365299
H	-4.215335	5.385396	-2.333844
H	-3.501264	5.351634	-3.928999
F	-0.161390	10.186762	1.632206
F	-0.646072	10.333734	-0.465386
F	-1.982311	9.303444	0.879600
H	-2.620858	7.141087	-0.384147
H	-1.572800	5.717177	-0.103730

C-H activation / Metallacycle / Coordination by OMe / Product

E = -1748.514148
G = -1747.702990

C	0.763138	3.861759	-2.983417
C	-0.434375	3.825280	-2.196189
C	-1.568647	3.649066	-3.011421
C	-1.082932	3.628470	-4.343323
C	0.345938	3.705703	-4.362644
Ce	-0.718902	6.311567	-3.514716
C	-1.603526	6.908369	-1.160995
O	-0.255128	7.497314	-1.137100
S	0.504157	7.853877	0.318826
O	0.160332	6.857170	1.352777
C	-3.008080	3.397002	-2.575133
C	-3.497863	2.078456	-3.204295
C	1.125375	3.421633	-5.664258
C	2.005864	2.164402	-5.511625
C	2.121717	3.767151	-2.251753
C	3.337537	4.324858	-3.005903
C	-0.350723	7.921916	-5.804963
C	-1.771408	7.773964	-5.876399
C	-2.313627	8.495334	-4.739432
C	-1.192598	9.054885	-4.048496
C	0.014096	8.742529	-4.711540
C	-3.730284	8.997922	-4.376800
C	-4.889358	8.048014	-4.713634
C	-2.422204	7.153241	-7.132687
C	-3.267779	5.903023	-6.829840
C	1.423041	9.231467	-4.390126
C	2.067284	9.803954	-5.665486
C	-3.924356	4.541767	-3.041776
C	-0.407356	9.454551	0.807654
F	-1.622123	9.174150	1.240977
O	1.891409	8.242487	-0.008779
F	0.281337	10.040113	1.770640
F	-0.486244	10.264677	-0.233927
C	2.285109	8.061671	-3.880516
C	1.393246	10.328589	-3.319081
C	-3.270939	8.196937	-7.887832
C	-1.340579	6.711255	-8.138835
C	-3.953896	10.349544	-5.094375
C	-3.858341	9.271491	-2.864538
C	-3.108554	3.272853	-1.049067
C	1.978271	4.613772	-6.136054
C	0.155210	3.096588	-6.817547
C	2.078158	4.547067	-0.921663
C	2.377628	2.284328	-1.900313
H	-1.821356	6.254708	-9.010629
H	-3.621952	7.775194	-8.837033
H	2.324568	7.249549	-4.616488
H	2.443213	1.656835	-2.792072
H	3.568955	3.782698	-3.922387
H	-3.628962	5.491988	-2.575030
H	0.341298	7.549999	-6.548170
H	-1.264261	9.688446	-3.175010
H	-0.457044	3.861166	-1.115696
H	-1.697329	3.443776	-5.214096
H	-4.525539	1.861379	-2.889790
H	-3.485891	2.124234	-4.297784
H	-2.862400	1.241778	-2.897158
H	-4.143712	3.067518	-0.755430
H	-2.485001	2.454444	-0.675341
H	-2.799031	4.194159	-0.546748
H	3.040998	4.450199	-0.408685
H	1.910542	5.615778	-1.086011
H	1.313876	4.182965	-0.232292
H	3.315472	2.180233	-1.341376

H	1.566493	1.892866	-1.278589
H	4.222109	4.255737	-2.363250
H	3.202805	5.381909	-3.255884
H	2.505796	4.364197	-7.064456
H	1.339713	5.479720	-6.343421
H	2.726045	4.914721	-5.402819
H	1.400480	1.308577	-5.195897
H	2.467429	1.913528	-6.473990
H	2.810641	2.288267	-4.787285
H	0.730349	2.907522	-7.730184
H	-0.437968	2.200973	-6.608713
H	-0.531300	3.920264	-7.032206
H	3.317796	8.375198	-3.687537
H	1.910337	7.677752	-2.920035
H	2.407836	10.689284	-3.118373
H	0.789316	11.181284	-3.645820
H	0.984167	9.957852	-2.376153
H	3.071578	10.186434	-5.448999
H	2.161576	9.045325	-6.448864
H	1.466628	10.626402	-6.066213
H	-3.703730	5.504147	-7.753484
H	-2.641849	5.116762	-6.394206
H	-4.085659	6.100573	-6.137554
H	-4.150216	8.519812	-7.330766
H	-2.672500	9.085207	-8.114839
H	-0.747300	7.559089	-8.494855
H	-0.657720	5.968241	-7.717462
H	-5.829311	8.486728	-4.360352
H	-5.006463	7.868781	-5.781950
H	-4.771971	7.081722	-4.213113
H	-4.941127	10.755905	-4.842848
H	-3.197651	11.076725	-4.782366
H	-3.893311	10.256724	-6.180718
H	-4.855361	9.673237	-2.653087
H	-3.737681	8.354048	-2.283327
H	-3.135952	10.006525	-2.500998
H	-4.967533	4.356303	-2.759105
H	-3.894054	4.656482	-4.130576
H	-2.322958	7.684857	-0.892391
H	-1.635816	6.095484	-0.431322

