Supporting Information

Chloride-mediated Chain Generation of Difluorocarbene from Me_3SiCF_2Cl for Efficient Preparation of *gem*-Difluorinated Cyclopropenes and Cyclopropanes

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General remarks:

Unless otherwise mentioned, solvents and reagents were purchased from commercial sources and used as received. The solvent THF and toluene were distilled from sodium. Tetrabutylammonium fluoride (TBAF) [either as 1.0 M THF solution with 5wt% water content (for reactions in THF), or as solid TBAF hydrate (for reactions in toluene)] and tetrabutylammonium chloride (hydrate) were bought from commercial sources and were used as received. ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a 400 MHz or 300 MHz NMR spectrometer. ^{1}H NMR chemical shifts were determined relative to internal $(CH_3)_4Si$ (TMS) at δ 0.0 or to the signal of a residual protonated solvent: $CHCl_3$ δ 7.26. ^{13}C NMR chemical shifts were determined relative to internal TMS at δ 0.0. ^{19}F NMR chemical shifts were determined relative to $CFCl_3$ at δ 0.0. Mass spectra were obtained on a mass spectrometer in the EI, ESI or MALDI mode. High-resolution mass data were recorded on a high-resolution mass spectrometer in the EI, ESI or MALDI mode.

Preparation of $TMSCF_2Cl$ (1):

$TMSCF_2Cl$ (**1**) was prepared by using literature procedures.[1] Compound **1** was obtained as a colorless liquid, b.p. 81–82 °C. ^{1}H NMR: δ 0.29 (s, 9H). ^{19}F NMR: δ –62.2 (s, 2F). The characterization data were consistent with those in the literature.[1]

Typical procedures for [2 + 1] cycloaddition between 1 and alkynes 4:

1,2-Diphenylethyne (**4f**, 0.178 g, 1.0 mmol), $TMSCF_2Cl$ (0.317, 2.0 mmol), nBu$_4$NCl (0.011 g, 0.04 mmol), and toluene (3.0 mL) were added into a pressure tube at room temperature. Then the reaction mixture was heated at 110 °C for 4 h. The reaction was quenched by adding saturated Na_2CO_3 solution (5 mL), followed by extraction with Et_2O (20 mL x 2). The organic phase was separated and dried over anhydrous K_2CO_3. After the removal of solvent under vacuum, the residue was subjected to silica gel column chromatography with petroleum ether/Et_3N (40/1 v/v) as eluent [The column should be eluted previously with petroleum ether/Et_3N (10/1 v/v)]. The product (3,3-difluorocycloprop-1-ene-1,2-diyl)dibenzene (**5f**) was obtained as a white solid (213 mg, yield: 93%), m.p. 58–59 °C. ^{1}H NMR: δ 7.86–7.73 (m, 4H), 7.61–7.45 (m, 6H). ^{19}F NMR: δ –112.7 (s, 2F). MS (EI, *m/z*, %): 228 (M^+, 81.58), 178 (100.00). The characterization data were consistent with the previous report.[2]

Characterization date for the isolated compounds (5):

1-(3,3-Difluorocycloprop-1-enyl)-4-methylbenzene (**5d**). Light yellow solid. m.p. 39–40 °C. IR (film): 2926, 1800, 1631, 1609, 1507, 1454, 1317, 1297, 1283, 1181, 1106, 1024, 826, 772, 503, 475 cm^{-1}. ^1H NMR: δ 7.55 (d, *J* = 8.4 Hz, 2H), 7.37 (t, *J* = 2.1 Hz, 1H), 7.28 (d, *J* = 8.7 Hz, 2H), 2.42 (s, 3H). ^{19}F NMR: δ –106.9 (s, 2F). ^{13}C NMR: δ 142.3, 133.8 (t, *J* = 10.2 Hz), 130.1, 129.8, 120.6, 112.1 (t, *J* = 12.5 Hz), 101.9 (t, *J* = 268.1 Hz), 21.6. MS (EI, *m/z*, %): 166 (M^+, 72.08), 115 (100.00), 151 (94.84), 116 (41.65). HRMS (EI): calcd. for $C_{10}H_8F_2$: 166.0594; Found: 166.0591.

2-(3,3-Difluorocycloprop-1-enyl)-6-methoxynaphthalene (**5e**). White solid. m.p. 84–85 °C. IR (film): 3125, 2973, 1717, 1625, 1601, 1484, 1390, 1292, 1272, 1202, 1166, 1029, 1006, 902, 859, 823, 785, 738, 478 cm^{-1}. ^1H NMR: δ 8.12–7.13 (m, 7H), 3.95 (s, 3H). ^{19}F NMR: δ –106.8 (s, 2F). ^{13}C NMR: δ 159.4, 136.2, 133.9 (t, *J* = 10.2 Hz), 131.0, 130.3, 128.3, 127.7, 126.5, 118.8, 118.3, 112.2 (t, *J* = 12.5 Hz), 105.9, 102.0 (t, *J* = 269.0 Hz), 55.4. MS (EI, *m/z*, %): 232 (M^+, 74.42), 182 (100.00). HRMS (EI): calcd. for $C_{14}H_{10}OF_2$: 232.0700; Found: 232.0705. Anal. Calcd. for $C_{14}H_{10}OF_2$: C, 72.41; H, 4.34; Found: C, 72.36; H, 4.29.

1-Butyl-3,3-difluoro-2-octylcycloprop-1-ene (**5f**). Colorless liquid. IR (film): 2933, 2860, 1806, 1467, 1311, 1109, 998, 809 cm^{-1}. ^1H NMR: δ 2.43–2.34 (m, 4H), 1.68–1.50 (m, 4H), 1.48–1.19 (m, 12H), 1.01–0.81 (m, 6H). ^{19}F NMR: δ –106.6 (s, 2F). ^{13}C NMR: δ 128.75 (t, *J* = 10.6 Hz), 128.68 (t, *J* = 10.8 Hz), 105.4 (t, *J* = 269.2 Hz), 31.8, 29.3, 29.11, 29.06, 28.9, 22.8, 22.6, 22.5, 22.2, 14.0, 13.6, 0.9. HRMS (EI): calcd. for $C_{15}H_{26}F_2$: 244.2003; Found: 244.2002.

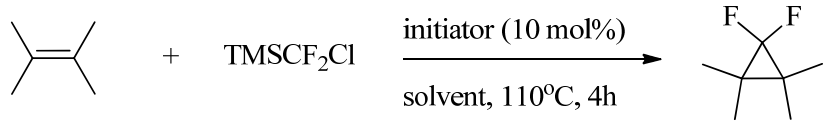
(3,3-Difluoro-2-phenylcycloprop-1-enyl)(phenyl)methyl acetate (**5h**). Light yellow solid. m.p. 39 °C. ^1H NMR: δ 7.52–7.37 (m, 10H), 6.89–6.84 (m, 1H), 2.20 (s, 3H). ^{19}F NMR: δ –108.1 (s, 2F). MS (EI, *m/z*, %): 257 (M^+ – COMe, 9.83), 105 (100.00), 43 (77.39), 258 (35.60). The characterization data were consistent with the previous report.[3]

(3,3-Difluoro-2-phenylcycloprop-1-enyl)methyl acetate (**5i**). Light yellow solid. m.p. 66–67 °C. ^1H NMR: δ 7.67–7.56 (m, 2H), 7.52–7.44 (m, 3H), 5.31–5.11 (m, 2H), 2.21 (s, 3H). ^{19}F NMR: δ –100.5 (s, 2F). MS (EI, *m/z*, %): 181 (M^+ – COMe, 39.15), 43 (100.00), 182 (35.43). The characterization data were consistent with the previous report. [3]

(2-Butyl-3,3-difluorocycloprop-1-enyl)benzene (**5j**). Colorless liquid. IR (film): 3064, 2962, 2935, 2876, 1888, 1797, 1467, 1450, 1320, 1283, 1006, 836, 765, 691, 612, 513, 447 cm^{-1}. ^1H NMR: δ 7.63–7.53 (m, 2H), 7.51–7.41 (m, 3H), 2.72–2.61 (m, 2H), 1.81–1.68 (m, 2H), 1.56–1.39 (m, 2H), 0.98 (t, *J* = 7.5 Hz, 3H). ^{19}F NMR: δ –109.4 (s, 2F). ^{13}C NMR: δ 130.4, 129.8, 128.9, 127.2 (t, *J* = 11.2 Hz), 125.8 (t, *J* = 10.9 Hz), 124.3, 103.7 (t, *J* = 269.8 Hz), 30.7, 23.2, 22.2, 13.6. MS (EI, *m/z*, %): 208 (M^+, 2.40), 115 (100.00), 165 (58.27), 129 (56.03). HRMS (EI): calcd. for $C_{13}H_{14}F_2$: 208.1064; Found: 208.1067.

(3,3-Difluoro-2-isobutylcycloprop-1-enyl)benzene (**5k**). Colorless liquid. IR (film): 2964, 1797, 1468, 1261, 1094, 1010, 869, 795, 763, 691 cm^{-1}. ^1H NMR: δ 7.62–7.54 (m, 2H), 7.49–7.41 (m, 3H), 2.62–2.53 (m, 2H), 2.17–2.00 (m, 1H), 1.06 (d, *J* = 6.0 Hz, 6H). ^{19}F NMR: δ –108.5 (s, 2F). ^{13}C NMR: δ 130.6, 129.8, 129.1, 126.6 (t, *J* = 12.6 Hz), 126.5 (t, *J* = 10.8 Hz), 124.5, 103.7 (t, *J* = 269.8 Hz), 32.7, 27.3, 22.3. HRMS (EI): calcd. for $C_{13}H_{14}F_2$: 208.1064; Found: 208.1063.

Survey of [2 + 1] cycloaddition reaction between 1 and alkenes 6:



6a (1.0 equiv) **1** (2.0 equiv) **7a**

entry[a]	solvent	initiator (10 mol%)[b]	yield (%)[b]
1	THF	*n*-Bu_4NCl	78
2	CH_3CN	*n*-Bu_4NCl	73
3	DMF	*n*-Bu_4NCl	50
4	toluene	*n*-Bu_4NCl	60
5	THF	None	0
6	THF	$MgCl_2$	0
7	THF	*n*-Bu_4NF	70
8	THF	*n*-Bu_4NCl	72
9[c]	**THF**	***n*-Bu_4NCl**	**80**

[a] Yields were determined by ^{19}F NMR spectroscopy using $PhCF_3$ as an internal standard. [b] The amount of initiator was caculated on the basis of the amountof reagent **1**. [c] 2 mol% of *n*-Bu_4NCl was usrd.

Typical procedure for [2 + 1] cycloaddition between 1 and alkenes 6:

1-Bromo-4-vinylbenzene (**6f**, 0.183 g, 1.0 mmol), $TMSCF_2Cl$ (0.476, 3.0 mmol), nBu_4NCl (0.022 g, 0.06 mmol), and THF (3.0 mL) were added into a pressure tube at room temperature. The reaction mixture was heated at 110 °C for 4 h. Then, the reaction was quenched by adding water (5 mL), followed by extraction with Et_2O (20 mL x 2). The organic phase was separated and dried over anhydrous $MgSO_4$. After the removal of solvent under vacuum, the residue was subjected to silica gel column chromatography with petroleum ether as eluent. The product 1-bromo-4-(2,2-difluorocyclopropyl) benzene (**7f**) was obtained as a colorless liquid (231 mg, yield: 99%). IR (film): 1495 147 1379 1419 1305 1232 1189 1041 1014 933 828 767 721 506 cm^{-1}. ^1H NMR: δ 7.46 (d, *J* = 8.4 Hz, 2H), 7.10 (d, *J* = 8.2 Hz, 2H), 2.78–2.62 (m, 1H), 1.91–1.76 (m, 1H), 1.65–1.51 (m, 1H). ^{19}F NMR: δ –126.6 (dtd, *J* = 154.9 Hz, *J* = 12.8 Hz, *J* = 3.8 Hz, 1F), δ –142.7 (ddd, *J* = 154.5 Hz, *J* = 13.0 Hz, *J* = 5.1 Hz, 1F). ^{13}C NMR: δ 132.7, 131.5, 129.7 (t, *J* = 1.9 Hz), 121.1, 112.2 (dd, *J* = 285.5 Hz, *J* = 286.7 Hz), 26.6 (t, *J* = 11.2 Hz), 17.1 (t, *J* = 11.4 Hz). MS (EI, *m/z*, %): 232 (M^+, 4.87), 153 (100.00), 234 (4.76), 133 (60.86). HRMS (EI): calcd. for $C_{13}H_{14}F_2$: 231.9699; Found: 231.9698.

Characterization date for the isolated compounds (7):

(2,2-Difluoro-1-methylcyclopropyl)benzene (**7b**). Colorless liquid. ^1H NMR: δ 7.38–7.26 (m, 5H), 1.73–1.63 (m, 1H), 1.54–1.50 (m, 3H), 1.45–1.35 (m, 1H). ^{19}F NMR: δ –131.7 (dd, *J* = 150.0 Hz, *J* = 13.2 Hz, 1F), δ –136.7 (dd, *J* = 150.0 Hz, *J* = 12.8 Hz, 1F). MS (EI, *m/z*, %): 168 (M^+, 28.30), 153 (100.00). The characterization data were consistent with the previous report.[4]

1-(2,2-Difluoro-1-methylcyclopropyl)-4-methoxybenzene (**7c**). Colorless liquid. ^1H NMR: δ 7.23 (d, *J* = 9.0 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H), 1.67–1.56 (m, 1H), 1.49 (s, 3H) , 1.41–1.30 (m, 1H). ^{19}F NMR: δ –133.1 (dd, *J* = 149.9 Hz, *J* = 13.4 Hz, 1F), δ –138.0 (dd, *J* = 149.7 Hz, *J* = 12.3 Hz, 1F). MS (EI, *m/z*, %): 198 (M^+, 25.39), 183 (100.00). The characterization data was consistent with the previous report.[5]

(2,2-Difluoro-1-pentylcyclopropyl)benzene (**7d**). Colorless liquid. IR (film): 3030 2931 2861 1605 1464 1447 1378 1311 1213 1151 1053 1016 960 905 700 640 cm^{-1}. ^1H NMR: δ 7.39–7.21 (m, 5H), 1.87–1.55 (m, 3H), 1.45–1.33 (m, 1H), 1.21 (s, 8H), 0.84 (t, *J* = 6.3 Hz, 3H). ^{19}F NMR: δ –130.7 (dd, *J* = 148.3 Hz, *J* = 13.5 Hz, 1F), δ –138.1 (dd, *J* = 148.9 Hz, *J* = 12.7 Hz, 1F). ^{13}C NMR: δ 129.44, 129.41, 128.3, 127.2,

125.8 (t, *J* = 287.4 Hz), 36.0 (dd, *J* = 9.7 Hz, *J* = 9.0 Hz), 34.6 (dd, *J* = 5.7 Hz, *J* = 2.8 Hz), 31.7, 29.1, 26.3 (d, *J* = 2.2 Hz), 22.6, 22.1 (t, *J* = 9.7 Hz), 14.0. MS (EI, *m/z*, %): 238 (M^+, 32.23), 153 (100.00), 167 (57.92). HRMS (EI): calcd. for $C_{15}H_{20}F_2$: 238.1533; Found: 238.1531.

(2,2-Difluorocyclopropyl)benzene (**7e**). Colorless liquid. ^{1}H NMR: δ 7.46–7.18 (m, 5H), 2.87–2.65 (m, 1H), 1.92–1.71 (m, 1H), 1.70–1.54 (m, 1H). ^{19}F NMR: δ 124.5–125.5 (m, 1F), 141.1–142.1 (m, 1F). MS (EI, *m/z*, %): 154 (M^+, 100.00), 133 (73.36). The characterization data was consistent with the previous report.[6]

4-((2,2-Difluorocyclopropyl)methyl)-1,2-dimethoxybenzene (**7g**). Colorless liquid. IR (film): 3006, 2939, 2837, 1592, 1517, 1473, 1286, 1265, 1239, 1197, 1158, 1144, 1024, 905, 801, 766 cm^{-1}. ^{1}H NMR: δ 6.85–6.74 (m, 3H), 3.88 (s, 3H), 3.87 (s, 3H), 2.84–2.65 (m, 2H), 1.86–1.68 (m, 1H), 1.54–1.40 (m, 1H), 1.14–1.01 (m, 1H). ^{19}F NMR: δ –127.5 (dt, *J* = 156.0 Hz, *J* = 13.3 Hz, 1F), δ –142.2 (ddd, *J* = 156.2 Hz, *J* = 13.4 Hz, *J* = 4.1 Hz, 1F). ^{13}C NMR: δ 149.0, 147.7, 132.2, 120.0, 114.4 (t, *J* =283.3 Hz), 111.5, 111.3, 55.9, 55.8, 32.4 (d, *J* = 3.6 Hz), 23.5 (t, *J* = 10.2 Hz), 16.3 (t, *J* = 10.9 Hz). MS (EI, *m/z*, %): 228 (M^+, 81.80), 151 (100.00), 187 (86.62). HRMS (EI): calcd. for $C_{12}H_{14}O_2F_2$: 228.0962; Found: 228.0960.

