Electronic Supplementary Information for

# Investigation of high Δε derivatives of the [*closo*-1-$CB_9H_{10}$]$^-$ anion for liquid crystal display applications.

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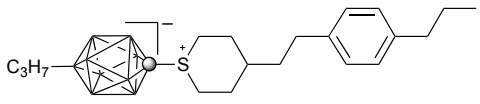
## 1. Synthetic Details

Reagents and solvents were obtained commercially or synthesized. $NEt_3$ was distilled over $CaH_2$ and DMF was stored over freshly activated 4 Å molecular sieves. All other reagents were used as supplied. Reactions were carried out under Ar and subsequent manipulations were conducted in air. NMR spectra were obtained at 128 MHz ($^{11}B$) and 400 MHz ($^{1}H$) in $CDCl_3$ or $CD_3CN$. $^{11}B$ chemical shifts were referenced to the solvent ($^{1}H$) or to an external sample of $B(OH)_3$ in MeOH ($^{11}B$, $\delta$ = 18.1 ppm). Optical microscopy and phase identification were performed using a PZO "Biopolar" polarized microscope equipped with a HCS400 Instec hot stage. Thermal analysis was obtained using a TA Instruments 2920 DSC. Transition temperatures and enthalpies were obtained using small samples and a heating rate of 5 $K \cdot min^{-1}$.

**Preparation of sulfonium derivative 3[n]. General procedure.**

To a solution of anhydrous $ZnCl_2$ (12 eq) in a dry THF (10 mL), a solution of $C_nH_{2n+1}MgBr$ (12 eq, 2M in $Et_2O$ or freshly prepared from $C_nH_{2n+1}Br$ in THF) was added at 0 °C under $N_2$ atmosphere. The mixture was stirred for 15 min at rt, NMP was added (5 mL) followed by $Pd_2dba_3$ (2 mol%), $[HPCy_3]^+[BF_4]^-$ (8 mol%) and iodide **3**[1] (1.0 mmol). The mixture was stirred overnight at rt, 10% HCl was added, the products were extracted ($Et_2O$), the extracts were dried ($Na_2SO_4$) and the solvent was evaporated. The resulting residue was purified using a short silica gel column (hexane/$CH_2Cl_2$, 1:1). The pure product was obtained in about 90% yield by triple recrystallization (toluene/*iso*-octane) as white crystals.

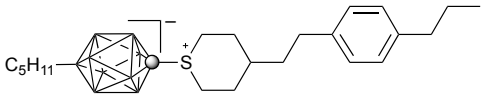
**Compound 3[3]b.**




Mp 225 °C (DSC); $^{1}H$ NMR (400 MHz, $CDCl_3$) $\delta$ 0.40-2.50 (br m, 8H), 0.95 (t, $J$ = 7.3 Hz, 3H), 1.18 (t, $J$ = 7.2 Hz, 3H), 1.64 (sext, $J$ = 7.5 Hz, 2H), 1.70-1.79 (m, 3H), 1.80-1.89 (m, 2H), 1.90-1.97 (m, 2H), 2.08 (t, $J$ = 7.9 Hz, 2H), 2.48-2.51 (m, 2H), 2.57 (t, $J$ = 7.7 Hz, 2H), 2.69 (t, $J$ = 7.5 Hz, 2H), 3.63 (br t, $J$ = 12.5 Hz, 2H), 4.05 (br d, $J$ = 12.1 Hz, 2H), 7.09 (d, $J$ = 8.0 Hz,

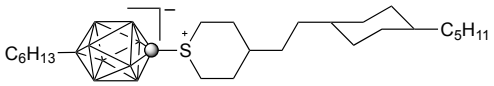
2H), 7.14 (d, $J$ = 8.1 Hz, 2H); $^{11}$B NMR (128 MHz, $CDCl_3$) δ -24.4 (d, $J$ = 143 Hz, 4B), -16.2 (d, $J$ = 145 Hz, 4B), 54.1 (s, 1B). Anal. Calcd. for $C_{20}H_{39}B_9S$: C, 58.75; H, 9.61. Found: C, 59.04; H, 9.31.