Methyl transfer / Metallacycle / Adduct of $MeOSO_2CF_3$

E = -1748.497231
G = -1747.685806

C	-1.264505	3.968443	-2.897934
C	-0.378092	4.998899	-2.513023
C	-0.683213	6.221461	-3.198980
C	-1.772294	5.921820	-4.098424
C	-2.090102	4.537190	-3.892139
Ce	0.388504	4.110505	-5.036574
C	-0.283330	1.951062	-3.836087
C	-1.093533	2.474059	-2.624250
C	-2.461802	1.793213	-2.468411
C	-0.028350	7.545276	-2.751323
C	0.960493	7.297122	-1.594359
C	-2.739924	6.778264	-4.942158
C	-3.279895	5.964012	-6.137585
C	2.359270	3.411900	-6.979140
C	2.936808	2.892438	-5.776441
C	3.328012	4.045042	-4.991431
C	2.939414	5.199089	-5.741435
C	2.382004	4.822358	-6.986188
C	3.237233	1.379656	-5.705352
C	4.550225	1.107504	-6.473285
C	2.082623	5.755950	-8.154179
C	3.387448	6.478532	-8.546677
C	4.170412	4.196593	-3.708537
C	5.555075	3.541189	-3.885186
O	-1.138197	3.026544	-7.024827
S	-1.963121	2.795349	-8.242573
C	-1.204922	1.278270	-9.098075
F	-1.980523	0.927845	-10.101318
O	-2.173774	3.828168	-9.261448
O	-3.431009	2.208678	-7.836844
C	-3.573518	1.466728	-6.593771
C	1.030327	6.810868	-7.774432
C	1.577105	4.977081	-9.375448
C	3.462981	3.640446	-2.459573
C	4.457018	5.682617	-3.417163
C	3.345908	0.775607	-4.297547
C	2.117994	0.582295	-6.410532
C	0.784398	8.237179	-3.861975
C	-1.090400	8.508448	-2.181763
C	-0.298881	2.249252	-1.332598
C	-2.155710	8.057729	-5.557941
C	-3.952803	7.151705	-4.060551
F	-0.008551	1.599325	-9.537021
F	-1.121061	0.291169	-8.226570
H	1.331373	7.378086	-6.888287
H	-3.656003	7.753333	-3.198097
H	-1.843046	8.789159	-4.813232
H	3.146040	6.220155	-5.448553
H	2.026732	2.801930	-7.808524
H	-2.901804	4.016570	-4.385556
H	0.376543	4.897251	-1.745211
H	-0.221500	1.175870	-1.126345
H	0.720914	2.637940	-1.415456
H	-0.780037	2.729521	-0.472775
H	-2.333971	0.713229	-2.330916
H	-3.017050	2.189916	-1.608616
H	-3.087102	1.941097	-3.356583
H	-3.969151	6.581092	-6.724521
H	-2.471555	5.652329	-6.808128
H	-3.834109	5.074517	-5.827216
H	-4.689225	7.724209	-4.638095
H	-4.442206	6.249527	-3.680323
H	-2.918303	8.540979	-6.179491
H	-1.300028	7.837125	-6.203301
H	1.208162	9.178764	-3.491883
H	1.619848	7.600714	-4.173985
H	0.192057	8.465290	-4.746661
H	-1.643069	8.026586	-1.368546
H	-0.608508	9.406607	-1.777049
H	-1.815326	8.834333	-2.927918
H	1.416910	8.248135	-1.299198
H	0.461440	6.880499	-0.714211
H	1.771941	6.621665	-1.881340
H	0.874527	7.524062	-8.592753
H	0.057835	6.345088	-7.568330
H	1.401767	5.660171	-10.213782
H	2.305905	4.227729	-9.700997
H	0.631018	4.468330	-9.166163
H	3.221969	7.140985	-9.405029
H	3.769648	7.085021	-7.719843
H	4.163725	5.755394	-8.816220
H	4.108798	3.730579	-1.577507
H	2.550887	4.213717	-2.256751
H	3.178341	2.594854	-2.564287
H	6.175645	3.728586	-3.000706
H	5.502551	2.461757	-4.025066
H	6.068781	3.965704	-4.754051
H	5.046661	5.763450	-2.497616
H	5.030763	6.152256	-4.222266
H	3.539762	6.260130	-3.267275
H	3.488810	-0.308143	-4.379812
H	4.190593	1.162194	-3.727127
H	2.430893	0.949866	-3.726038
H	4.773987	0.033501	-6.485989
H	4.469010	1.451390	-7.509552
H	5.400115	1.624296	-6.020164
H	2.320578	-0.491286	-6.324732
H	1.146435	0.781578	-5.946226
H	2.051658	0.808028	-7.478375
H	-0.982689	1.583330	-4.613387
H	0.348038	1.097151	-3.566852