4-((2,2-Difluorocyclopropyl)methyl)-2-methoxyphenol (**7h**). Colorless liquid. IR (film): 3545, 3031, 2941, 2848, 1641, 1516, 1474, 1434, 1272, 1236, 1201, 1153, 1125, 1023, 904, 810, 561 cm^{-1}. ^{1}H NMR: δ 6.88–6.71 (m, 3H), 5.51 (s, 1H), 3.89 (s, 3H), 2.81–2.63 (m, 2H), 1.85–1.66 (m, 1H), 1.54–1.39 (m, 1H), 1.14–0.99 (m, 1H). ^{19}F NMR: δ –127.4 (dt, *J* = 156.4 Hz, *J* = 13.1 Hz, 1F), δ –142.2 (ddd, *J* = 156.0 Hz, *J* = 12.6 Hz, *J* = 4.3 Hz, 1F). ^{13}C NMR: δ 146.5, 144.2, 131.6, 120.8, 114.4, 114.4 (t, *J* =282.9 Hz), 110.7, 55.8, 32.5 (d, *J* = 4.4 Hz), 23.6 (t, *J* = 11.0 Hz), 16.3 (t, *J* = 10.9 Hz). MS (EI, *m/z*, %): 214 (M^+, 77.21), 173 (100.00). HRMS (EI): calcd. for $C_{11}H_{12}O_2F_2$: 214.0805; Found: 214.0806.

4-((2,2-Difluorocyclopropyl)methyl)-1-(difluoromethoxy)-2-methoxybenzene (**7i**). Colorless liquid. IR (film): 3018, 2944, 2851, 1600, 1515, 1475, 1423, 1385, 1127, 1036, 985, 970, 904, 802 cm^{-1}. ^{1}H NMR: δ 7.10 (d, *J* = 8.4 Hz, 1H), 6.86–6.85 (m, 3H), 3.88 (s, 3H), 2.77 (d, *J* = 7.8 Hz, 2H), 1.86–1.68 (m, 1H), 1.57–1.43 (m, 1H), 1.45–1.03 (m, 1H). ^{19}F NMR: δ –80.6 (d, *J* = 75.2 Hz, 2F), –127.6 (dt, *J* = 156.4 Hz, *J* = 13.8 Hz 1F), –142.1 (ddd, *J* = 156.8 Hz, *J* = 13.1 Hz, *J* = 3.2 Hz 1F). ^{13}C NMR: δ 151.1, 138.5, 122.4, 120.4, 116.2 (t, *J* = 258.4 Hz), 114.2 (t, *J* = 283.3 Hz), 112.6, 55.9, 32.6 (d, *J* = 2.3 Hz), 23.2 (t, *J* = 10.9 Hz), 16.3 (t, *J* = 11.0 Hz). MS (EI, *m/z*, %): 264 (M^+, 53.95), 137 (100.00). HRMS (EI): calcd. for $C_{12}H_{12}O_2F_4$: 264.0773; Found: 264.0769.

1-(3,3-Difluoro-2-phenylcycloprop-1-enyl)-4-(2,2-difluorocyclopropyl)benzene (**9**). White solid. m.p. 98–99 °C. IR (film): 1784, 1611, 1466, 1268, 1237, 1192, 1043, 995, 960, 845, 831, 769, 686, 605, 544, 492 cm^{-1}. ^1H NMR: δ 7.81–7.70 (m, 4H), 7.56–7.48 (m, 3H), 7.38 (d, *J* = 8.1 Hz, 2H), 2.88–2.73 (m, 1H), 1.98–1.83 (m, 1H), 1.76–1.63 (m, 1H). ^{19}F NMR: δ –112.7 (s, 2F), δ –126.1 (dtd, *J* = 154.4 Hz, *J* = 12.8 Hz, *J* = 3.8 Hz, 1F), δ –142.6 (ddd, *J* = 154.4 Hz, *J* = 13.6 Hz, *J* = 4.5 Hz, 1F). ^{13}C NMR: δ 155.9, 147.5, 147.2, 139.3, 132.9, 131.6, 131.5, 129.4, 128.9, 123.6, 122.4, 112.1 (t, *J* = 287.4 Hz), 127.3 (t, *J* = 11.0 Hz), 17.6 (t, *J* = 10.5 Hz). MS (EI, *m/z*, %): 304 (M^+, 46.56), 151 (100.00). HRMS (EI): calcd. for $C_{18}H_{12}F_4$: 304.0875; Found: 304.0872.

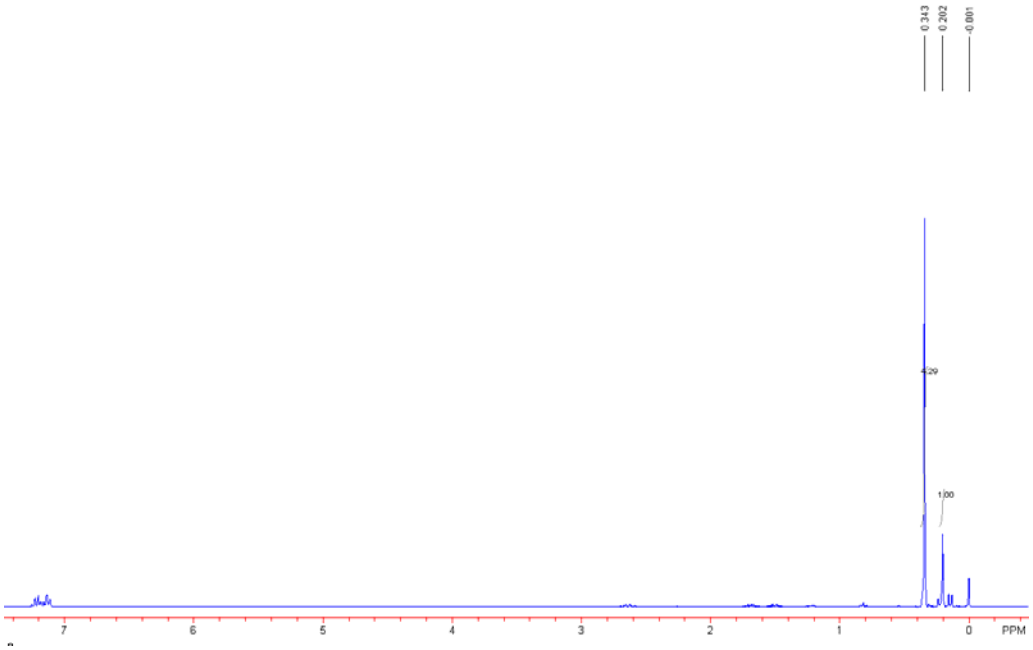
Typical procedure for difluoromethylation of phenols using compound 1:

A pressure tube was charged with 4-allyl-2-methoxyphenol (**6h**, 0.164 g, 1 mmol), aqueous KOH (25 wt.%, 0.8 mL) and toluene (2 mL). To this solution $TMSCF_2Cl$ (0.397 g, 2.5 mmol) was added at –78 °C, then the tube was sealed. The mixture was heated to 50 °C for 4h. Then the mixture was extracted with Et_2O (20 mL x 2), and the combined organic phase was separated and dried over $MgSO_4$. After the removal of solvents under vacuum, the crude product was further purified by silica gel column chromatography to give product 4-allyl-1-(difluoromethoxy)-2-methoxybenzene (**10**) as a colorless liquid (175 mg, yield: 82%). IR (film): 2980 1641 1599 1511 1467 1421 1382 1274 1216 1123 1935 919 cm^{-1}. ^1H NMR: δ 7.07 (d, *J* = 8.2 Hz, 1H), 6.80–6.25 (m, 3H), 6.02–5.87 (m, 1H), 5.14–5.10 (m, 1H), 5.09–5.06 (m, 1H), 3.86 (s, 3H), 3.36 (d, *J* = 6.9 Hz, 2H). ^{19}F NMR: δ –80.6 (d, *J* = 56.8 Hz, 2F). ^{13}C NMR: δ 150.9, 138.9, 136.9, 122.2, 120.2, 116.3 (t, *J* = 258.3 Hz), 112.9, 55.9, 39.9. MS (EI, *m/z*, %): 214 (M^+, 100.00), 91 (55.30), 147 (53.70). HRMS (EI): calcd. for $C_{11}H_{12}O_2F_2$: 214.0805 ; Found: 214.0807.

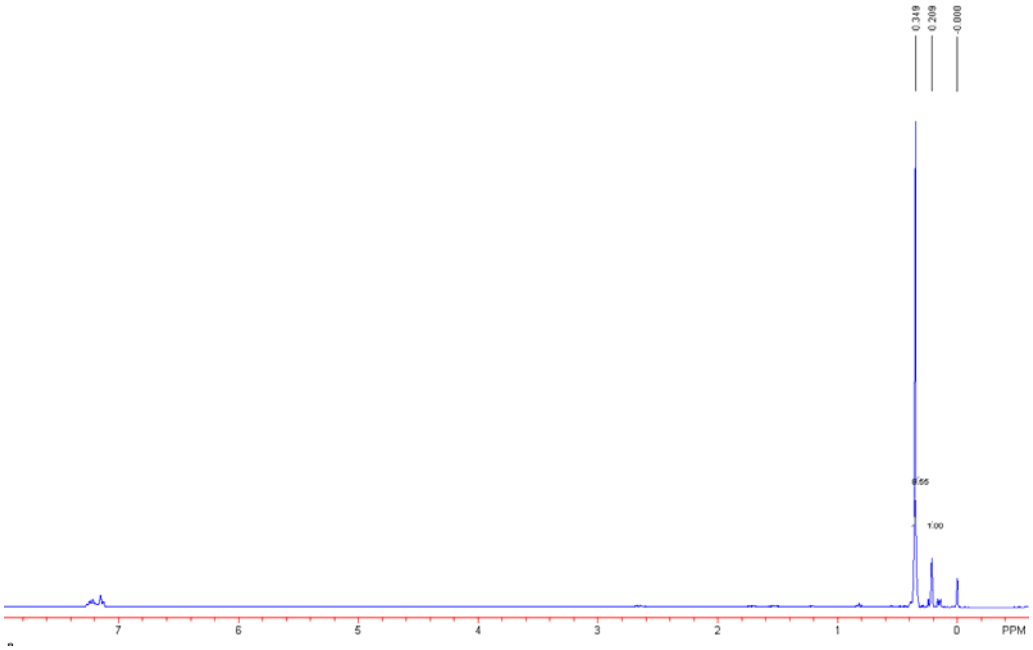
Determination of the formation of TMSCl in the [2 + 1] cycloaddition between $TMSCF_2Cl$ (1) and alkene (6b):

Styrene **6b** (0.104 g, 1.0 mmol), $TMSCF_2Cl$ (0.476, 3.0 mmol), and nBu$_4$NCl (0.022 g, 0.06 mmol) (without solvent) were mixed in a pressure tube at room temperature. Then reaction mixture was heated at 110 °C for 4 h. The reaction mixture was characterized by ^1H NMR spectroscopy. (After the authentic TMSCl was added to the mixture, the peak of TMSCl was identical with that observed in the reaction mixture).

A: ^{1}H NMR (from the reaction mixture):



B: ^{1}H NMR (the authentic TMSCl was added to the reaction mixture):



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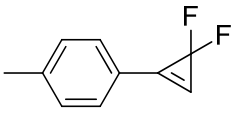
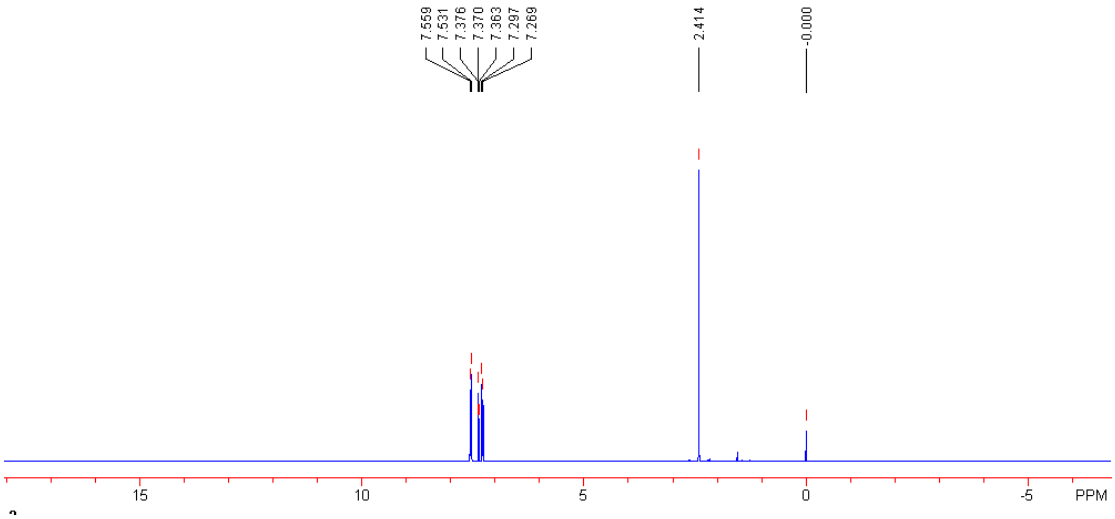
^{1}H, ^{19}F, and ^{13}C NMR spectra of all new products:

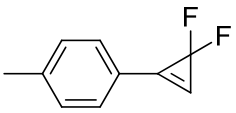
^{1}H NMR



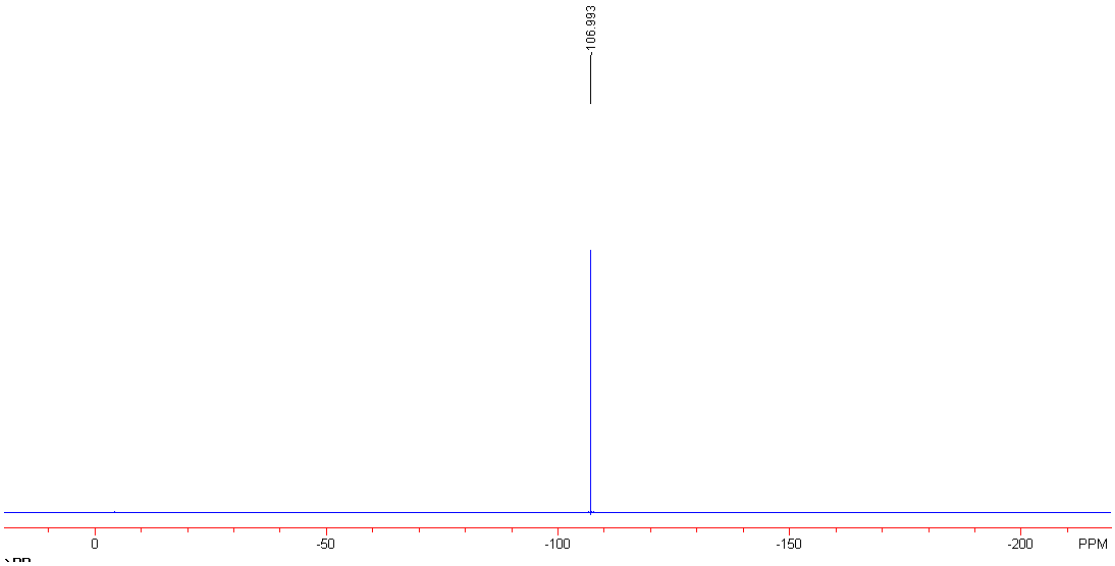
5d



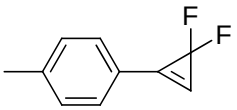
^{19}F NMR



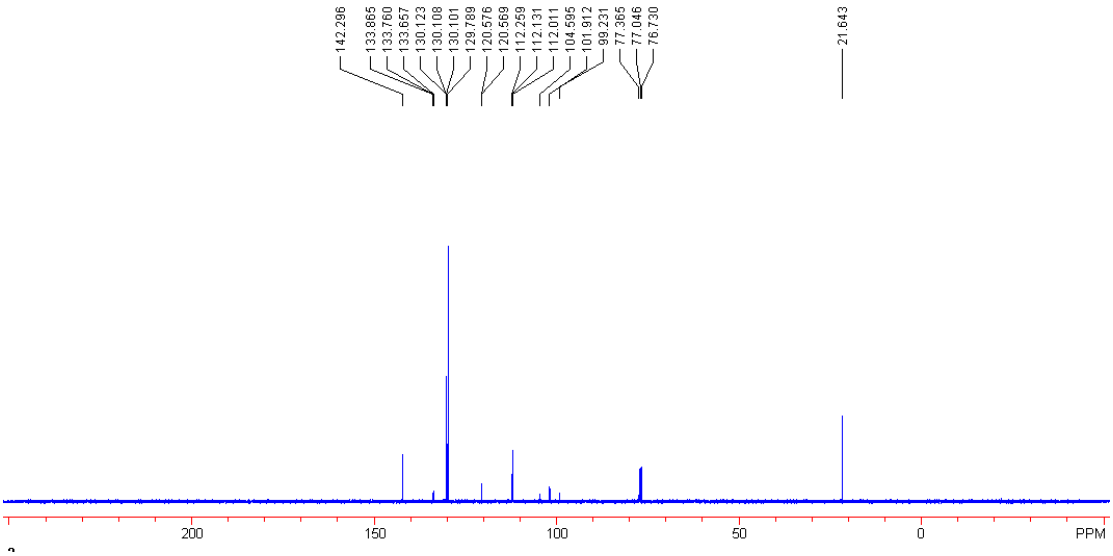
5d



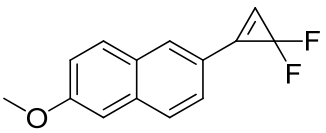
^{13}C NMR


F
F

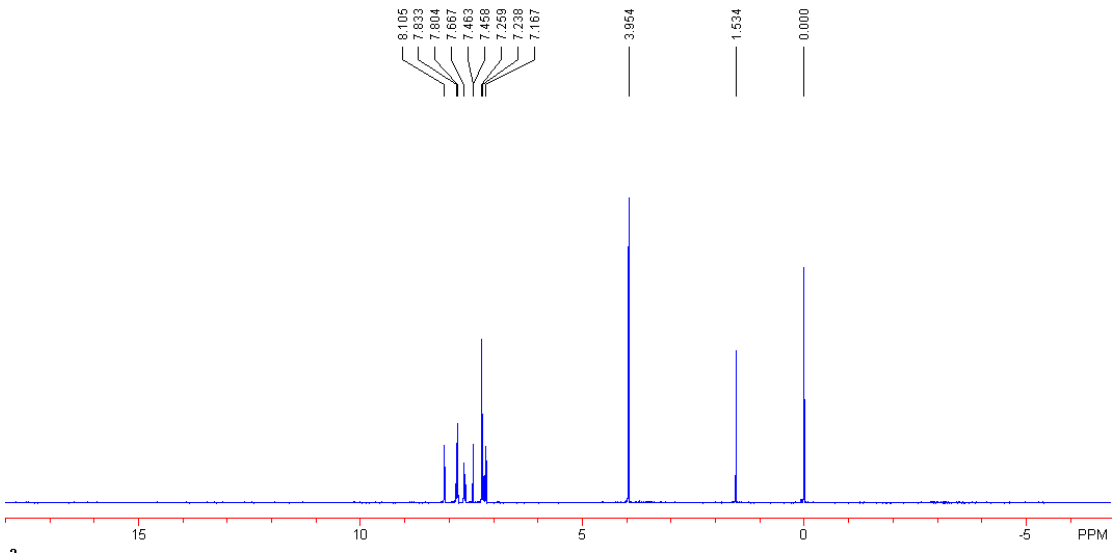
5d


142.296
133.865
133.760
133.657
130.123
130.108
130.101
129.789
120.576
120.569
112.259
112.131
112.011
104.595
101.912
99.231
77.365
77.046
76.730
21.643
200
150
100
50
0
PPM

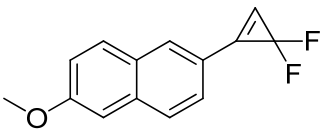
^{1}H NMR


F
F
O

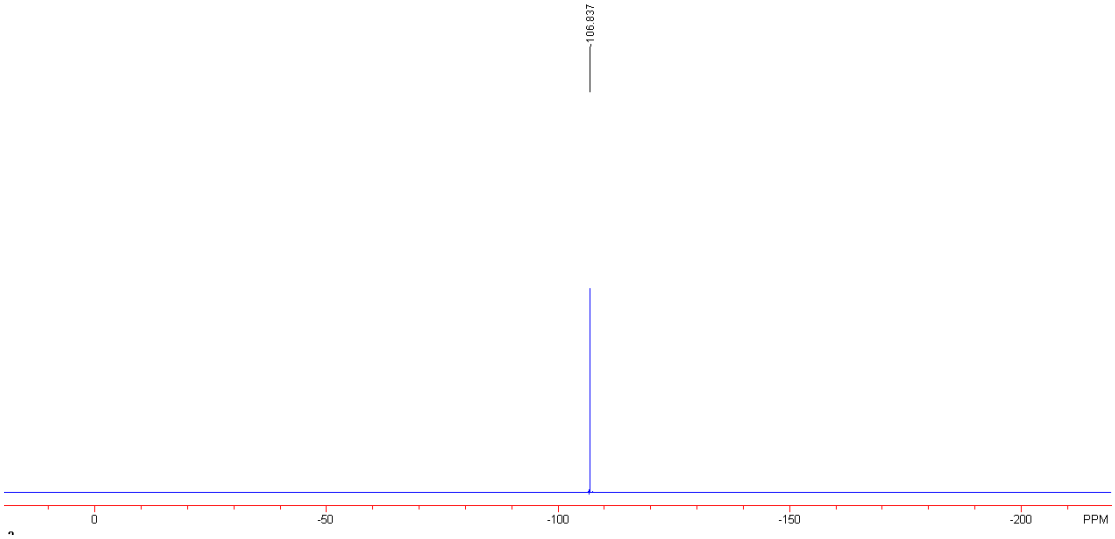
5e


8.105
7.833
7.804
7.667
7.463
7.458
7.259
7.238
7.167
3.954
1.534
0.000
15
10
5
0
-5
PPM

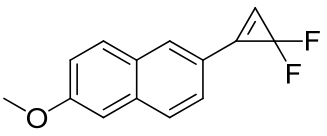
^{19}F NMR



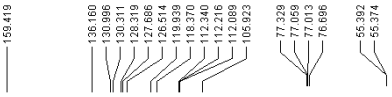
5e

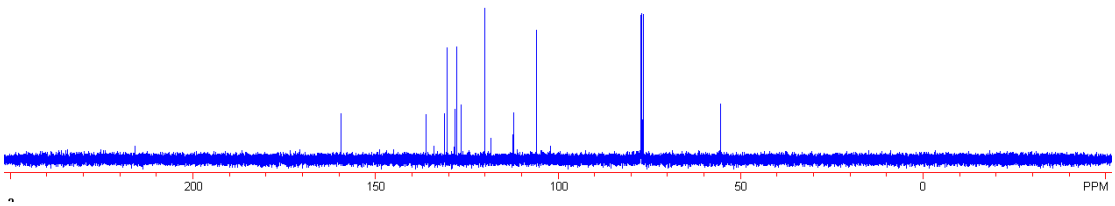


^{13}C NMR

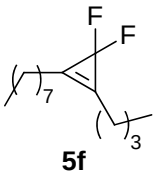

F
F
O

5e

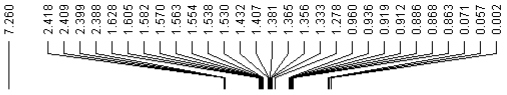

159.419
136.160
130.996
130.311
128.319
127.686
126.514
119.939
118.370
112.340
112.216
112.089
105.923
77.329
77.059
77.013
76.696
55.392
55.374

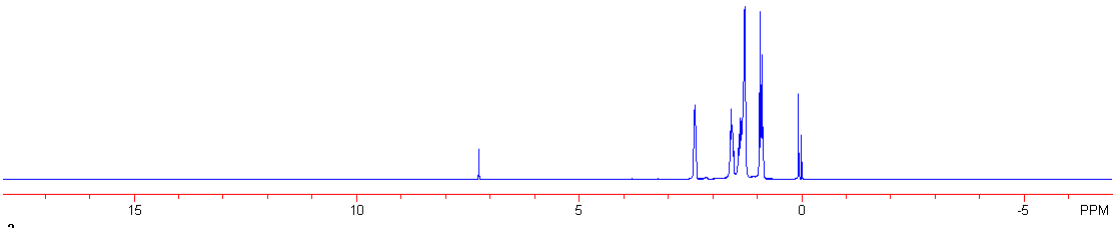

200
150
100
50
0
PPM

^{1}H NMR

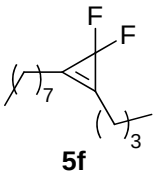

F
F
7
3

5f

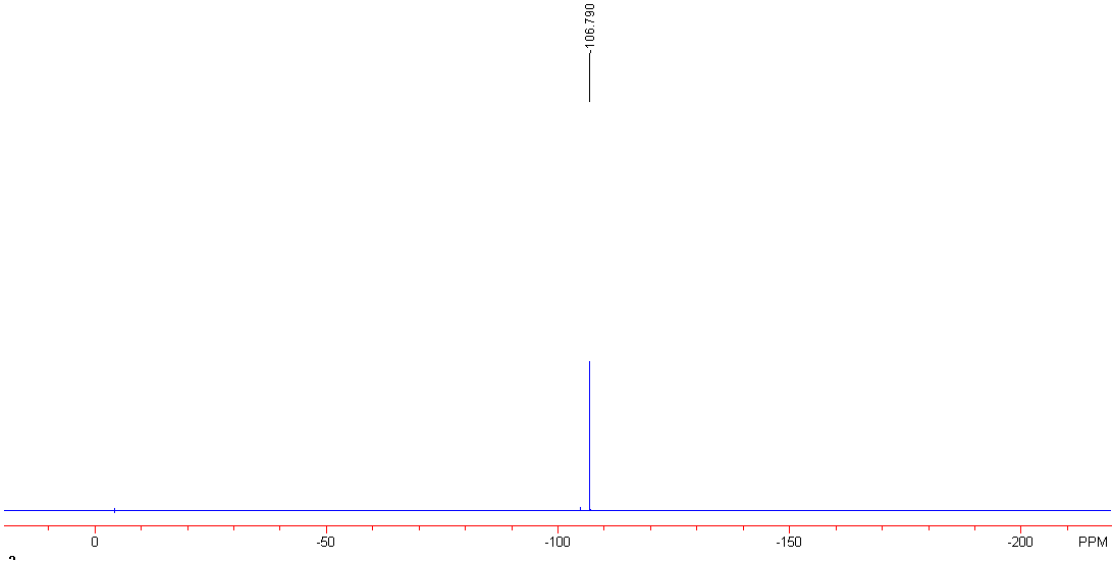

7.260
2.418
2.409
2.399
2.388
1.628
1.605
1.582
1.570
1.563
1.554
1.538
1.530
1.432
1.407
1.381
1.365
1.356
1.333
1.278
0.960
0.936
0.919
0.912
0.886
0.868
0.863
0.071
0.057
0.002


15
10
5
0
-5
PPM

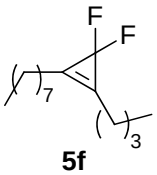
^{19}F NMR



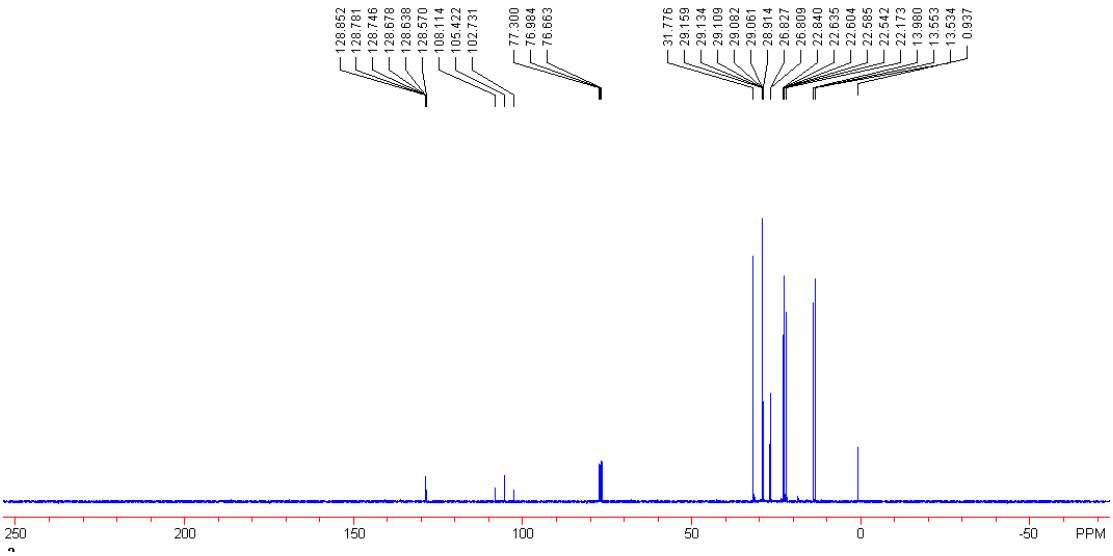
5f



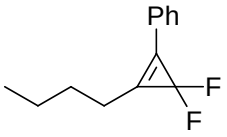
^{13}C NMR


F
F
7
3

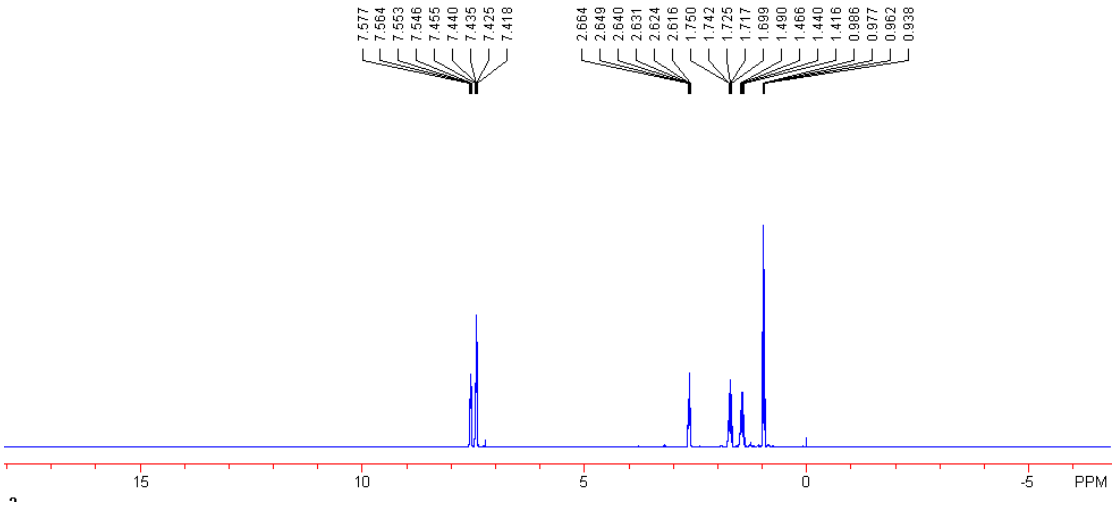
5f


128.852
128.781
128.746
128.678
128.638
128.570
108.114
105.422
102.731
77.300
76.984
76.663
31.776
29.159
29.134
29.109
29.082
29.061
28.814
26.827
26.809
22.840
22.635
22.604
22.585
22.542
22.173
13.980
13.553
13.534
0.937
250
200
150
100
50
0
-50
PPM

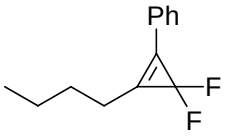
^{1}H NMR


Ph
F
F

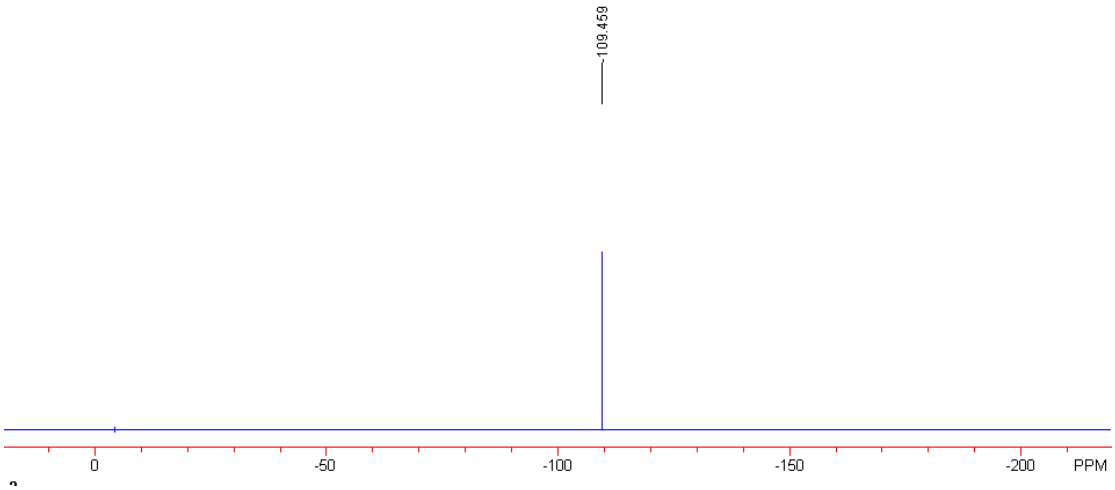
5j


7.577
7.564
7.553
7.546
7.455
7.440
7.435
7.425
7.418
2.664
2.649
2.640
2.631
2.624
2.616
1.750
1.742
1.725
1.717
1.699
1.490
1.466
1.440
1.416
0.986
0.977
0.962
0.938
15
10
5
0
-5
PPM