H	-4.624504	1.580663	-6.330515
H	-3.333378	0.415950	-6.763076
H	-2.937928	1.888327	-5.814951

Methyl transfer / Metallacycle / TS

E = -1748.469104
G = -1747.653017

C	2.765901	2.734719	-5.762164
C	2.244304	3.275445	-6.983406
C	2.307126	4.685707	-6.980817
C	2.808235	5.039842	-5.706110
C	3.143445	3.872108	-4.947821
Ce	0.196701	4.081672	-5.181004
O	-1.136311	3.832535	-7.564106
S	-2.202901	2.946760	-8.173619
O	-3.436110	3.569933	-8.683842
C	2.096585	5.640501	-8.152756
C	1.001866	6.677508	-7.845617
C	3.997196	4.003580	-3.667064
C	3.341014	3.394823	-2.414998
C	3.100496	1.224415	-5.721518
C	3.259031	0.583972	-4.333941
C	-0.401698	5.006495	-2.627262
C	-0.730553	6.227612	-3.309088
C	-1.887742	5.938736	-4.123392
C	-2.217778	4.564041	-3.880598
C	-1.336672	3.993087	-2.932663
C	-0.033197	7.549038	-2.913829
C	0.782404	8.177114	-4.059623
C	-1.209370	2.513144	-2.580362
C	-0.629320	2.335544	-1.166983
C	-2.888600	6.812651	-4.908984
C	-2.273667	7.998802	-5.666715
C	-0.266795	1.925347	-3.654144
C	-1.500787	1.715182	-5.811420
O	-2.453409	1.689185	-7.262488
C	-2.583878	1.828527	-2.602431
C	-3.970909	7.324302	-3.931054
C	-3.622366	5.978782	-5.979798
C	-1.048682	8.575214	-2.371375
C	0.953508	7.310948	-1.753320
C	1.709658	4.875564	-9.423674
C	3.421638	6.383982	-8.416721
C	4.258069	5.487001	-3.340129
C	5.396173	3.391339	-3.892644
C	2.004540	0.394481	-6.421167
C	4.409391	1.017476	-6.518933
C	-1.363650	2.131398	-9.660124
H	1.223668	7.235321	-6.929989
H	-3.557338	7.960093	-3.146305
H	-1.819227	8.743031	-5.013250
H	3.031522	6.052855	-5.400103
H	1.938593	2.680986	-7.834384
H	-3.099901	4.076561	-4.276709
H	0.393360	4.906746	-1.901095
H	-0.536052	1.269338	-0.932195
H	0.369101	2.775530	-1.081630
H	-1.270634	2.800892	-0.408148
H	-2.474256	0.759622	-2.385891
H	-3.244877	2.261092	-1.843815
H	-3.095264	1.917821	-3.565123
H	-4.318548	6.623102	-6.527060
H	-2.931779	5.551372	-6.710962
H	-4.217870	5.167754	-5.552291
H	-4.727800	7.904038	-4.472859
H	-4.473562	6.482543	-3.444263
H	-3.056331	8.510202	-6.238147
H	-1.515035	7.663543	-6.381799
H	1.211283	9.134877	-3.740965
H	1.614672	7.523562	-4.340942
H	0.184871	8.360845	-4.952543
H	-1.641651	8.138776	-1.561247
H	-0.516688	9.445009	-1.968612
H	-1.735519	8.941146	-3.133889
H	1.444818	8.255747	-1.497568
H	0.442919	6.947055	-0.856293
H	1.739423	6.597178	-2.013166
H	0.913444	7.404340	-8.661782
H	0.020917	6.198128	-7.740553
H	1.584514	5.571811	-10.260123
H	2.481260	4.150776	-9.703627
H	0.765793	4.342796	-9.290624
H	3.320162	7.054780	-9.278158
H	3.723048	6.987290	-7.554775
H	4.228771	5.675496	-8.628645
H	4.011714	3.486628	-1.552324
H	2.417444	3.930106	-2.170394
H	3.092521	2.340974	-2.531206
H	6.033034	3.583978	-3.021138
H	5.374520	2.313084	-4.048665
H	5.874730	3.845693	-4.766376
H	4.831253	5.556692	-2.409652
H	4.840027	5.981288	-4.124118
H	3.331272	6.048653	-3.196319
H	3.457601	-0.486791	-4.458156
H	4.089819	0.992841	-3.759947
H	2.346141	0.678463	-3.739304
H	4.686075	-0.043812	-6.534479
H	4.288816	1.353251	-7.553672
H	5.241337	1.577817	-6.085496
H	2.306258	-0.658343	-6.452039
H	1.065428	0.446351	-5.861857
H	1.822004	0.702220	-7.453471
H	-0.301347	0.829761	-3.684098
H	0.778505	2.160603	-3.373106
F	-1.093794	3.046470	-10.571726
F	-0.238945	1.552034	-9.266150
F	-2.171746	1.222116	-10.168442
H	-1.842711	0.777277	-5.397180
H	-0.516432	1.692196	-6.257317
H	-1.941293	2.602074	-5.375345

Methyl transfer / Metallacycle / Product

E = -1748.621081
G = -1747.803810

C	1.920442	-2.036286	2.099438
C	1.991356	-0.793218	2.771179
C	2.148485	0.283938	1.833850
C	2.122240	-0.320929	0.515423
C	1.938854	-1.722446	0.719866
Ce	-0.579735	-0.773965	1.562916
O	-1.677780	-2.833916	0.440789
S	-1.900809	-2.225253	-0.946584
C	-0.922212	-3.367148	-2.095509
C	2.671604	1.638921	2.363478
C	2.398936	2.863867	1.479994
C	2.453122	0.216515	-0.896950
C	1.491484	1.312107	-1.392317
C	2.033774	-3.440230	2.694094
C	0.705133	-4.207920	2.602109
C	-2.233438	-0.155741	3.887772
C	-1.784143	1.077284	3.311965
C	-2.426005	1.315423	2.073145
C	-3.229787	0.174813	1.838968
C	-3.186355	-0.722711	2.950026
C	-1.812360	-0.548262	5.320124
C	-3.007032	-0.532778	6.294293
C	-2.486902	2.618785	1.280662
C	-1.982814	2.430290	-0.158332
C	-4.346425	-1.743671	3.091391
C	-5.499618	-0.986084	3.796331
O	-1.153290	-0.889239	-0.959189

O	-3.272581	-2.234870	-1.493138
C	-3.957338	3.082969	1.229988
C	-1.667156	3.718180	1.968087
C	-4.894090	-2.165688	1.712725
C	-4.074201	-3.038846	3.889958
C	-3.183881	-4.082630	3.222305
C	-1.110471	-1.915878	5.365783
C	-0.800893	0.466629	5.886950
C	2.063443	1.971869	3.739252
C	4.198407	1.502731	2.572501
C	3.104330	-4.223105	1.908593
C	2.478687	-3.374132	4.162419
C	3.912528	0.714694	-0.948582
C	2.364437	-0.911499	-1.943835
H	2.067237	-0.679480	3.844723
H	-1.133748	1.779487	3.812782
H	1.911185	-2.455303	-0.073626
H	-3.884081	0.052663	0.985443
F	-1.586511	-4.499580	-2.241805
F	-0.770559	-2.786379	-3.273426
F	0.271565	-3.632177	-1.582224
H	1.835333	1.701713	-2.357865
H	0.492151	0.896111	-1.550913
H	1.412352	2.156606	-0.709546
H	4.178190	0.975978	-1.979536
H	4.088816	1.597949	-0.334153
H	4.598523	-0.070293	-0.613318
H	2.587765	-0.497051	-2.932568
H	3.085546	-1.712539	-1.753459
H	1.362053	-1.341112	-1.989194
H	-2.092888	3.357441	-0.732938
H	-0.919367	2.166292	-0.176572
H	-2.533333	1.643492	-0.683037
H	-1.717914	4.645097	1.386837
H	-2.050560	3.930786	2.971453
H	-0.611224	3.446473	2.062705
H	-4.035799	4.043783	0.707650
H	-4.586750	2.361499	0.700716
H	-4.362659	3.207626	2.239211
H	2.752101	3.765531	1.992605
H	2.910846	2.823361	0.519177
H	1.329218	2.994308	1.290275
H	4.615164	2.438229	2.965099
H	4.418210	0.705481	3.289491
H	4.719473	1.263848	1.643237
H	2.469181	2.923582	4.099317
H	0.976714	2.075609	3.681136
H	2.297441	1.221681	4.498724
H	2.593193	-4.386432	4.565021
H	3.440257	-2.860172	4.260218
H	1.751091	-2.853818	4.792728
H	3.250124	-5.214076	2.353861
H	2.814040	-4.369467	0.863912
H	4.064068	-3.696993	1.921583
H	0.817730	-5.232786	2.975306
H	-0.069490	-3.734034	3.216005
H	0.340915	-4.267363	1.571728
H	-5.660450	-2.936455	1.853694
H	-5.378419	-1.335994	1.190763
H	-4.123189	-2.573721	1.058562
H	-6.396559	-1.616277	3.829974
H	-5.249962	-0.700888	4.820041
H	-5.747695	-0.072821	3.247018
H	-5.053436	-3.498154	4.081957
H	-3.679436	-2.793674	4.878407
H	-0.484777	0.142389	6.884087
H	0.095120	0.541725	5.264774
H	-1.234897	1.466093	5.989563
H	-2.650875	-0.682828	7.320240
H	-3.523368	0.431628	6.254835
H	-3.736965	-1.315758	6.087754
H	-0.844579	-2.181444	6.396081
H	-1.720322	-2.723571	4.961983
H	-0.176353	-1.875741	4.792678
H	-2.967894	-4.905149	3.912754
H	-3.654115	-4.511969	2.333852
H	-2.228665	-3.663450	2.895635

Methyl transfer / Cp'_2CeOMe / Adduct of $MeOSO_2CF_3$

E = -1864.256516
G = -1863.392680

C	-0.372155	0.392100	0.906543
C	-0.309312	0.020106	2.290554
C	1.095100	-0.056119	2.624248
C	1.811861	0.281344	1.430523
C	0.925502	0.617170	0.387356
Ce	0.708814	-2.240729	0.554818
O	3.146470	-3.380965	1.533856
S	4.557693	-3.385740	2.011882
C	5.378159	-4.938141	1.285349
F	4.905672	-5.996181	1.907301
C	-1.596240	0.124310	3.137384
C	-2.837418	-0.241011	2.298172
C	1.852498	-0.208553	3.962369
C	1.673518	-1.592064	4.614238
C	1.273485	1.355357	-0.899573
C	2.755052	1.179565	-1.257977
C	-0.417643	-4.249604	-1.139272
C	-1.507534	-3.386495	-0.898092
C	-1.850241	-3.583161	0.465319
C	-1.030209	-4.590112	1.053403
C	-0.091686	-5.005312	0.025114
C	-2.377745	-2.720523	-1.959187
C	-3.513591	-3.708470	-2.306596
C	-1.337984	-5.132117	2.464108
C	-0.207521	-4.832697	3.466350
C	0.892301	-6.185776	-0.113791
C	1.660498	-6.566582	1.160466
O	4.902125	-3.362041	3.437898
O	5.430713	-2.220125	1.287495
C	5.111827	-1.847603	-0.088485
C	-3.009984	-1.416937	-1.453934
C	-1.584561	-2.430893	-3.241110
C	-2.613096	-4.476588	3.029757
C	-1.646021	-6.642607	2.435999
C	0.114136	-7.419992	-0.622206
C	1.967629	-5.863239	-1.173891
C	-1.652440	-0.763708	4.388346
C	-1.775529	1.601274	3.560686
C	3.367880	-0.021381	3.750181
C	1.451739	0.899795	4.958030
C	0.419639	0.877041	-2.081393
C	0.995723	2.856225	-0.666821
F	5.120192	-5.017052	-0.006394
F	6.679084	-4.847275	1.474917
O	2.080334	-2.163947	-1.166167
H	4.040291	-1.948397	-0.298672
H	5.414758	-0.803607	-0.158749
H	5.711308	-2.460872	-0.763889
H	0.071117	-4.361466	-2.097092
H	-2.702085	-3.128114	0.950147
H	2.888042	0.360850	1.364366
H	-1.290197	0.628904	0.384447
H	1.254254	3.441268	-1.558282
H	-0.061088	3.030551	-0.440149
H	1.584998	3.235304	0.174428
H	2.982991	1.701888	-2.194165
H	3.405775	1.599170	-0.482861
H	2.989645	0.118916	-1.380970
H	0.645123	1.461366	-2.981317
H	0.623457	-0.174831	-2.301075
H	-0.650390	0.989147	-1.879172
H	-2.703404	1.725689	4.132966
H	-0.947765	1.957827	4.176547
H	-1.831728	2.245540	2.677664