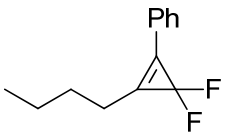
^{19}**F** NMR



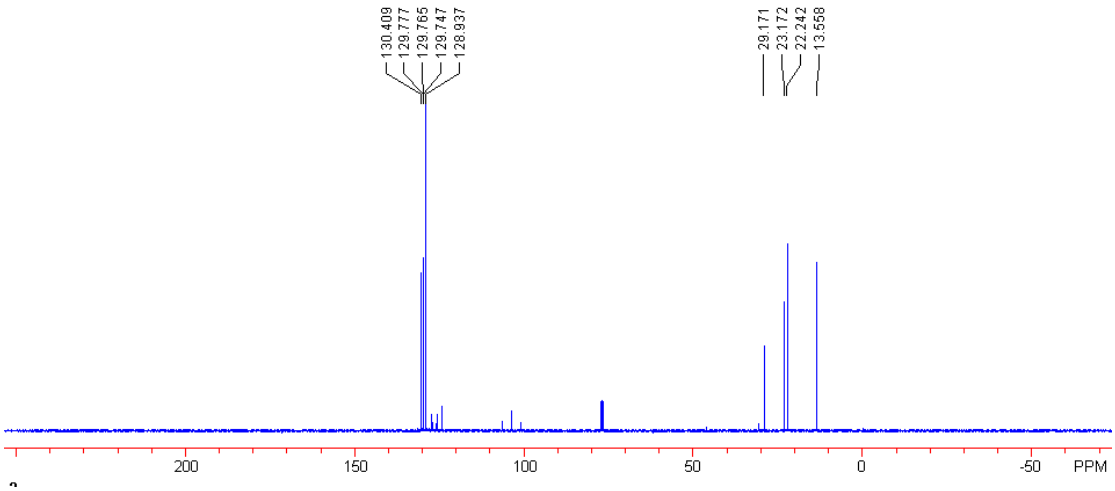
5j



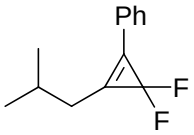
^{13}C NMR


Ph
F
F

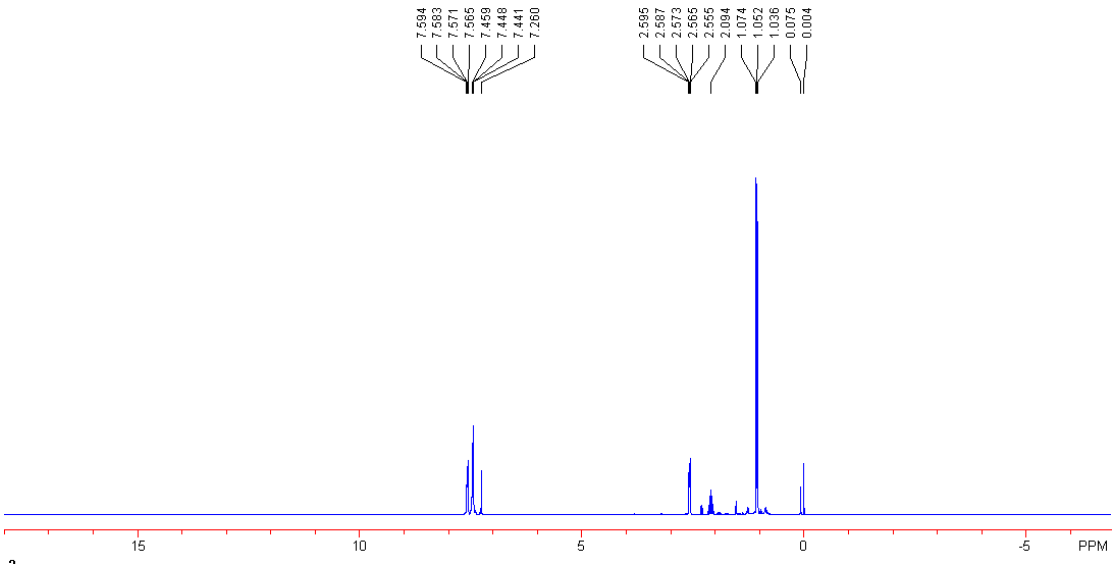
5j


130.409
129.777
129.765
129.747
128.937
29.171
23.172
22.242
13.558
200
150
100
50
0
-50
PPM

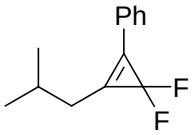
^{1}H NMR


Ph
F
F

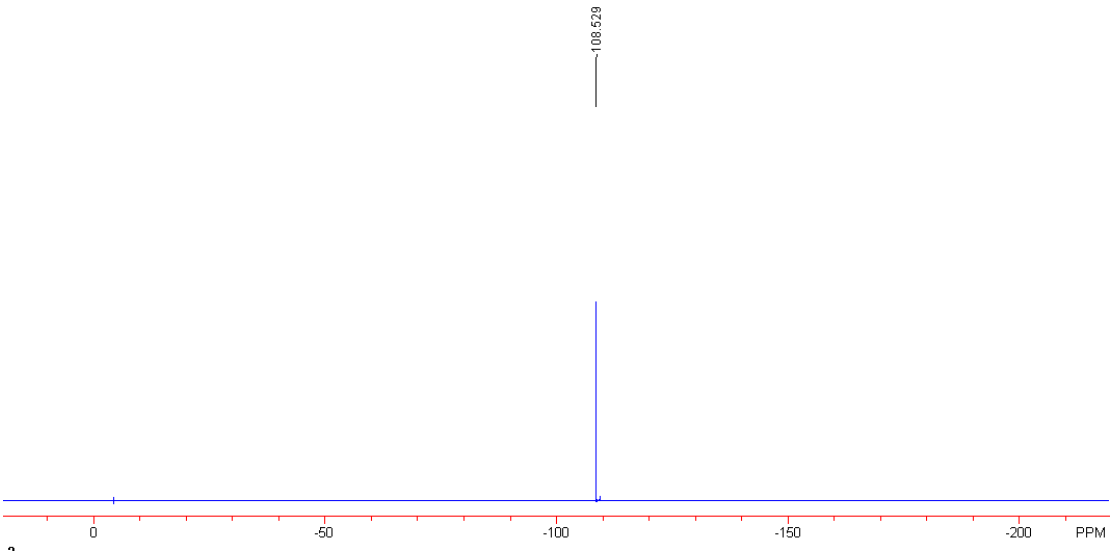
5k


7.594
7.583
7.571
7.565
7.459
7.448
7.441
7.260
2.595
2.587
2.573
2.565
2.555
2.094
1.074
1.052
1.036
0.075
0.004
15
10
5
0
-5
PPM

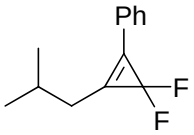
^{19}F NMR



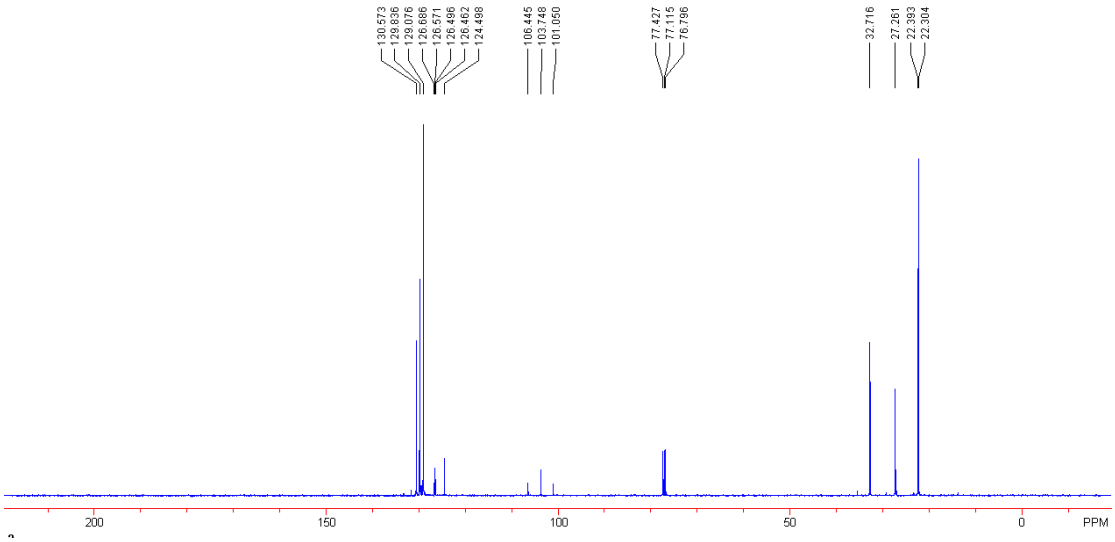
5k



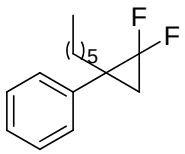
^{13}C NMR


Ph
F
F

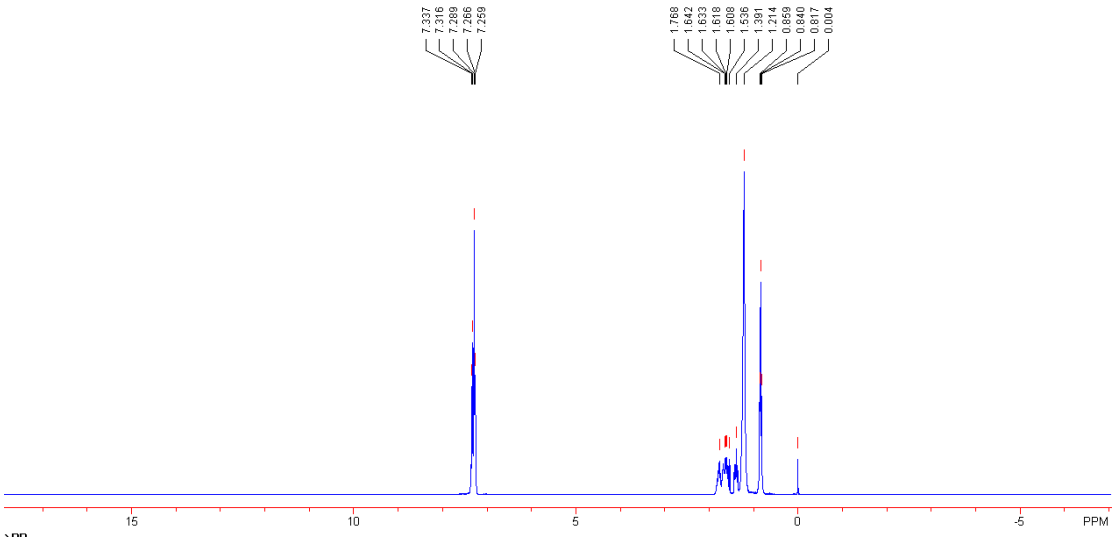
5k


130.573
129.836
129.076
126.666
126.571
126.496
126.462
124.498
106.445
103.748
101.050
77.427
77.115
76.796
32.716
27.261
22.393
22.304
200
150
100
50
0
PPM

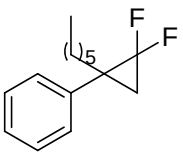
^{1}H NMR


F
F
5

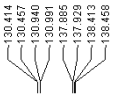
7d

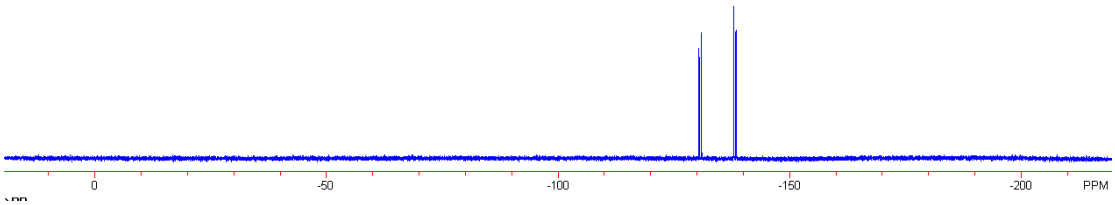

7.337
7.316
7.289
7.266
7.259
1.768
1.642
1.633
1.618
1.608
1.536
1.391
1.214
0.859
0.840
0.817
0.004
15
10
5
0
-5
PPM

^{19}F NMR

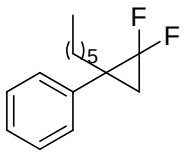

F
F
5

7d

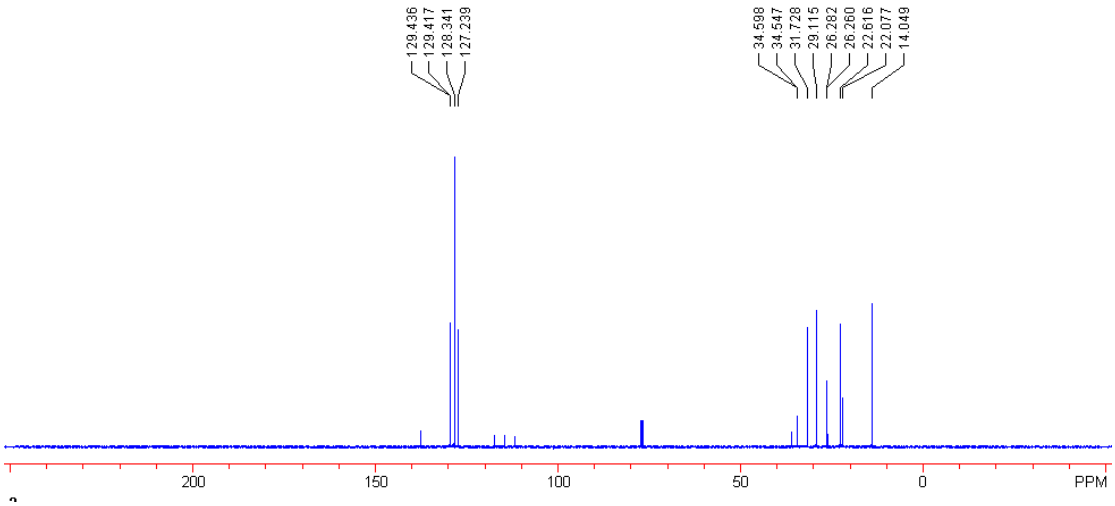

130.414
130.457
130.940
130.991
137.885
137.929
138.413
138.458


0
-50
-100
-150
-200
PPM

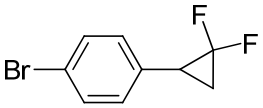
^{13}C NMR


F
F
5

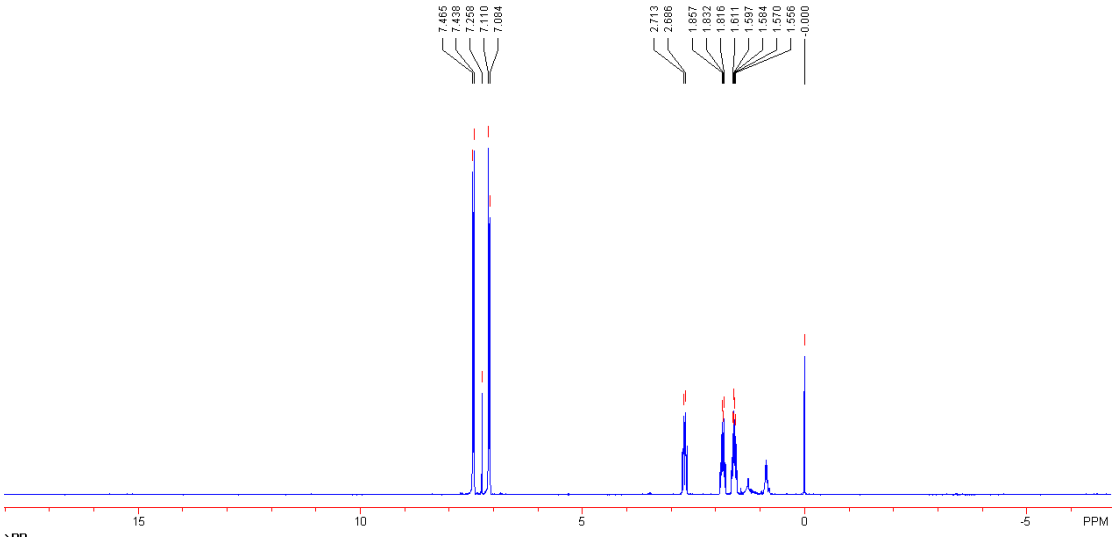
7d


129.436
129.417
128.341
127.239
34.598
34.547
31.728
29.115
26.282
26.260
22.616
22.077
14.049
200
150
100
50
0
PPM

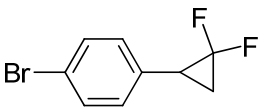
^{1}H NMR


F
F
Br

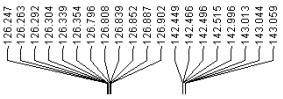
7f


7.465
7.438
7.258
7.110
7.084
2.713
2.686
1.857
1.832
1.816
1.611
1.597
1.584
1.570
1.556
0.000
15
10
5
0
-5
PPM

^{19}F NMR


F
F
Br

7f


-126.247
-126.263
-126.292
-126.304
-126.339
-126.354
-126.796
-126.808
-126.839
-126.852
-126.887
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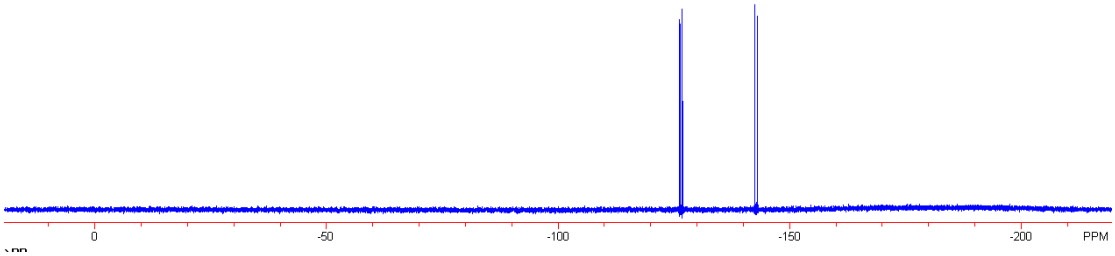
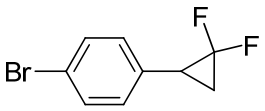
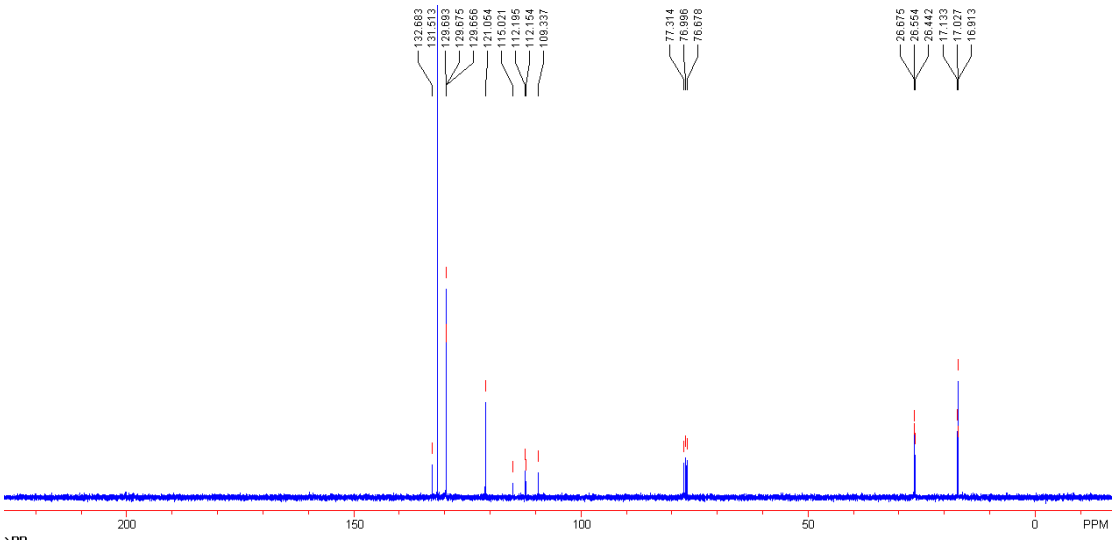
-142.515
-142.996
-143.013
-143.044
-143.059