H	-3.733316	-0.195021	2.927084
H	-2.996773	0.448950	1.465857
H	-2.761067	-1.251157	1.888878
H	-2.633720	-0.661954	4.865755
H	-1.518110	-1.820148	4.138558
H	-0.906849	-0.497784	5.137154
H	2.214958	-1.637817	5.566707
H	0.630156	-1.832500	4.816475
H	2.088078	-2.378085	3.974481
H	2.090669	0.850432	5.847857
H	1.581680	1.887835	4.504450
H	0.418998	0.821076	5.296741
H	3.887827	-0.158543	4.703912
H	3.784318	-0.748666	3.050055
H	3.603828	0.981969	3.382286
H	-3.671418	-0.992504	-2.218012
H	-3.610239	-1.580705	-0.553716
H	-2.246726	-0.670060	-1.217469
H	-4.167487	-3.291730	-3.082675
H	-3.105693	-4.655400	-2.674147
H	-4.125970	-3.926779	-1.425908
H	-2.231982	-1.956005	-3.986713
H	-0.741829	-1.759323	-3.053479
H	-1.192198	-3.350107	-3.687550
H	-0.452833	-5.227650	4.459835
H	0.750240	-5.260264	3.167946
H	-0.073875	-3.750122	3.578028
H	-1.954429	-6.978285	3.433273
H	-2.466677	-6.852063	1.742200
H	-0.794309	-7.252613	2.137407
H	-2.805717	-4.866483	4.035041
H	-2.524109	-3.390516	3.113251
H	-3.488454	-4.700691	2.412178
H	2.373490	-7.366609	0.930786
H	2.226780	-5.716165	1.548377
H	1.017423	-6.935486	1.958728
H	0.795267	-8.265952	-0.778373
H	-0.660648	-7.735629	0.080070
H	-0.374665	-7.196218	-1.575584
H	2.700577	-6.676957	-1.211494
H	1.546390	-5.769667	-2.178160
H	2.494725	-4.933092	-0.942708
C	2.461079	-2.433043	-2.474723
H	3.464460	-2.891968	-2.519044
H	1.773060	-3.129775	-2.978576
H	2.501366	-1.515587	-3.085554

Methyl transfer / Cp'$_2$CeOMe / TS

E = -1864.216449
G = -1863.349315

C	-0.331752	0.339710	0.887453
C	-0.260024	-0.015931	2.277917
C	1.144485	-0.037366	2.617558
C	1.852787	0.308275	1.420101
C	0.957188	0.610541	0.371010
Ce	0.803614	-2.242872	0.579051
O	3.066313	-3.445185	1.993875
S	4.566700	-3.343133	2.207367
C	5.214302	-5.092956	1.908148
F	4.646374	-5.934575	2.754321
C	-1.549297	0.081029	3.124112
C	-2.786114	-0.311138	2.292114
C	1.901693	-0.138166	3.961894
C	1.756416	-1.510018	4.645996
C	1.276539	1.391021	-0.898949
C	2.756102	1.262749	-1.285265
C	-0.315656	-4.184979	-1.188987
C	-1.408330	-3.332122	-0.919268
C	-1.731272	-3.557618	0.444461
C	-0.908871	-4.582300	1.000193
C	0.015068	-4.976637	-0.047230
C	-2.320956	-2.682166	-1.955660
C	-3.426344	-3.710233	-2.286801
C	-1.195333	-5.142976	2.408989
C	-0.048198	-4.850753	3.394242
C	0.976854	-6.169841	-0.225607
C	1.766156	-6.577778	1.026222
O	5.056373	-2.968975	3.547559
O	5.252823	-2.568825	1.037767
C	3.980622	-2.221337	-0.247064
C	-2.990051	-1.407815	-1.425914
C	-1.571472	-2.349733	-3.252230
C	-2.463858	-4.497260	3.000131
C	-1.503248	-6.653137	2.368559
C	0.163100	-7.380204	-0.736314
C	2.031295	-5.855709	-1.307858
C	-1.591123	-0.784932	4.390917
C	-1.748558	1.563397	3.520211
C	3.410804	0.094527	3.750175
C	1.461119	0.981864	4.927801
C	0.413850	0.937446	-2.083596
C	0.971622	2.877121	-0.608675
F	4.937548	-5.465189	0.664150
F	6.522178	-5.107174	2.083432
O	2.220036	-2.044945	-1.287736
H	3.512929	-1.497431	0.397068
H	4.645033	-1.825203	-1.005579
H	3.697499	-3.253195	-0.312583
H	0.155351	-4.286879	-2.156814
H	-2.581340	-3.119382	0.946743
H	2.922120	0.463198	1.371644
H	-1.256060	0.543581	0.363553
H	1.206889	3.496854	-1.482668
H	-0.085142	3.022530	-0.362482
H	1.565419	3.239033	0.236767
H	2.959112	1.839601	-2.194508
H	3.413720	1.651359	-0.500513
H	3.010264	0.216651	-1.473286
H	0.617357	1.556069	-2.965293
H	0.632203	-0.101884	-2.344401
H	-0.655132	1.024773	-1.864200
H	-2.679131	1.682453	4.088819
H	-0.928174	1.943497	4.130925
H	-1.814810	2.191158	2.626044
H	-3.680182	-0.273831	2.923682
H	-2.959324	0.369168	1.454646
H	-2.694706	-1.322832	1.891992
H	-2.573930	-0.689324	4.866100
H	-1.439264	-1.843860	4.162762
H	-0.849646	-0.492930	5.133546
H	2.286232	-1.509689	5.605782
H	0.717526	-1.773509	4.844310
H	2.202372	-2.298260	4.033934
H	2.109328	0.980325	5.811817
H	1.549223	1.962953	4.449477
H	0.435933	0.870145	5.280295
H	3.929478	-0.012003	4.707919
H	3.860286	-0.630943	3.070035
H	3.615398	1.101265	3.371841
H	-3.687915	-1.007347	-2.169934
H	-3.558919	-1.597623	-0.510876
H	-2.249233	-0.633615	-1.208787
H	-4.111931	-3.310849	-3.044156
H	-2.992876	-4.638456	-2.672278
H	-4.010840	-3.958250	-1.395185
H	-2.260696	-1.916449	-3.985317
H	-0.771826	-1.623924	-3.079815
H	-1.133119	-3.243901	-3.706981
H	-0.271398	-5.268749	4.383270
H	0.909826	-5.256853	3.069644
H	0.076346	-3.769015	3.530509
H	-1.798243	-6.996607	3.366931
H	-2.334070	-6.856225	1.684937
H	-0.656103	-7.261226	2.054934
H	-2.639465	-4.899607	4.003367
H	-2.377542	-3.412157	3.096810