0
-50
-100
-150
-200
PPM

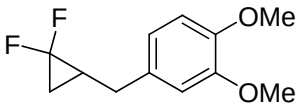
^{13}C NMR


F
F
Br

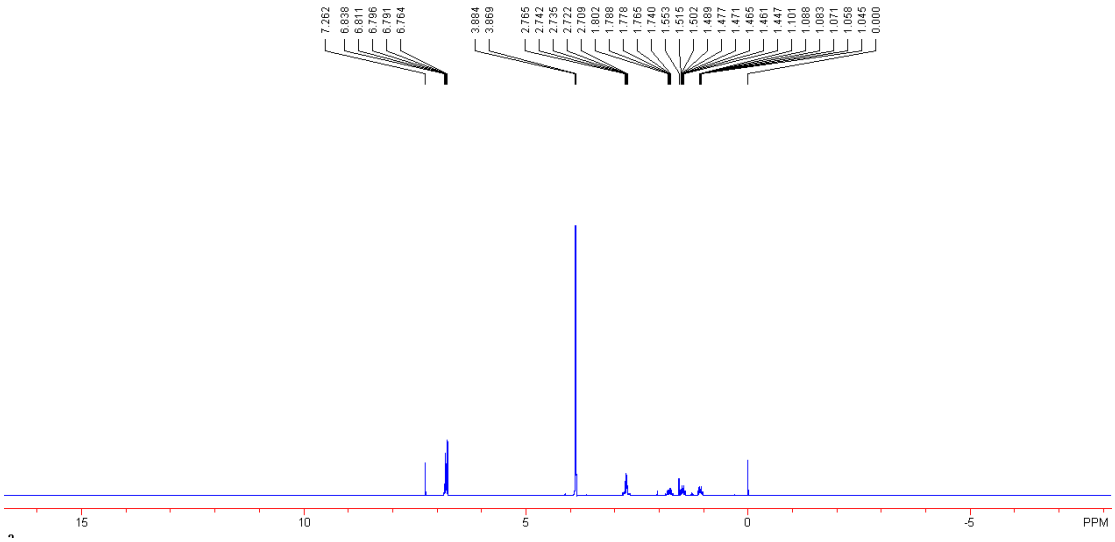
7f


132.683
131.513
129.693
129.675
129.656
121.054
115.021
112.195
112.154
109.337
77.314
76.996
76.678
26.675
26.554
26.442
17.133
17.027
16.913
200
150
100
50
0
PPM

^{1}H NMR


F
F
OMe
OMe

7g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6.811
6.796
6.791
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2.742
2.735
2.722
2.709
1.802
1.788
1.778
1.765
1.740
1.553
1.515
1.502
1.489
1.477
1.471
1.465
1.461
1.447
1.101
1.088
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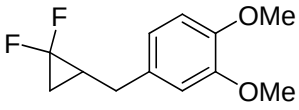
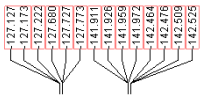
1.071
1.058
1.045
0.000
15
10
5
0
-5
PPM

^{19}F NMR


F
F
OMe
OMe

7g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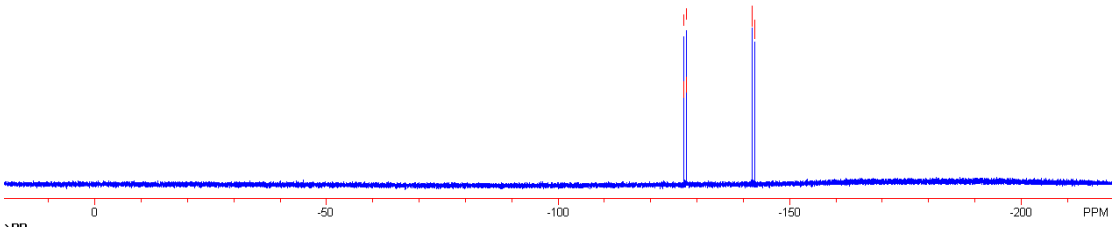
-127.680
-127.727
-127.773
-141.911
-141.926
-141.959
-141.972
-142.464
-142.476
-142.509
-142.525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-50
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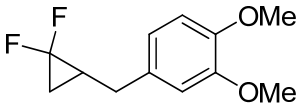
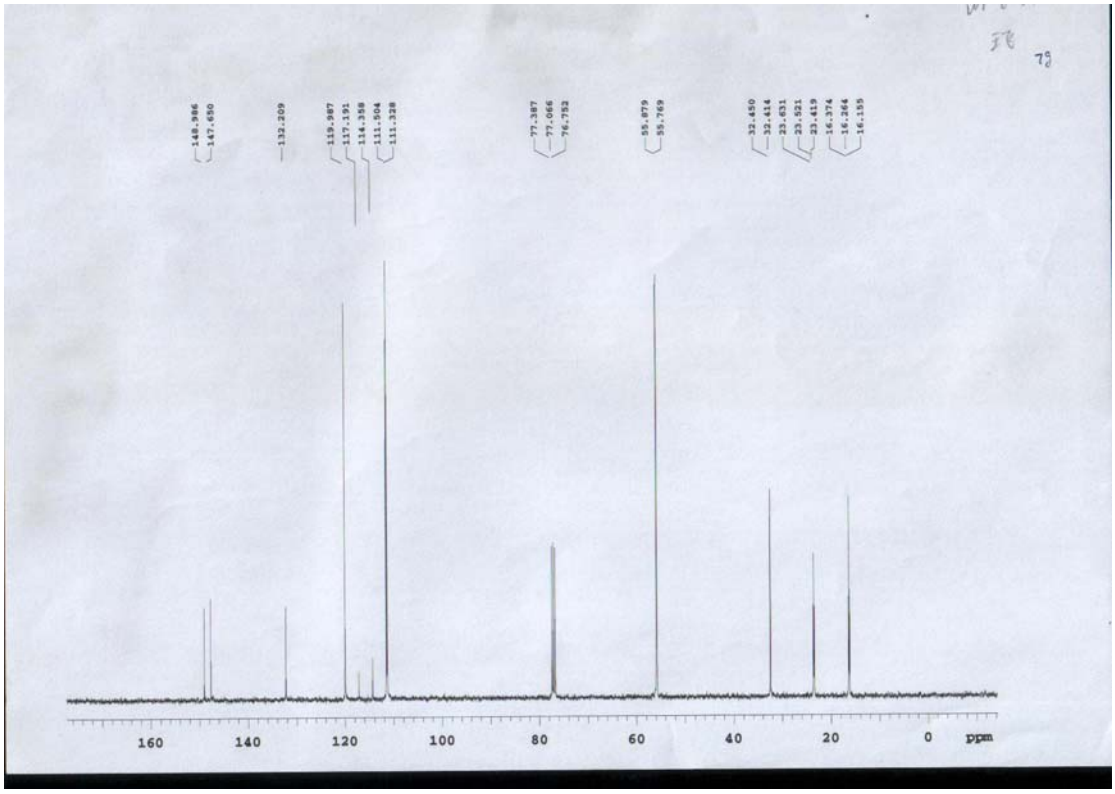
-150
-200
PPM

^{13}C NMR


F
F
OMe
OMe

7g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117.191
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111.504
111.328
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77.066
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55.769
32.450
32.414
23.631
23.521
23.419
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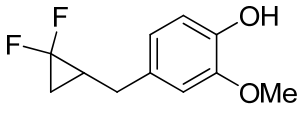
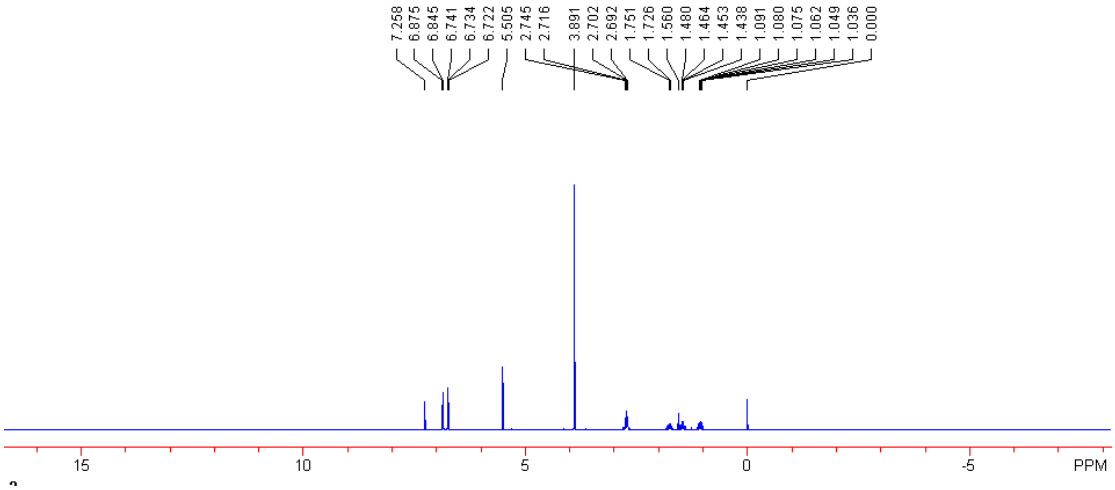
16.264
16.155
160
140
120
100
80
60
40
20
0
ppm

^{1}H NMR


F
F
OH
OMe

7h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3.891
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1.726
1.560
1.480
1.464
1.453
1.438
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1.062
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1.036
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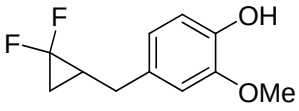
10
5
0
-5
PPM

^{19}F NMR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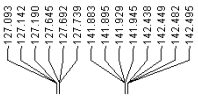
F
OH
OMe

7h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-127.692
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-141.929
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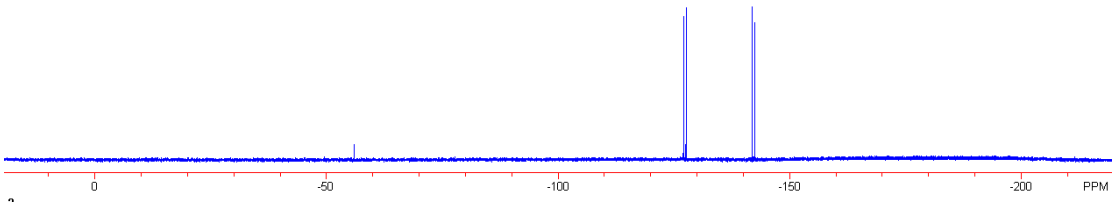
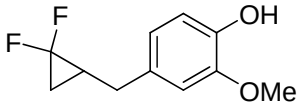
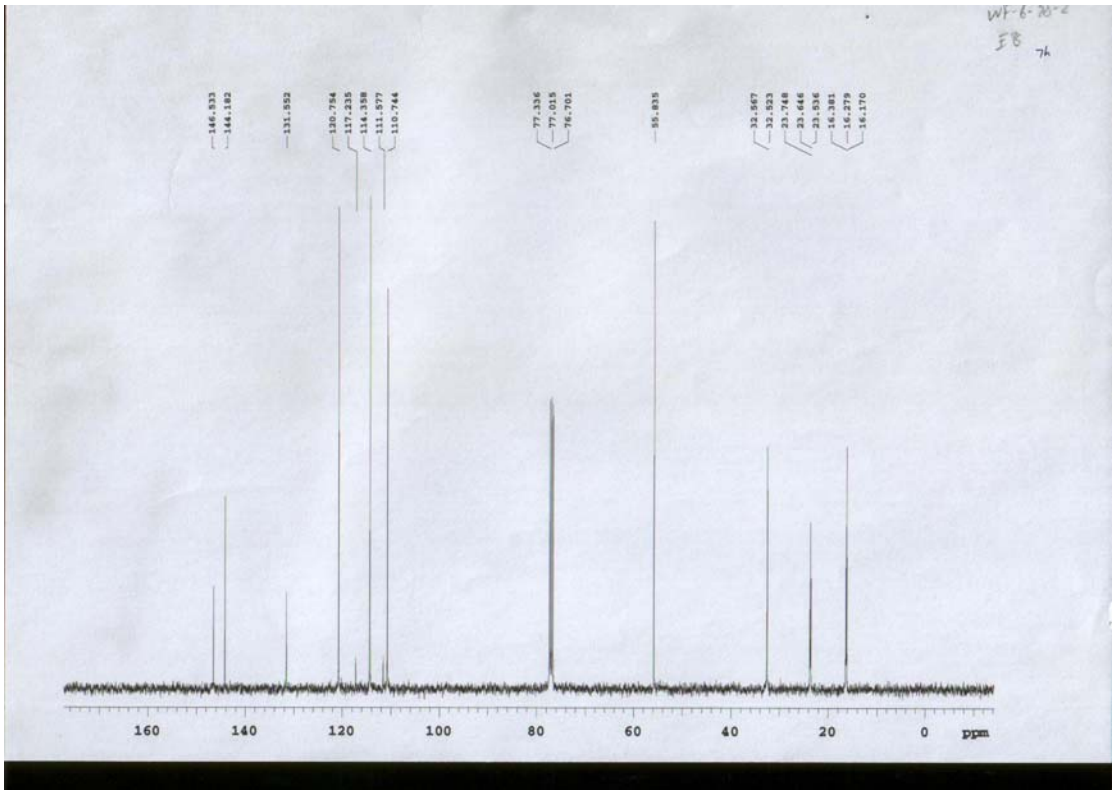
-142.438
-142.449
-142.482
-142.495


0
-50
-100
-150
-200
PPM

^{13}C NMR


F
F
OH
OMe

7h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114.358
111.577
110.744
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77.015
76.701
55.835
32.567
32.523
23.748
23.646
23.536
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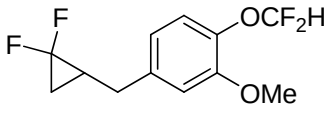
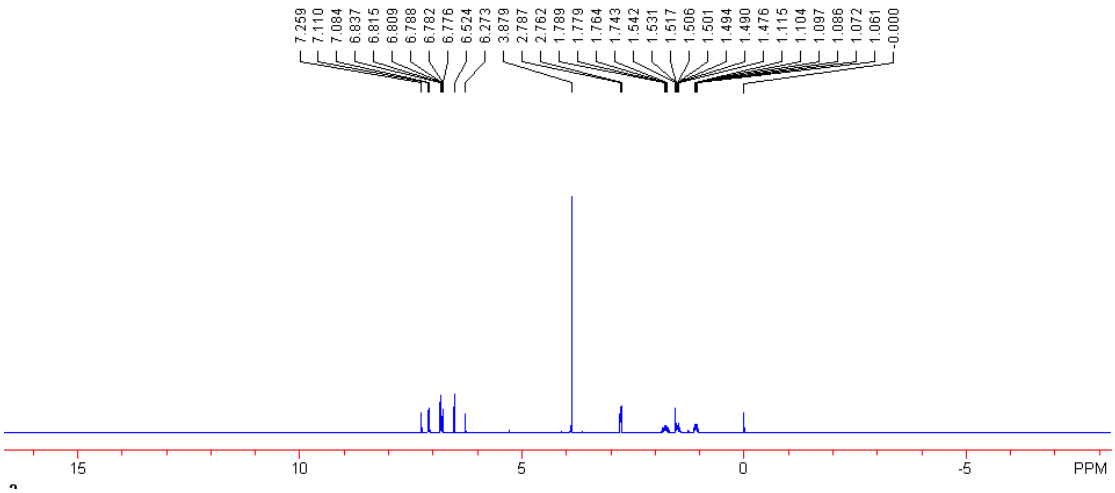
16.279
16.170
160
140
120
100
80
60
40
20
0
ppm

^{1}H NMR


F
F
OCF2H
OMe

7i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7.110
7.084
6.837
6.815
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6.788
6.782
6.776
6.524
6.273
3.879
2.787
2.762
1.789
1.779
1.764
1.743
1.542
1.531
1.517
1.506
1.501
1.494
1.490
1.476
1.115
1.104
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1.086
1.072
1.061
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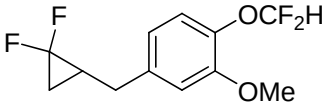
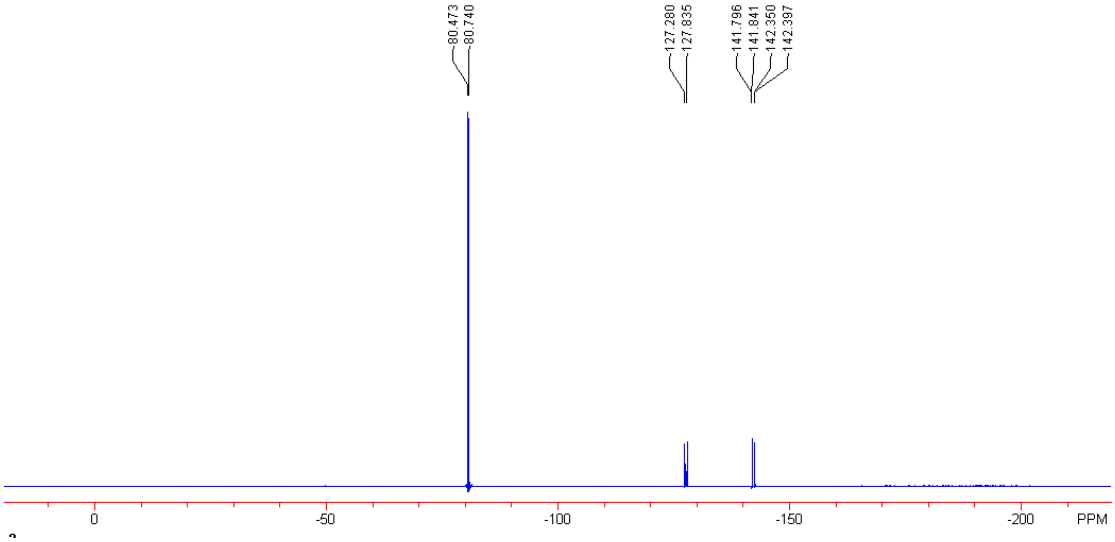
15
10
5
0
-5
PPM

^{19}F NMR


F
F
OCF2H
OMe

7i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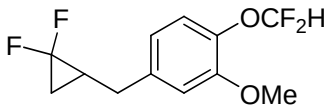
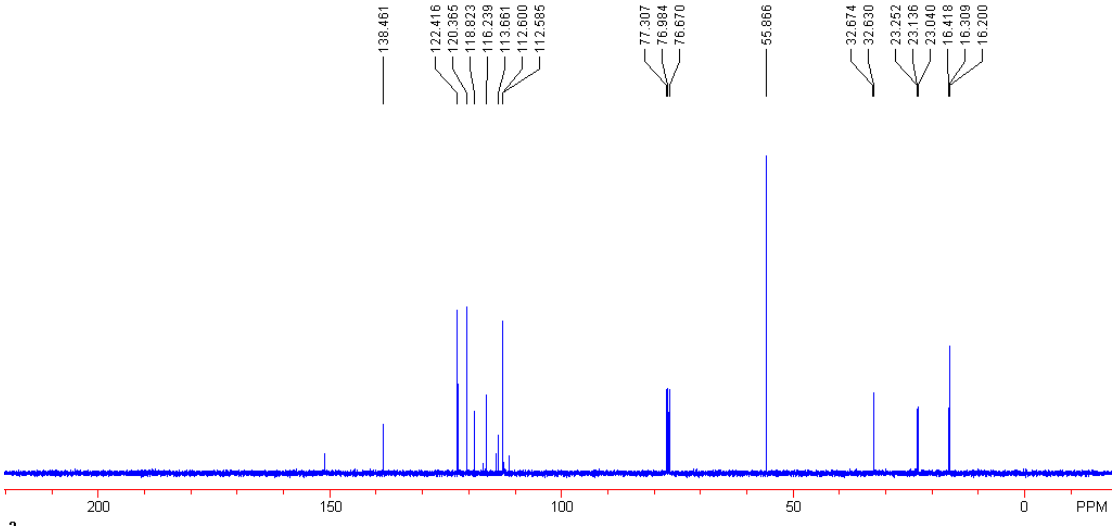
-142.397
0
-50
-100
-150
-200
PPM

^{13}C NMR


F
F
OCF2H
OMe

7i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76.984
76.670
55.866
32.674
32.630
23.252
23.136
23.040
16.418
16.309
16.200
200
150
100
50
0
PPM

Summary of Computational results:

Density functional theory (DFT) calculations were conducted at the B3LYP/6-311+G** level of theory using Gaussian 09.[c1-c3] Tetramethylethylene (**6a**) was chosen as the model substrate. The self-consistent reaction field (SCRF) method, polarizable continuum model (PCM), using the integral equation formalism variant was applied to include the solvent effects in THF and toluene.[c4]

C1. Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai,T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
C2. (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648. (b) C. Lee, W. Yang, and R. G. Parr, *Phys. Rev. B.*, 1988, **37**, 785.
C3. (a) A. D. McLean and G. S. Chandler, *J. Chem. Phys.*, 1980, **72**, 5639. (b) K. Raghavachari, J. S. Binkley, R. Seeger, and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650.
C4. (a) S. Miertuš, E. Scrocco, J. Tomasi, *Chem. Phys.*, 1981, **55**, 117. (b) S. Miertuš, J. Tomasi, *Chem. Phys.*, 1982, **65**, 239.

I. Reactions in THF:
Me_3SiCF_2Cl (**1**) in THF

Zero-point correction= 0.122363 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1107.309943
Sum of electronic and thermal Enthalpies= -1107.297143
Sum of electronic and thermal Free Energies= -1107.347711

H	0.48086500	-2.31773300	-1.22972800
C	0.48497700	-2.29285000	-0.13727300
H	1.52378700	-2.27161900	0.20242900
H	0.03414100	-3.22307200	0.22193700
Si	-0.47886500	-0.82797500	0.52580500
C	-0.42312200	-0.71884800	2.39874100
H	0.60508800	-0.70679300	2.76951700
H	-0.92706500	-1.58697600	2.83461900
H	-0.92938200	0.17978000	2.76061100
C	-2.22771900	-0.73411200	-0.14364600
H	-2.24309900	-0.76079100	-1.23583500
H	-2.73387000	0.17722400	0.18556600
H	-2.80635600	-1.58814800	0.22183000
C	0.45488400	0.77949900	-0.09740100
F	1.75616400	0.81135300	0.32656100
F	-0.11477700	1.92489900	0.38888600
Cl	0.49398300	0.94587100	-1.91046000

Cl^- in THF

Zero-point correction= 0.000000 (Hartree/Particle)
Sum of electronic and zero-point Energies= -460.400964
Sum of electronic and thermal Enthalpies= -460.398603
Sum of electronic and thermal Free Energies= -460.415986

$Me_3SiCF_2Cl^{\bullet -}$ radical anion in THF

Zero-point correction= 0.120071 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1107.333686
Sum of electronic and thermal Enthalpies= -1107.320707
Sum of electronic and thermal Free Energies= -1107.372317

H	0.47462600	-2.31576100	-1.24358900
C	0.49858800	-2.29316900	-0.14721600
H	1.54367900	-2.24803900	0.18553000
H	0.06453700	-3.22866500	0.22230100
Si	-0.49371300	-0.85351100	0.53699400
C	-0.42005200	-0.71730500	2.40984100
H	0.61526500	-0.71572200	2.77376400
H	-0.93204300	-1.58583000	2.84227200
H	-0.92523200	0.18928300	2.76675500
C	-2.23739700	-0.72211300	-0.14799700
H	-2.24570300	-0.76085800	-1.24399600
H	-2.72734300	0.20401900	0.17977600
H	-2.82561200	-1.56742300	0.22613300
C	0.44361300	0.76150900	-0.08957300
F	1.74304100	0.80841200	0.34451200
F	-0.13443500	1.91348800	0.37606900
Cl	0.50781500	0.92139200	-1.90941600

Cl· radical in THF

Zero-point correction= 0.000000 (Hartree/Particle)
Sum of electronic and zero-point Energies= -460.167804
Sum of electronic and thermal Enthalpies= -460.165444
Sum of electronic and thermal Free Energies= -460.183481

Cl-Me_3Si-CF_2Cl^- transition state (10) in THF

Imaginary Frequency: -94.7684 cm^{-1}
Zero-point correction= 0.120259 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1567.676866
Sum of electronic and thermal Enthalpies= -1567.661365
Sum of electronic and thermal Free Energies= -1567.721954

Si	1.15911400	-0.02329500	-0.00124100
C	0.72768600	-0.88891200	1.60837400
H	1.20464800	-0.37396900	2.44743900
H	1.10875100	-1.91381300	1.58665400
H	-0.34802100	-0.92005700	1.77639000
C	1.23681200	1.85797500	-0.00414400

H	1.77548400	2.20143400	0.88381100
H	0.25358900	2.32634400	-0.01536500
H	1.79387900	2.19754600	-0.88214400
C	0.72726300	-0.89214500	-1.60894300
H	1.20373500	-0.37883900	-2.44928800
H	-0.34857500	-0.92353900	-1.77622200
H	1.10824400	-1.91703300	-1.58545000
C	-1.69237200	0.56918400	0.00072000
F	-2.22052500	1.25228300	1.07027400
F	-2.22429100	1.25423300	-1.06578100
Cl	-2.97363200	-1.17154400	0.00130300
Cl	3.36390400	-0.40205100	-0.00024100

CF_2Cl^- (**11**) in THF

Zero-point correction= 0.007271 (Hartree/Particle)
Sum of electronic and zero-point Energies= -698.172663
Sum of electronic and thermal Enthalpies= -698.166895
Sum of electronic and thermal Free Energies= -698.201733

C	0.33558700	-0.58246500	-0.66386300
F	1.47638900	-0.46006800	0.03060100
F	-0.33900600	-1.51141400	0.02972500
Cl	-0.84662900	1.46921600	0.30990300

Me_3SiCl in THF

Zero-point correction= 0.111924(Hartree/Particle)
Sum of electronic and zero-point Energies= -869.509012
Sum of electronic and thermal Enthalpies= -869.499433
Sum of electronic and thermal Free Energies= -869.541605

Si	-0.34476300	-0.00000500	-0.12221600
C	-0.24226500	0.00004900	-1.99141500
H	0.28137500	-0.88621900	-2.35874000
H	0.28138400	0.88633200	-2.35869200
H	-1.25039600	0.00006600	-2.41861500
C	-1.14073000	1.55573500	0.54946500
H	-0.62155200	2.45024300	0.19582800
H	-1.13367600	1.56318800	1.64244600
H	-2.18229200	1.61410500	0.21660300
C	-1.14074100	-1.55577800	0.54937400
H	-0.62157000	-2.45027000	0.19568400
H	-2.18230300	-1.61412000	0.21651000
H	-1.13368500	-1.56329400	1.64234800
Cl	1.66990300	-0.00003300	0.59017900

CF_2 in THF

Zero-point correction= 0.006636 (Hartree/Particle)
Sum of electronic and zero-point Energies= -237.769038
Sum of electronic and thermal Enthalpies= -237.765086

Sum of electronic and thermal Free Energies= -237.793100

C	0.00000000	-0.02370300	-0.59687900
F	0.00000000	1.04201600	0.15867400
F	0.00000000	-1.02631300	0.24033000

Tetramethylethylene (**6a**) in THF

Zero-point correction= 0.162432(Hartree/Particle)
Sum of electronic and zero-point Energies= -235.762198
Sum of electronic and thermal Enthalpies= -235.752470
Sum of electronic and thermal Free Energies= -235.795929

C	-0.03319300	-0.01783900	0.67525000
C	0.02888600	0.01839200	-0.67053300
C	-0.10772100	1.20794000	1.55965600
H	-0.10911300	2.15220900	1.01921700
H	0.73823000	1.22401400	2.25750200
H	-1.01353300	1.17561900	2.17726400
C	-0.03717900	-1.29018600	1.49439400
H	-0.94565500	-1.34505500	2.10644100
H	0.80576600	-1.29242200	2.19601600
H	0.02032400	-2.20244400	0.90456900
C	0.10329700	-1.20738800	-1.55493900
H	-0.74219400	-1.22289000	-2.25335400
H	0.10368800	-2.15168100	-1.01454100
H	1.00954000	-1.17562000	-2.17194500
C	0.03299100	1.29074500	-1.48966500
H	-0.02363000	2.20302500	-0.89978900
H	-0.81037700	1.29344500	-2.19078100
H	0.94112400	1.34513400	-2.10226100

Tetramethylethylene + CF_2 Transition State in THF

Imaginary Frequency: -239.4254 cm^{-1}
Zero-point correction= 0.171842 (Hartree/Particle)
Sum of electronic and zero-point Energies= -473.515205
Sum of electronic and thermal Enthalpies= -473.503031
Sum of electronic and thermal Free Energies= -473.551513

C	-1.52510000	-1.27378400	0.12170400
C	0.56601600	0.12879300	0.02486700
C	-0.75073800	0.53300400	-0.16634000
F	-1.13411500	-1.75766200	1.32882100
F	-0.97966100	-2.14921100	-0.76224900
C	-1.27441000	0.82276000	-1.56411900
H	-0.94749300	1.81742200	-1.88511300
H	-2.36527900	0.80966600	-1.55779900
H	-0.93777900	0.09693400	-2.30247800
C	-1.48932900	1.31164400	0.91085000
H	-1.32375800	0.91494300	1.91118800
H	-2.56206200	1.28140900	0.71474600

H	-1.16992100	2.35896500	0.89838100
C	1.17966500	0.02722700	1.38799800
H	2.25995300	0.17693100	1.33795700
H	1.01286700	-0.98669900	1.78544200
H	0.76449000	0.72906900	2.10907100
C	1.38830400	-0.44973900	-1.08663100
H	2.45419600	-0.34571100	-0.87754900
H	1.17909500	-0.00518900	-2.05878300
H	1.17728600	-1.52756500	-1.17085400

2,2-difluorotetramethylcyclopropane in THF

Zero-point correction= 0.176072 (Hartree/Particle)
Sum of electronic and zero-point Energies= -473.597274
Sum of electronic and thermal Enthalpies= -473.585633
Sum of electronic and thermal Free Energies= -473.632045

C	0.82630000	0.24794100	0.20519800
C	-0.57477000	-0.41038400	0.53510200
C	-0.26939800	0.17460200	-0.79641100
F	-0.14741900	-0.63586900	-1.89484900
F	-0.90359400	1.31807000	-1.20767900
C	-0.67008600	-1.92240000	0.66966600
H	-0.06620100	-2.45821600	-0.06061000
H	-1.70822100	-2.24086700	0.53702500
H	-0.35195900	-2.23113100	1.66981200
C	-1.54113600	0.32234200	1.45361900
H	-1.26753100	0.15451600	2.49945300
H	-2.55403100	-0.06446100	1.30794900
H	-1.57198800	1.39627900	1.27760200
C	1.17163900	1.59740100	0.81541400
H	1.97212700	2.07035100	0.23890100
H	1.53162800	1.46676100	1.84014800
H	0.32981200	2.28726300	0.83471700
C	2.04328500	-0.64735900	0.02965500
H	2.82111500	-0.10971700	-0.52050900
H	1.82861700	-1.56366100	-0.51758800
H	2.45397900	-0.91983600	1.00634400

Tetramethylethylene + CF_2Cl^- Transition State in THF

Imaginary Frequency: -309.1547 cm^{-1}
Zero-point correction= 0.171350 (Hartree/Particle)
Sum of electronic and zero-point Energies= -933.902494
Sum of electronic and thermal Enthalpies= -933.888219
Sum of electronic and thermal Free Energies= -933.943209

C	0.29037600	-1.03784300	-0.33439000
F	1.38210800	-1.02147900	-1.13865300
F	0.77300900	-1.46923000	0.85694500
Cl	-0.81528300	-3.07230600	-1.12800700
C	-0.40882700	0.75568700	-0.14835300

C	-0.98745400	0.93604500	-1.54923600
H	-0.22078400	0.92952100	-2.32381700
H	-1.53075300	1.88764700	-1.60963400
H	-1.67693900	0.11848500	-1.76811900
C	-1.51962600	0.48418000	0.86219200
H	-1.13802000	0.17814100	1.83612900
H	-2.15921600	-0.32111400	0.49551200
H	-2.12696100	1.38790300	0.99938600
C	0.71540900	1.50261700	0.23783100
C	1.74490300	1.96724500	-0.75854900
H	2.24407300	2.87805700	-0.40244300
H	1.32981600	2.18741600	-1.74344600
H	2.54007100	1.21242700	-0.90939000
C	1.22556400	1.50309100	1.65480300
H	1.74911400	2.44213300	1.87809000
H	1.95492900	0.68892000	1.82747900
H	0.43904800	1.38338600	2.40149100

F^- in THF

Zero-point correction= 0.000000 (Hartree/Particle)
Sum of electronic and zero-point Energies= -100.007894
Sum of electronic and thermal Enthalpies= -100.005533
Sum of electronic and thermal Free Energies= -100.022052

(F)$Me_3SiCF_2Cl^-$ (**12**) in THF

Zero-point correction= 0.123062 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1207.338006
Sum of electronic and thermal Enthalpies= -1207.323542
Sum of electronic and thermal Free Energies= -1207.377806

Si	-0.15262100	-1.03582800	0.03391800
C	-0.21079200	1.11291500	0.16075700
F	-1.27527600	1.70970400	-0.48674400
F	-0.29048700	1.62692600	1.44046900
Cl	1.30917700	2.00372800	-0.57705900
C	-0.10523200	-0.93219400	-1.87130900
H	0.86520000	-1.29100400	-2.23094000
H	-0.26915300	0.06416200	-2.28389800
H	-0.86196500	-1.60842400	-2.28081600
C	-1.84629000	-1.04993200	0.91890600
H	-1.82578000	-0.46124400	1.84062900
H	-2.14294600	-2.07126500	1.16699800
H	-2.62192400	-0.61667100	0.27860800
C	1.43456700	-1.07299000	1.09232700
H	2.28249800	-1.36769600	0.46444100
H	1.32996000	-1.84284500	1.86269200
H	1.68825300	-0.12813300	1.57532900
F	-0.10444200	-2.83868200	-0.08305700

F-Me_3Si-CF_2Cl^- transition state (**13**) in THF

Imaginary Frequency: -69.3061cm^{-1}
Zero-point correction= 0.121351 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1207.334778
Sum of electronic and thermal Enthalpies= -1207.319931
Sum of electronic and thermal Free Energies= -1207.377438