H	-3.348570	-4.717192	2.394203
H	2.470541	-7.376622	0.769806
H	2.341374	-5.737791	1.420159
H	1.135115	-6.957266	1.828832
H	0.824704	-8.236676	-0.914857
H	-0.603686	-7.689350	-0.023053
H	-0.338891	-7.135551	-1.677839
H	2.743986	-6.683963	-1.378059
H	1.590342	-5.727183	-2.299726
H	2.595271	-4.948391	-1.070939
C	2.396882	-2.332349	-2.645117
H	3.033818	-3.219925	-2.793993
H	1.439300	-2.534107	-3.142153
H	2.871641	-1.489529	-3.172321

Methyl transfer / Cp'_2CeOMe / Adduct of CH_3OCH_3

E = -1864.294808
G = -1863.426832

C	-0.278289	0.301188	0.876147
C	-0.253864	-0.028116	2.269972
C	1.145460	-0.044373	2.656098
C	1.893056	0.268731	1.478597
C	1.027819	0.548543	0.391649
Ce	0.885600	-2.294443	0.711740
O	2.855246	-3.435438	1.638336
S	4.223001	-3.356528	2.374619
C	5.139952	-4.880494	1.722738
F	4.664124	-5.990161	2.265041
C	-1.567929	0.114633	3.074442
C	-2.786317	-0.288653	2.222358
C	1.844996	-0.112105	4.032919
C	1.643160	-1.456150	4.755739
C	1.361979	1.374005	-0.848071
C	2.842760	1.273916	-1.232628
C	-0.269050	-4.186668	-1.120206
C	-1.354190	-3.322567	-0.842332
C	-1.670040	-3.554744	0.520029
C	-0.861917	-4.602240	1.061731
C	0.047216	-5.003071	0.008856
C	-2.288510	-2.693359	-1.874272
C	-3.351501	-3.762093	-2.217431
C	-1.154686	-5.174744	2.464462
C	0.005595	-4.929013	3.447005
C	0.987707	-6.209351	-0.192151
C	1.755365	-6.667855	1.054082
O	4.115263	-3.598105	3.833851
O	5.051535	-2.217022	1.880526
C	3.975129	-2.206149	-1.176749
C	-3.008542	-1.452047	-1.335211
C	-1.560929	-2.313072	-3.169936
C	-2.402158	-4.505705	3.073701
C	-1.505175	-6.674926	2.396601
C	0.151521	-7.385630	-0.744018
C	2.062174	-5.882381	-1.251332
C	-1.664687	-0.704716	4.368732
C	-1.754938	1.613590	3.410381
C	3.364926	0.093710	3.879519
C	1.378271	1.047753	4.938566
C	0.502258	0.978882	-2.055415
C	1.056915	2.847999	-0.496678
F	5.031848	-4.970184	0.398508
F	6.421365	-4.766923	2.035603
O	2.555276	-2.206337	-1.382077
H	4.178564	-1.972172	-0.133665
H	4.441816	-1.452763	-1.822382
H	4.383789	-3.193477	-1.416775
H	0.176644	-4.315896	-2.097035
H	-2.513445	-3.114596	1.031116
H	2.969099	0.378025	1.456090
H	-1.183985	0.496019	0.318498
H	1.296097	3.504160	-1.342511
H	-0.000163	2.983179	-0.247509
H	1.648336	3.171389	0.365422
H	3.055073	1.927752	-2.085840
H	3.496373	1.583363	-0.411532
H	3.109075	0.253318	-1.513766
H	0.710324	1.636489	-2.907109
H	0.711980	-0.047544	-2.371266
H	-0.567292	1.056050	-1.836541
H	-2.693396	1.763956	3.957965
H	-0.940603	2.007240	4.020142
H	-1.799450	2.207335	2.491932
H	-3.698195	-0.195003	2.821664
H	-2.915244	0.349387	1.344784
H	-2.709846	-1.322917	1.882155
H	-2.664468	-0.584740	4.800970
H	-1.514392	-1.772111	4.183637
H	-0.950163	-0.393349	5.129275
H	2.102273	-1.418984	5.750530
H	0.592113	-1.711140	4.889358
H	2.136099	-2.270497	4.219558
H	1.995661	1.071452	5.843762
H	1.495695	2.009987	4.429071
H	0.340549	0.959676	5.259624
H	3.837399	0.002420	4.862919
H	3.837016	-0.642983	3.228180
H	3.596716	1.093151	3.495707
H	-3.715617	-1.070249	-2.080266
H	-3.576378	-1.673470	-0.427266
H	-2.297932	-0.653828	-1.104213
H	-4.056811	-3.380222	-2.965643
H	-2.882365	-4.666259	-2.618021
H	-3.920026	-4.046999	-1.326804
H	-2.279051	-1.943520	-3.910109
H	-0.831093	-1.515625	-2.999882
H	-1.049466	-3.171295	-3.618319
H	-0.213880	-5.378165	4.422871
H	0.956691	-5.330354	3.099307
H	0.143679	-3.854213	3.622384
H	-1.800980	-7.029612	3.390700
H	-2.347461	-6.840821	1.716746
H	-0.678200	-7.299473	2.062979
H	-2.578157	-4.915649	4.073659
H	-2.287835	-3.424302	3.183321
H	-3.298310	-4.696165	2.474420
H	2.450761	-7.468520	0.780056
H	2.337365	-5.848002	1.474770
H	1.110988	-7.063474	1.838047
H	0.795350	-8.252596	-0.935633
H	-0.630536	-7.694309	-0.046741
H	-0.333972	-7.107423	-1.685192
H	2.755931	-6.724793	-1.340363
H	1.634953	-5.717716	-2.244883
H	2.643602	-5.000413	-0.968018
C	2.263144	-2.409606	-2.761287
H	2.655072	-3.378031	-3.095081
H	1.183075	-2.392889	-2.889414
H	2.714338	-1.609632	-3.361498

Methyl transfer / Cp'_2CeF / Adduct of $MeOSO_2CF_3$

E = -1773.535824
G = -1772.710114

C	-0.298458	0.385495	0.979168
C	-0.309154	0.003714	2.362598
C	1.078648	-0.115714	2.758615
C	1.857017	0.201553	1.600650
C	1.029923	0.559801	0.517664
Ce	0.686630	-2.252249	0.720185
O	3.020531	-3.220630	1.701557
S	4.407968	-2.996697	1.188013
C	5.491276	-3.981482	2.389690
F	5.364837	-3.436918	3.583565

C	-1.627864	0.123123	3.155837
C	-2.841462	-0.201899	2.262577
C	1.774569	-0.309814	4.125819
C	1.545352	-1.703926	4.739386
C	1.468493	1.227526	-0.780913
C	2.981969	1.083785	-0.992348
C	-0.351920	-4.178859	-1.115364
C	-1.467834	-3.351780	-0.865234
C	-1.841445	-3.615771	0.479015
C	-1.013812	-4.631563	1.041942
C	-0.045658	-4.987701	0.018120
C	-2.322503	-2.661014	-1.923631
C	-3.458469	-3.637531	-2.301975
C	-1.313844	-5.211950	2.438699
C	-0.198133	-4.880980	3.447499
C	0.949247	-6.155582	-0.153776
C	1.766857	-6.525746	1.094605
O	4.973144	-1.644467	1.047276
O	4.706970	-3.922925	-0.112448
C	4.944269	-3.229697	-1.381158
C	-2.956350	-1.363473	-1.405557
C	-1.511255	-2.355264	-3.190501
C	-2.615745	-4.613202	3.006004
C	-1.555748	-6.732960	2.394135
C	0.172416	-7.399390	-0.641741
C	1.979808	-5.821717	-1.254150
C	-1.752959	-0.793687	4.380670
C	-1.791996	1.594399	3.602415
C	3.302277	-0.155110	3.981393
C	1.352927	0.785116	5.127020
C	0.747101	0.635047	-2.000242
C	1.121078	2.727581	-0.676439
F	5.101053	-5.237948	2.424208
F	6.745037	-3.906123	1.991247
F	2.212012	-2.189553	-0.872905
H	5.773290	-2.529894	-1.267471
H	5.213266	-4.040133	-2.057561
H	4.022417	-2.731584	-1.685063
H	0.176915	-4.220016	-2.057036
H	-2.712134	-3.196815	0.964532
H	2.937028	0.216513	1.571242
H	-1.183919	0.649029	0.414664
H	1.445841	3.262523	-1.577355
H	0.042407	2.877526	-0.562681
H	1.615702	3.182106	0.188202
H	3.273379	1.558800	-1.936189
H	3.546989	1.571472	-0.190959
H	3.268673	0.029475	-1.031529
H	1.017434	1.185067	-2.909615
H	1.036032	-0.410981	-2.144519
H	-0.341347	0.694761	-1.895883
H	-2.738423	1.727965	4.141068
H	-0.981308	1.919886	4.256943
H	-1.799605	2.257167	2.731448
H	-3.761460	-0.124273	2.852481
H	-2.942197	0.489119	1.422033
H	-2.783593	-1.217111	1.860926
H	-2.747612	-0.677589	4.826076
H	-1.640120	-1.846446	4.103669
H	-1.027138	-0.570966	5.162077
H	2.039143	-1.775369	5.716212
H	0.490817	-1.935395	4.888402
H	1.981926	-2.480960	4.101584
H	1.948807	0.701432	6.043786
H	1.526658	1.779304	4.702667
H	0.303969	0.724468	5.416426
H	3.773832	-0.311138	4.957899
H	3.729206	-0.882379	3.287801
H	3.578830	0.845381	3.635124
H	-3.613690	-0.928892	-2.167504
H	-3.560848	-1.538074	-0.510283
H	-2.194058	-0.619388	-1.156829
H	-4.095832	-3.206488	-3.083893
H	-3.049985	-4.582162	-2.674673
H	-4.087810	-3.863287	-1.435152
H	-2.143394	-1.851492	-3.930204
H	-0.657647	-1.705035	-2.979702
H	-1.131599	-3.271090	-3.654395
H	-0.413221	-5.320073	4.429550
H	0.781421	-5.241776	3.129523
H	-0.129441	-3.796572	3.597709
H	-1.872263	-7.088236	3.382015
H	-2.349699	-6.973980	1.680022
H	-0.669511	-7.301360	2.114289
H	-2.802570	-5.027518	4.002603
H	-2.566448	-3.525787	3.109856
H	-3.477325	-4.856251	2.376306
H	2.463013	-7.335395	0.846976
H	2.360635	-5.678089	1.447797
H	1.152844	-6.879341	1.922986
H	0.864006	-8.228417	-0.837556
H	-0.565790	-7.741891	0.085790
H	-0.359084	-7.173411	-1.571561
H	2.733560	-6.615810	-1.298814
H	1.520092	-5.762411	-2.244530
H	2.487879	-4.874694	-1.057609