Si	1.49369100	-0.10134100	-0.00029000
C	1.52306600	1.78777300	-0.00684800
H	2.55829500	2.14106500	0.03230700
H	1.05871900	2.19050800	-0.91050900
H	0.98701900	2.20154800	0.85046000
C	1.04218900	-0.98795300	-1.59703500
H	1.64087200	-1.90002000	-1.68753900
H	-0.01308900	-1.25622100	-1.63802300
H	1.27165000	-0.35570400	-2.46103700
C	1.04347400	-0.97141600	1.60594600
H	1.64462600	-1.88071600	1.70704600
H	1.26930400	-0.32930600	2.46358700
H	-0.01102500	-1.24278300	1.64810200
F	3.17988500	-0.38998700	-0.00179800
C	-1.21555200	0.55937700	-0.00290700
F	-1.72212300	1.25448200	1.06855200
F	-1.73273600	1.25592200	-1.06807200
Cl	-2.52884400	-1.14523000	0.00237900

Me_3SiF in THF

Zero-point correction= 0.112714 (Hartree/Particle)
Sum of electronic and zero-point Energies= -509.168757
Sum of electronic and thermal Enthalpies= -509.159471
Sum of electronic and thermal Free Energies= -509.200458

Si	-0.00281200	0.00524100	-0.00252600
C	-1.74514100	-0.08811100	0.67122300
H	-1.74465300	-0.09804500	1.76485800
H	-2.25478500	-0.99062000	0.32195400
H	-2.33151100	0.77622900	0.34375200
C	0.94962300	1.46702800	0.67129800
H	1.98541100	1.45905800	0.32019800
H	0.95986100	1.46119400	1.76494700
H	0.49219700	2.40651200	0.34522200
C	0.05071800	-0.08737600	-1.86957500
H	1.08153700	-0.10078900	-2.23478700
H	-0.45050600	0.77968900	-2.31130900
H	-0.45244300	-0.98737400	-2.23421600
F	0.77962400	-1.35271500	0.55128200

CF_3^- in THF

Zero-point correction= 0.008780(Hartree/Particle)
Sum of electronic and zero-point Energies= -337.816683

Sum of electronic and thermal Enthalpies= -337.811945
Sum of electronic and thermal Free Energies= -337.842957

C	-0.25523700	0.44258400	0.18056700
F	-0.14796500	0.25740900	-1.24021900
F	1.11898500	0.25721700	0.55337100
F	-0.78305600	-0.84039200	0.55391700

II. Reactions in Toluene:

Me_3SiCF_2Cl (1) in Toluene

Zero-point correction= 0.122535 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1107.308261
Sum of electronic and thermal Enthalpies= -1107.295463
Sum of electronic and thermal Free Energies= -1107.346135

Si	-0.17675200	0.00000000	1.07209300
C	-1.98296000	0.00000000	1.58571500
H	-2.06133400	0.00000000	2.67747200
H	-2.50459100	-0.88539200	1.21318900
H	-2.50459100	0.88539200	1.21318900
C	0.71263500	1.56453800	1.59977800
H	1.74980000	1.57373300	1.25614600
H	0.72020200	1.63903000	2.69179100
H	0.21472500	2.45580000	1.20886300
C	0.71263500	-1.56453800	1.59977800
H	1.74980000	-1.57373300	1.25614600
H	0.21472500	-2.45580000	1.20886300
H	0.72020200	-1.63903000	2.69179100
C	-0.20656200	0.00000000	-0.88527700
F	-0.86667100	1.08942200	-1.38267600
F	-0.86667100	-1.08942200	-1.38267600
Cl	1.44983200	0.00000000	-1.63725600

Cl^- in Toluene

Zero-point correction= 0.000000 (Hartree/Particle)
Sum of electronic and zero-point Energies= -460.368569
Sum of electronic and thermal Enthalpies= -460.366209
Sum of electronic and thermal Free Energies= -460.383592

$Me_3SiCF_2Cl^{\bullet -}$ radical anion in Toluene

Zero-point correction= 0.120501(Hartree/Particle)
Sum of electronic and zero-point Energies= -1107.317603
Sum of electronic and thermal Enthalpies= -1107.304687
Sum of electronic and thermal Free Energies= -1107.355996

Si	-0.17102800	0.00000000	1.11468500
C	-1.99240500	0.00000000	1.58299000
H	-2.08316200	0.00000000	2.67412700
H	-2.50280900	-0.89283900	1.19933000

H	-2.50280900	0.89283900	1.19933000
C	0.71928300	1.58224700	1.59444700
H	1.76086800	1.58030300	1.25041200
H	0.72247500	1.67624900	2.68490200
H	0.20959000	2.46219600	1.17959600
C	0.71928300	-1.58224700	1.59444700
H	1.76086800	-1.58030300	1.25041200
H	0.20959000	-2.46219600	1.17959600
H	0.72247500	-1.67624900	2.68490200
C	-0.21017600	0.00000000	-0.85490400
F	-0.86929800	1.08945700	-1.35915500
F	-0.86929800	-1.08945700	-1.35915500
Cl	1.45097800	0.00000000	-1.62903400

Cl· radical in Toluene

Zero-point correction= 0.000000 (Hartree/Particle)
Sum of electronic and zero-point Energies= -460.167407
Sum of electronic and thermal Enthalpies= -460.165046
Sum of electronic and thermal Free Energies= -460.183084

Cl-Me$_3$Si-CF$_2$Cl$^-$ transition state (**10**) in Toluene

Imaginary Frequency: - 78.3556 cm^{-1}
Zero-point correction= 0.120607(Hartree/Particle)
Sum of electronic and zero-point Energies= -1567.654733
Sum of electronic and thermal Enthalpies= -1567.639459
Sum of electronic and thermal Free Energies= -1567.698028

Si	1.20647700	-0.03160400	-0.00756100
C	0.73654900	-0.87998900	1.59932500
H	1.18551700	-0.35238600	2.44605900
H	1.12426000	-1.90269900	1.60004900
H	-0.34399000	-0.91297400	1.73127200
C	1.25954900	1.84955700	-0.03572000
H	1.66918800	2.22385600	0.90715500
H	0.27300900	2.28645100	-0.18523400
H	1.92007200	2.18359700	-0.84111200
C	0.74099400	-0.89224700	-1.60806900
H	1.23519800	-0.40404000	-2.45318400
H	-0.33725000	-0.87626400	-1.76409100
H	1.07648800	-1.93283100	-1.58017700
C	-1.74463100	0.57791600	0.03410500
F	-2.26588400	1.18765100	1.15772300
F	-2.31698600	1.32123800	-0.97950100
Cl	-2.95751700	-1.17221900	-0.04675400
Cl	3.39465100	-0.41921200	0.01186100

CF$_2$Cl$^-$ (**11**) in Toluene

Zero-point correction= 0.007371(Hartree/Particle)
Sum of electronic and zero-point Energies= -698.145448

Sum of electronic and thermal Enthalpies= -698.139903
Sum of electronic and thermal Free Energies= -698.173818

C	0.70947000	0.51317700	-0.06334000
F	0.45308000	0.43179100	-1.40183300
F	-0.15954900	1.49000300	0.32822100
Cl	-0.51790300	-1.35023900	0.64448900

Me_3SiCl in Toluene

Zero-point correction= 0.112040(Hartree/Particle)
Sum of electronic and zero-point Energies= -869.507332
Sum of electronic and thermal Enthalpies= -869.497757
Sum of electronic and thermal Free Energies= -869.539939

Si	0.33436700	0.00000000	-0.11856200
C	0.24299800	0.00000000	-1.98978700
H	1.25158600	0.00000000	-2.41615400
H	-0.28053100	0.88522500	-2.35984300
H	-0.28053100	-0.88522500	-2.35984300
C	1.14057900	1.55414700	0.54853700
H	2.18214500	1.61162000	0.21514600
H	1.13460800	1.56426000	1.64152500
H	0.62308600	2.45034500	0.19665300
C	1.14057900	-1.55414700	0.54853700
H	2.18214500	-1.61162000	0.21514600
H	0.62308600	-2.45034500	0.19665300
H	1.13460800	-1.56426000	1.64152500
Cl	-1.66979100	0.00000000	0.58998400

CF_2 in Toluene

Zero-point correction= 0.006685(Hartree/Particle)
Sum of electronic and zero-point Energies= -237.768415
Sum of electronic and thermal Enthalpies= -237.764467
Sum of electronic and thermal Free Energies= -237.792478

C	0.25511300	-0.41167400	0.34255600
F	0.21035700	-0.37527300	-0.96315800
F	-0.38684500	0.66007200	0.72622700

Tetramethylethylene (**6a**) in Toluene

Zero-point correction= 0.162535(Hartree/Particle)
Sum of electronic and zero-point Energies= -235.761657
Sum of electronic and thermal Enthalpies= -235.751897
Sum of electronic and thermal Free Energies= -235.796100

C	-0.03320100	-0.01773700	0.67501900
C	0.02889100	0.01829800	-0.67030700
C	-0.10742800	1.20790600	1.55917900
H	-0.10926900	2.15202500	1.01856600
H	0.73911400	1.22481900	2.25631500

H	-1.01307600	1.17608400	2.17706300
C	-0.03752700	-1.28973800	1.49420000
H	-0.94689100	-1.34564700	2.10486200
H	0.80479000	-1.29199500	2.19658400
H	0.02125100	-2.20190100	0.90445600
C	0.10286700	-1.20736300	-1.55447200
H	-0.74280200	-1.22316200	-2.25268300
H	0.10276500	-2.15152500	-1.01392700
H	1.00935100	-1.17663000	-2.17118800
C	0.03348000	1.29030600	-1.48947000
H	-0.02326000	2.20252800	-0.89961500
H	-0.80983900	1.29363300	-2.19065400
H	0.94203400	1.34509900	-2.10142700

Tetramethylethylene + CF_2 Transition State in Toluene

Imaginary Frequency: - 243.5704cm^{-1}
Zero-point correction= 0.171450 (Hartree/Particle)
Sum of electronic and zero-point Energies= -473.523489
Sum of electronic and thermal Enthalpies= -473.511095
Sum of electronic and thermal Free Energies= -473.560793

C	-1.53674400	-1.25696900	0.14671100
C	0.56133000	0.11516100	0.03195400
C	-0.75715100	0.52097100	-0.16015900
F	-1.14537600	-1.74723700	1.35315500
F	-1.02108900	-2.15134500	-0.73945200
C	-1.27029800	0.80734700	-1.56320600
H	-0.94662200	1.80559400	-1.87727600
H	-2.36108200	0.78710900	-1.56728800
H	-0.92068200	0.08695400	-2.30104800
C	-1.49124900	1.32755600	0.90014100
H	-1.32429700	0.96118200	1.91156800
H	-2.56457600	1.29165500	0.70764100
H	-1.17051900	2.37376300	0.85587700
C	1.18696300	0.01604200	1.38863100
H	2.23559300	0.32256700	1.34540900
H	1.17936100	-1.03393000	1.72102300
H	0.68621200	0.60547600	2.15320100
C	1.38462900	-0.45170700	-1.08584200
H	2.44655900	-0.43313700	-0.83543100
H	1.24215000	0.07061200	-2.03223000
H	1.10911700	-1.50445700	-1.25427000

2,2-difluorotetramethylcyclopropane in Toluene

Zero-point correction= 0.176228(Hartree/Particle)
Sum of electronic and zero-point Energies= -473.595796
Sum of electronic and thermal Enthalpies= -473.584158
Sum of electronic and thermal Free Energies= -473.630576

C	0.82623400	0.24776900	0.20564900

C	-0.57438100	-0.41032100	0.53563900
C	-0.26977400	0.17479100	-0.79700900
F	-0.14643600	-0.63691800	-1.89110600
F	-0.90252800	1.31753700	-1.20377600
C	-0.66975100	-1.92232300	0.66982100
H	-0.06777200	-2.45722700	-0.06260400
H	-1.70791500	-2.24092700	0.53749000
H	-0.35078500	-2.23331200	1.66921800
C	-1.54100600	0.32242400	1.45380600
H	-1.26724100	0.15834000	2.50039900
H	-2.55357000	-0.06591400	1.30969900
H	-1.57477200	1.39556900	1.27392100
C	1.17164000	1.59741400	0.81533300
H	1.97305000	2.06972400	0.23952000
H	1.52996000	1.46918300	1.84116700
H	0.33040000	2.28799200	0.83071200
C	2.04306500	-0.64760400	0.02971800
H	2.82216100	-0.10899700	-0.51775500
H	1.82855200	-1.56088800	-0.52251800
H	2.45303700	-0.92468700	1.00563500

Tetramethylethylene + CF_2Cl^- Transition State in Toluene

Imaginary Frequency: -310.9030 cm^{-1}
Zero-point correction= 0.171410(Hartree/Particle)
Sum of electronic and zero-point Energies= -933.876305
Sum of electronic and thermal Enthalpies= -933.861993
Sum of electronic and thermal Free Energies= -933.917240

C	0.29311900	-1.03599600	-0.34393100
F	1.31944800	-1.03322100	-1.23031700
F	0.87042600	-1.43066400	0.81766300
Cl	-0.85117900	-3.09968300	-0.99483400
C	-0.40766400	0.75645400	-0.15262100
C	-0.97959800	0.94322100	-1.55542000
H	-0.20925700	0.93964900	-2.32635700
H	-1.52220700	1.89531900	-1.61423600
H	-1.66839500	0.12693300	-1.78109000
C	-1.52331900	0.47966300	0.85115600
H	-1.14649500	0.16960900	1.82568900
H	-2.16043100	-0.32446100	0.47766900
H	-2.13202000	1.38233300	0.98921800
C	0.71434400	1.50200900	0.24251800
C	1.74817700	1.97196200	-0.74689900
H	2.24630100	2.88041900	-0.38344000
H	1.33715100	2.19807300	-1.73217100
H	2.54356000	1.21761900	-0.89894900
C	1.21790000	1.49552000	1.66182500
H	1.74028900	2.43348600	1.89221100
H	1.94652400	0.68056500	1.83393600
H	0.42788400	1.37212100	2.40420300

F^- in Toluene

Zero-point correction= 0.000000 (Hartree/Particle)
Sum of electronic and zero-point Energies= -99.968381
Sum of electronic and thermal Enthalpies= -99.966020
Sum of electronic and thermal Free Energies= -99.982539

(F)$Me_3SiCF_2Cl^-$ (**12**) in Toluene

Zero-point correction= 0.123402 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1207.316052
Sum of electronic and thermal Enthalpies= -1207.301704
Sum of electronic and thermal Free Energies= -1207.355543

Si	-0.16149300	-1.05371700	0.03398700
C	-0.19041100	1.10749400	0.15194200
F	-1.25270300	1.71647200	-0.48735700
F	-0.25057800	1.62833900	1.43000000
Cl	1.33680500	1.97538300	-0.60665800
C	-0.11418100	-0.92921800	-1.87094000
H	0.91802600	-1.05339800	-2.21693400
H	-0.48283800	0.01872600	-2.26652700
H	-0.69841000	-1.74696200	-2.30144500
C	-1.85458000	-1.03419900	0.92330700
H	-1.82576800	-0.42781400	1.83332300
H	-2.15542500	-2.05005900	1.18942600
H	-2.62797000	-0.60618000	0.27669300
C	1.42460000	-1.09426200	1.09660200
H	2.27492300	-1.37249300	0.46427600
H	1.32233700	-1.88038900	1.85070200
H	1.67045000	-0.15526300	1.59500200
F	-0.13003800	-2.84193000	-0.07414600

F-Me_3Si-CF_2Cl^- transition state (**13**) in Toluene

Imaginary Frequency: -58.9705cm^{-1}
Zero-point correction= 0.121684 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1207.312082
Sum of electronic and thermal Enthalpies= -1207.297377
Sum of electronic and thermal Free Energies= -1207.353942

Si	1.55292100	-0.10821700	0.00425400
C	1.54270900	1.77909500	-0.03602300
H	2.56898000	2.14967900	-0.12877100
H	0.95909200	2.15802500	-0.87757700
H	1.10793500	2.19499800	0.87648300
C	1.07836900	-1.00095200	-1.57832800
H	1.61766100	-1.95210200	-1.63715100
H	0.00779200	-1.19994200	-1.62410600
H	1.36045500	-0.40531600	-2.45274900
C	1.05965600	-0.95809900	1.60673500
H	1.63298500	-1.88484500	1.71399100

H	1.29410200	-0.32216400	2.46657800
H	-0.00326200	-1.19623600	1.63393500
F	3.22950200	-0.38856200	0.02703500
C	-1.29746400	0.57903900	0.01739600
F	-1.83614500	1.14895400	1.14961100
F	-1.81503800	1.38102200	-0.97583800
Cl	-2.57082700	-1.14437800	-0.18115500

Me_3SiF in Toluene

Zero-point correction= 0.112870(Hartree/Particle)
Sum of electronic and zero-point Energies= -509.166917
Sum of electronic and thermal Enthalpies= -509.157635
Sum of electronic and thermal Free Energies= -509.198633

Si	0.00052100	-0.00058500	-0.00006300
C	-1.74444000	-0.08742000	0.67050400
H	-1.74595800	-0.09839100	1.76411000
H	-2.25558700	-0.98952600	0.32245200
H	-2.33098100	0.77706100	0.34341800
C	0.94863200	1.46676400	0.67053600
H	1.98484400	1.46024500	0.32070800
H	0.96077500	1.46220100	1.76415100
H	0.49125300	2.40647000	0.34475600
C	0.05034200	-0.08671800	-1.86855100
H	1.08049600	-0.10082400	-2.23557800
H	-0.45082500	0.78029200	-2.31065800
H	-0.45183000	-0.98646900	-2.23508800
F	0.77988000	-1.35317800	0.55162200