Methyl transfer / Cp'_2CeF / TS

E = -1773.480092
G = -1772.652781

C	-0.293203	0.362833	0.939020
C	-0.248020	-0.058614	2.312604
C	1.154071	-0.127657	2.666801
C	1.884384	0.244497	1.492129
C	1.006061	0.619057	0.447438
Ce	0.769623	-2.235050	0.644955
O	3.172543	-3.222620	1.420587
S	4.669851	-3.109056	1.134998
C	5.390616	-4.742102	1.762051
F	5.047950	-4.893564	3.030175
C	-1.548813	0.034142	3.141059
C	-2.779748	-0.292797	2.270333
C	1.893393	-0.324450	4.010244
C	1.720664	-1.739476	4.592192
C	1.350967	1.471718	-0.770138
C	2.777941	1.227521	-1.280227
C	-0.112524	-4.349811	-1.026053
C	-1.225161	-3.486948	-0.935206
C	-1.699793	-3.622934	0.393852
C	-0.944445	-4.607055	1.105523
C	0.085986	-5.067119	0.194163
C	-1.960665	-2.827869	-2.096804
C	-3.120525	-3.764970	-2.499240
C	-1.411083	-5.106749	2.488758
C	-0.390768	-4.798327	3.598819
C	1.043718	-6.279400	0.200546
C	1.692868	-6.606601	1.554267
O	5.401369	-2.047902	1.860812
O	4.955981	-3.179007	-0.385243
C	3.386356	-2.416709	-1.222826
C	-2.552262	-1.468571	-1.698449
C	-1.039565	-2.643487	-3.311734
C	-2.731744	-4.422121	2.893148
C	-1.737567	-6.613725	2.468253
C	0.266452	-7.511847	-0.316312
C	2.214400	-6.066532	-0.779951
C	-1.633507	-0.886285	4.365648
C	-1.716533	1.502043	3.599051
C	3.409339	-0.111085	3.833547
C	1.456838	0.733174	5.044891
C	0.370140	1.251774	-1.929600
C	1.248287	2.944002	-0.309743
F	4.930508	-5.759181	1.056944
F	6.705064	-4.694477	1.659536
F	1.623515	-1.776838	-1.524565

H	3.457003	-1.581954	-0.548777
H	3.803099	-2.279723	-2.212905
H	2.907610	-3.354935	-1.015937
H	0.470609	-4.490627	-1.925867
H	-2.596855	-3.151418	0.770415
H	2.961901	0.337572	1.455621
H	-1.205909	0.605411	0.411866
H	1.476090	3.622264	-1.140947
H	0.240741	3.173073	0.051721
H	1.951715	3.150487	0.503339
H	3.024126	1.957161	-2.059700
H	3.523388	1.340338	-0.485982
H	2.866219	0.232084	-1.719667
H	0.622552	1.915277	-2.764680
H	0.416000	0.221054	-2.290285
H	-0.660515	1.479619	-1.638040
H	-2.655391	1.622195	4.153381
H	-0.899066	1.830035	4.243336
H	-1.745312	2.171046	2.733318
H	-3.682780	-0.272908	2.889827
H	-2.929815	0.433007	1.467022
H	-2.702391	-1.284935	1.818324
H	-2.611605	-0.767520	4.845253
H	-1.534050	-1.938039	4.085013
H	-0.879764	-0.667735	5.120850
H	2.260188	-1.826153	5.542771
H	0.677979	-1.994004	4.783944
H	2.145505	-2.489710	3.915141
H	2.077527	0.644982	5.944074
H	1.592838	1.742425	4.642635
H	0.417981	0.634989	5.358943
H	3.903949	-0.255790	4.800102
H	3.859448	-0.816604	3.133252
H	3.638505	0.905996	3.499459
H	-3.142298	-1.053335	-2.523433
H	-3.214392	-1.554318	-0.830727
H	-1.765473	-0.747729	-1.457710
H	-3.666512	-3.353356	-3.356667
H	-2.742844	-4.754000	-2.777490
H	-3.828845	-3.895461	-1.674642
H	-1.578930	-2.130838	-4.116016
H	-0.149992	-2.059787	-3.059169
H	-0.707065	-3.608898	-3.708433
H	-0.734277	-5.190962	4.563384
H	0.594007	-5.220614	3.399317
H	-0.271506	-3.716138	3.717486
H	-2.186129	-6.906660	3.424647
H	-2.459076	-6.839945	1.676497
H	-0.862873	-7.245080	2.316209
H	-3.030637	-4.770072	3.887684
H	-2.642599	-3.334478	2.943393
H	-3.541483	-4.666951	2.198534
H	2.410521	-7.424650	1.426481
H	2.240974	-5.745572	1.947562
H	0.977123	-6.930264	2.309199
H	0.923235	-8.389627	-0.347554
H	-0.592478	-7.754865	0.311210
H	-0.105393	-7.329848	-1.329697
H	2.853264	-6.955973	-0.783392
H	1.885337	-5.908584	-1.809943
H	2.844656	-5.227665	-0.474642