CF_3^- in Toluene

Zero-point correction= 0.008823 (Hartree/Particle)
Sum of electronic and zero-point Energies= -337.788257
Sum of electronic and thermal Enthalpies= -337.783522
Sum of electronic and thermal Free Energies= -337.814535

C	-0.25589100	0.44379600	0.18102800
F	-0.14807100	0.25737600	-1.24173200
F	1.12018700	0.25707700	0.55397700
F	-0.78349800	-0.84143200	0.55436400

III. Reactions in gas phase:

Me_3SiCF_2Cl (1) in Gas Phase

Zero-point correction= 0.122786 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1107.306093
Sum of electronic and thermal Enthalpies= -1107.293311
Sum of electronic and thermal Free Energies= -1107.343841

Si	-0.08952100	0.15507900	1.06437100
C	-0.99412800	1.71829700	1.58391600

H	-0.48573100	2.61385200	1.21717400
H	-1.04287000	1.78484300	2.67532900
H	-2.01838300	1.73120500	1.20232800
C	1.70873800	0.16967300	1.60059100
H	2.23129300	1.04751000	1.21133900
H	2.23862400	-0.72097500	1.25420600
H	1.77705900	0.19763000	2.69263500
C	-0.99561500	-1.39792200	1.60183700
H	-0.48024200	-2.29961500	1.26232900
H	-2.01436700	-1.42094800	1.20589000
H	-1.06104200	-1.43911800	2.69362700
C	-0.10305800	0.17830400	-0.88876300
F	0.52879100	1.28357500	-1.38313600
F	-1.37611500	0.22326400	-1.38158400
Cl	0.70389500	-1.27152000	-1.62951600

Cl^- in Gas Phase

Zero-point correction= 0.000000 (Hartree/Particle)
Sum of electronic and zero-point Energies= -460.303727
Sum of electronic and thermal Enthalpies= -460.301367
Sum of electronic and thermal Free Energies= -460.318750

$Me_3SiCF_2Cl^{\bullet -}$ radical anion in Gas Phase

Zero-point correction= 0.121072(Hartree/Particle)
Sum of electronic and zero-point Energies= -1107.287392
Sum of electronic and thermal Enthalpies= -1107.274490
Sum of electronic and thermal Free Energies= -1107.325891

Si	-0.08722500	0.15049500	1.10607000
C	-0.99818300	1.72614200	1.58041700
H	-0.47878500	2.61518800	1.20199800
H	-1.04833500	1.80246600	2.67096200
H	-2.02418800	1.72477200	1.19249300
C	1.72451000	0.17336800	1.59848600
H	2.22923700	1.06166700	1.19841200
H	2.25000000	-0.72118100	1.24451700
H	1.80242200	0.20275500	2.68941500
C	-1.00677900	-1.41076500	1.59876800
H	-0.48404000	-2.31000900	1.25284300
H	-2.02507400	-1.41472300	1.19015000
H	-1.07977800	-1.45954900	2.68924800
C	-0.10460400	0.18091700	-0.86334600
F	0.52881500	1.28267300	-1.36950400
F	-1.37544000	0.22487700	-1.36802100
Cl	0.70477500	-1.27595700	-1.63033700

$Cl^{\cdot}$ radical in Gas Phase

Zero-point correction= 0.000000 (Hartree/Particle)
Sum of electronic and zero-point Energies= -460.166883

Sum of electronic and thermal Enthalpies= -460.164522
Sum of electronic and thermal Free Energies= -460.182560

(Cl)$Me_3SiCF_2Cl^-$ in Gas Phase

Zero-point correction= 0.123119(Hartree/Particle)
Sum of electronic and zero-point Energies= -1567.634720
Sum of electronic and thermal Enthalpies= -1567.619708
Sum of electronic and thermal Free Energies= -1567.676718

Si	0.16867800	0.54540100	0.77371500
Cl	0.22566700	0.27086800	4.40370400
C	0.18288300	0.65509900	-1.20322500
F	1.31926400	1.24347500	-1.69316700
F	0.13215200	-0.57620500	-1.80231600
Cl	-1.22139300	1.61423200	-1.91203300
C	0.30998100	2.31942200	1.35620800
H	1.22777000	2.78897700	0.98964100
H	0.33330700	2.29255400	2.45024000
H	-0.54206400	2.92164800	1.02887900
C	1.68071000	-0.49926400	1.14761100
H	2.59863400	-0.02822900	0.78364700
H	1.60194600	-1.49561100	0.70269500
H	1.73272800	-0.59567100	2.23709200
C	-1.45068200	-0.29204000	1.20080900
H	-1.46595400	-0.41160400	2.28889500
H	-1.52861300	-1.27658500	0.72983500
H	-2.31092400	0.30871400	0.89304200

Cl-Me_3Si-CF_2Cl^- transition state (**10**) in Gas Phase

Imaginary Frequency: - 62.1942cm^{-1}
Zero-point correction= 0.120457(Hartree/Particle)
Sum of electronic and zero-point Energies= -1567.613120
Sum of electronic and thermal Enthalpies= -1567.597661
Sum of electronic and thermal Free Energies= -1567.658494

Si	1.27910800	-0.04485300	-0.00669700
C	0.74875300	-0.86812300	1.59215200
H	1.12628600	-0.31093100	2.45473600
H	1.15801900	-1.88141700	1.63960500
H	-0.33871300	-0.91952000	1.64548100
C	1.31316500	1.83585700	-0.04652900
H	1.72455400	2.22462100	0.88995300
H	0.31084500	2.23887700	-0.18681300
H	1.95819400	2.17692100	-0.86183900
C	0.73623900	-0.90226100	-1.58131200
H	1.10799000	-0.36514000	-2.45911500
H	-0.35266600	-0.95301600	-1.62227300
H	1.14017900	-1.91832100	-1.61103700
C	-1.81142500	0.63134700	0.04916100

F	-2.39916100	1.13636600	1.19491300
F	-2.40209700	1.40622100	-0.93324100
Cl	-2.89030300	-1.18195100	-0.17524600
Cl	3.44672600	-0.45087500	0.00424600

CF_2Cl^- (**11**) in Gas Phase

Zero-point correction= 0.007443(Hartree/Particle)
Sum of electronic and zero-point Energies= -698.092687
Sum of electronic and thermal Enthalpies= -698.087236
Sum of electronic and thermal Free Energies= -698.120823

C	0.69822000	0.48502800	-0.04999600
F	0.44951400	0.42179900	-1.40474400
F	-0.16664100	1.48710700	0.33559600
Cl	-0.49599600	-1.30920200	0.62668100

Me_3SiCl in Gas Phase

Zero-point correction= 0.112227(Hartree/Particle)
Sum of electronic and zero-point Energies= -869.505232
Sum of electronic and thermal Enthalpies= -869.495680
Sum of electronic and thermal Free Energies= -869.537819

Si	-0.32209600	-0.00000500	-0.11454700
C	-0.24427600	0.00004900	-1.98833700
H	0.27884000	-0.88409900	-2.36174300
H	0.27884500	0.88421600	-2.36169300
H	-1.25373000	0.00006400	-2.41306500
C	-1.14053200	1.55208200	0.54761800
H	-0.62491200	2.45051600	0.19865000
H	-1.13701800	1.56440000	1.64063800
H	-2.18171700	1.60837500	0.21259500
C	-1.14054400	-1.55212500	0.54752800
H	-0.62493200	-2.45054300	0.19850600
H	-2.18172900	-1.60838900	0.21250200
H	-1.13702800	-1.56450600	1.64054700
Cl	1.66951800	-0.00003400	0.58956000

CF_2 in Gas Phase

Zero-point correction= 0.006749 (Hartree/Particle)
Sum of electronic and zero-point Energies= -237.767613
Sum of electronic and thermal Enthalpies= -237.763667
Sum of electronic and thermal Free Energies= -237.791677

C	0.25559400	-0.41245000	0.34319300
F	0.21005700	-0.37478200	-0.96330300
F	-0.38702600	0.66035600	0.72573500

Tetramethylethylene (**6a**) in Gas Phase

Zero-point correction= 0.162751 (Hartree/Particle)
Sum of electronic and zero-point Energies= -235.760940
Sum of electronic and thermal Enthalpies= -235.751233
Sum of electronic and thermal Free Energies= -235.794532

C	-0.03312900	-0.01792900	0.67477200
C	0.02913000	0.01838900	-0.66994400
C	-0.10135000	1.20786600	1.55873800
H	-0.04004100	2.15194900	1.02150500
H	0.71411900	1.19079600	2.29172400
H	-1.03393300	1.21196400	2.13632100
C	-0.04393100	-1.29021100	1.49291900
H	-0.92672500	-1.31432400	2.14310200
H	0.82830800	-1.32584100	2.15711000
H	-0.04727400	-2.20262000	0.90059900
C	0.11101600	-1.20685000	-1.55344900
H	-0.76020800	-1.25837100	-2.21795200
H	0.17008700	-2.14787600	-1.01070300
H	0.99107000	-1.14496900	-2.20489700
C	0.02577800	1.29027900	-1.48873100
H	-0.08735600	2.19928000	-0.90203300
H	-0.78948500	1.26589300	-2.22176800
H	0.95517500	1.37757700	-2.06481200

Tetramethylethylene + CF_2 Transition State in Gas Phase

Imaginary Frequency: - 260.4629cm^{-1}
Zero-point correction= 0.171837(Hartree/Particle)
Sum of electronic and zero-point Energies= -473.521195
Sum of electronic and thermal Enthalpies= -473.508925
Sum of electronic and thermal Free Energies= -473.558167

C	-1.51957500	-1.26035100	0.09921000
C	0.56795300	0.12470100	0.02244900
C	-0.75571300	0.51821000	-0.16710900
F	-1.16732800	-1.75220300	1.31279900
F	-0.97859700	-2.14432400	-0.77531100
C	-1.27806000	0.83259200	-1.56124500
H	-0.95055900	1.83334900	-1.86307300
H	-2.36882800	0.81708300	-1.55431800
H	-0.94336900	0.12026700	-2.31349900
C	-1.48886200	1.29865200	0.91401100
H	-1.31173000	0.90940500	1.91536600
H	-2.56326800	1.25938900	0.72911200
H	-1.17479200	2.34781100	0.89074700
C	1.17895600	0.02542900	1.38817700
H	2.26630400	0.10876500	1.33336800
H	0.95220700	-0.96036500	1.82561000
H	0.81069600	0.77677500	2.08577300
C	1.39494300	-0.45400000	-1.08531400
H	2.45716500	-0.26729600	-0.91254400
H	1.13398600	-0.07310800	-2.07135800

H	1.26069900	-1.54757500	-1.11373900

2,2-difluorotetramethylcyclopropane in Gas Phase

Zero-point correction= 0.176401(Hartree/Particle)
Sum of electronic and zero-point Energies= -473.593860
Sum of electronic and thermal Enthalpies= -473.582224
Sum of electronic and thermal Free Energies= -473.628650

C	0.82601800	0.24761000	0.20575200
C	-0.57411200	-0.41021600	0.53558200
C	-0.27025100	0.17517800	-0.79858600
F	-0.14485400	-0.63800200	-1.88737700
F	-0.90124600	1.31708500	-1.19978900
C	-0.66875300	-1.92208100	0.66959500
H	-0.07174200	-2.45561100	-0.06784200
H	-1.70743500	-2.24111500	0.54188300
H	-0.34469800	-2.23595400	1.66671900
C	-1.53992800	0.32317200	1.45378300
H	-1.26301600	0.16735900	2.50106300
H	-2.55175400	-0.06939700	1.31558200
H	-1.57949300	1.39477500	1.26612300
C	1.17056300	1.59699700	0.81596000
H	1.97565200	2.06788100	0.24398600
H	1.52300700	1.47164200	1.84444600
H	0.33039100	2.28897100	0.82355300
C	2.04216900	-0.64835000	0.02985500
H	2.82403100	-0.10852000	-0.51259600
H	1.82773600	-1.55720900	-0.52965600
H	2.44988100	-0.93259000	1.00492300

Tetramethylethylene + CF_2Cl^- Transition State in Gas Phase

Imaginary Frequency: -309.6489 cm^{-1}
Zero-point correction= 0.171280(Hartree/Particle)
Sum of electronic and zero-point Energies= -933.829448
Sum of electronic and thermal Enthalpies= -933.815106
Sum of electronic and thermal Free Energies= -933.869467

C	0.29311900	-1.03599600	-0.34393100
F	1.31944800	-1.03322100	-1.23031700
F	0.87042600	-1.43066400	0.81766300
Cl	-0.85117900	-3.09968300	-0.99483400
C	-0.40766400	0.75645400	-0.15262100
C	-0.97959800	0.94322100	-1.55542000
H	-0.20925700	0.93964900	-2.32635700
H	-1.52220700	1.89531900	-1.61423600
H	-1.66839500	0.12693300	-1.78109000
C	-1.52331900	0.47966300	0.85115600
H	-1.14649500	0.16960900	1.82568900
H	-2.16043100	-0.32446100	0.47766900
H	-2.13202000	1.38233300	0.98921800

C	0.71434400	1.50200900	0.24251800
C	1.74817700	1.97196200	-0.74689900
H	2.24630100	2.88041900	-0.38344000
H	1.33715100	2.19807300	-1.73217100
H	2.54356000	1.21761900	-0.89894900
C	1.21790000	1.49552000	1.66182500
H	1.74028900	2.43348600	1.89221100
H	1.94652400	0.68056500	1.83393600
H	0.42788400	1.37212100	2.40420300

F^- in Gas Phase

Zero-point correction= 0.000000 (Hartree/Particle)
Sum of electronic and zero-point Energies= -99.888693
Sum of electronic and thermal Enthalpies= -99.886333
Sum of electronic and thermal Free Energies= -99.902852

(F)$Me_3SiCF_2Cl^-$ (12) in Gas Phase

Zero-point correction= 0.123145(Hartree/Particle)
Sum of electronic and zero-point Energies= -1207.274408
Sum of electronic and thermal Enthalpies= -1207.259756
Sum of electronic and thermal Free Energies= -1207.315456

Si	-0.16163800	-1.06806900	0.03488200
C	-0.19707600	1.10850100	0.14567200
F	-1.26014400	1.71505800	-0.49432100
F	-0.26059100	1.62570000	1.42455700
Cl	1.33151900	1.98707000	-0.61131900
C	-0.11173400	-0.94473800	-1.87106500
H	0.92849500	-1.00785900	-2.20968600
H	-0.52964900	-0.01714600	-2.26680700
H	-0.64540500	-1.79678200	-2.30106300
C	-1.85946900	-1.03070100	0.91958200
H	-1.77952700	-0.54773400	1.89881200
H	-2.22930600	-2.04909400	1.05951700
H	-2.59726500	-0.46394300	0.34275700
C	1.42866200	-1.08649800	1.09556600
H	2.26914300	-1.40264200	0.46771200
H	1.31723500	-1.84540200	1.87637900
H	1.69041500	-0.13297100	1.55612300
F	-0.13091800	-2.84222100	-0.04604600

F-Me_3Si-CF_2Cl^- transition state (13) in Gas Phase

Imaginary Frequency: -54.4719 cm^{-1}
Zero-point correction= 0.121315 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1207.269141
Sum of electronic and thermal Enthalpies= -1207.254131
Sum of electronic and thermal Free Energies= -1207.312675

Si	1.56979800	-0.18555700	-0.06388000

C	-1.44328300	0.73528400	0.06240800
F	-1.88375600	1.54211300	1.09589000
F	-2.06749800	1.31102000	-1.02603500
Cl	-2.68436000	-0.98885100	0.35271500
C	1.06982400	-1.05884600	1.51736000
H	1.43848000	-2.09005300	1.50296000
H	-0.01594900	-1.07707300	1.62179000
H	1.50321300	-0.56013100	2.39064100
C	1.66782200	1.69331700	0.04648300
H	1.54799400	2.15015000	-0.94041300
H	2.64821700	1.98416200	0.44010400
H	0.88655500	2.09501000	0.69196100
C	0.86265500	-0.93605500	-1.63160600
H	-0.21399700	-1.08173600	-1.54193900
H	1.34170100	-1.90294600	-1.82069000
H	1.05514700	-0.29133300	-2.49519100
F	3.20499500	-0.58199800	-0.20307600

Me_3SiF in Gas Phase

Zero-point correction= 0.113077(Hartree/Particle)
Sum of electronic and zero-point Energies= -509.164502
Sum of electronic and thermal Enthalpies= -509.155228
Sum of electronic and thermal Free Energies= -509.196223

Si	0.00495200	-0.00810000	0.00264600
C	-1.74329300	-0.08648700	0.66978000
H	-1.74670500	-0.09805900	1.76339200
H	-2.25712500	-0.98777700	0.32360800
H	-2.32940500	0.77851600	0.34307200
C	0.94727600	1.46628000	0.66992700
H	1.98425300	1.46187000	0.32238600
H	0.96041500	1.46339400	1.76354800
H	0.48967300	2.40588300	0.34392800
C	0.04997700	-0.08617800	-1.86774500
H	1.07926800	-0.10048900	-2.23722600
H	-0.45161400	0.78064200	-2.30988400
H	-0.45093700	-0.98576600	-2.23643100
F	0.78038500	-1.35380800	0.55131900

CF_3^- in Gas Phase

Zero-point correction= 0.008835(Hartree/Particle)
Sum of electronic and zero-point Energies= -337.731374
Sum of electronic and thermal Enthalpies= -337.726635
Sum of electronic and thermal Free Energies= -337.757663

C	-0.25645100	0.44449300	0.18139400
F	-0.14814800	0.25790000	-1.24409600
F	1.12311300	0.25798700	0.55484600
F	-0.78578700	-0.84356200	0.55549200