**Compound 3[5]b.**



Mp 195 °C; $^1$H NMR (400 MHz, $CDCl_3$) δ 0.40-2.50 (br m, 8H), 0.94 (t, $J$ = 7.3 Hz, 6H), 1.44 (sext, $J$ = 7.3 Hz, 2H), 1.53-1.60 (m, 3H), 1.64 (sext, $J$ = 7.5 Hz, 2H), 1.71-1.79 (m, 2H), 1.80-1.85 (m, 2H), 1.86-1.96 (m, 2H), 2.05-2.11 (m, 2H), 2.50-2.55 (m, 2H), 2.57 (t, $J$ = 7.7 Hz, 2H), 2.70 (t, $J$ = 7.5 Hz, 2H), 3.66 (br t, $J$ = 12.2 Hz, 2H), 4.07 (br d, $J$ = 12.1 Hz, 2H), 7.08 (d, $J$ = 8.0 Hz, 2H), 7.14 (d, $J$ = 8.1 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 13.8, 14.3, 19.5 (br), 22.9, 24.5, 29.7 (2C), 31.8, 32.1, 34.8, 35.5, 37.4, 37.6, 44.0 (2C), 128.0, 128.7, 137.9, 140.7; $^{11}$B NMR (128 MHz, $CDCl_3$) δ -24.5 (d, $J$ = 141 Hz, 4B), -16.2 (d, $J$ = 141 Hz, 4B), 54.7 (s, 1B). Anal. Calcd. for $C_{22}H_{43}B_9S$: C, 60.48; H, 9.92. Found: C, 60.61; H, 9.77.

**Compound 3[6]c**.



Mp 258 °C; $^1$H NMR (400 MHz, $CDCl_3$) δ 0.40-2.50 (br m, 8H), 0.88 (t, $J$ = 7.1 Hz, 3H), 0.91 (t, $J$ = 7.0 Hz, 3H), 1.12-1.20 (m, 4H), 1.21-1.33 (m, 13H), 1.34-1.47 (m, 6H), 1.55-1.62 (m, 2H), 1.69-1.86 (m, 6H), 1.86-1.98 (m, 2H), 2.08 (t, $J$ = 8.1 Hz, 2H), 2.50 (br d, $J$ = 15.4 Hz, 2H), 3.68 (br t, $J$ = 12.7, Hz, 2H), 4.07 (br d, $J$ = 12.1 Hz, 2H); $^{11}$B NMR (400 MHz, $CDCl_3$) δ -24.5 (d, $J$ = 141 Hz, 4B), -16.2 (d, $J$ = 141 Hz, 4B), 54.7 (s, 1B). HRMS, calcd. for $C_{25}H_{55}B_9S$ *m/z* 486.4873; found *m/z* 486.4893.

**Preparation of Esters 4[n]. General procedure.**

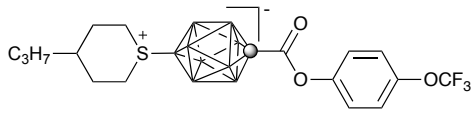
**Method A. Esters of phenols.** The sulfonium acid (0.16 mmol) was suspended in $CH_2Cl_2$ (1 mL) and was treated with $(COCl)_2$ (3 eq) and anhydrous DMF (catalytic amount). The suspension began to bubble and became homogenous and was stirred vigorously for 30 min at rt.

The light yellow solution was evaporated to dryness. The residue was redissolved in anhydrous $CH_2Cl_2$ (1 mL) and the appropriate phenol **10** (1.1 eq) and freshly distilled $NEt_3$ (3 eq) were added. The mixture was stirred at rt overnight. The reaction mixture was washed with 5% HCl, dried ($Na_2SO_4$) and evaporated to dryness. The product was isolated by column chromatography ($SiO_2$), the eluent was filtered through a cotton plug and the solvent evaporated to give the desired ester in about 60% yield. The resulting esters were purified further by repeated recrystallization.

**Method B. Esters of cyclohexanols.** The acid chloride derived from the sulfonium acid was generated as in Method A. The crude acid chloride, excess alcohol **11** (5 eq), and freshly distilled pyridine (5 eq) were stirred and heated for 3 days at 90 °C, protected from moisture. At times, the reaction was cooled to rt, and minimal amount of anhydrous $CH_2Cl_2$ was added to wash the sides of the flask. The product was purified as in Method A.

* NMR spectra of all esters **4[n]** recorded at ambient temperature show the presence of minor quantities (about 20%) of the *cis* isomer, (**4[n]-*cis***) with characteristic signals at 2.08-2.15 (m), 2.28-2.35 (m) and 3.55-3.65 (m) ppm in the $^1$H NMR spectra. The B(10) signals of the *cis* isomers are shifted upfield by about 1 ppm relative to the *trans* isomers in $^{11}$B NMR spectra. In addition, in compounds **4[n]h** the pyrimidine ring of the *cis* isomer is shifted downfield by about 0.01 ppm relative to the *trans* isomer **4[n]h-*trans***.

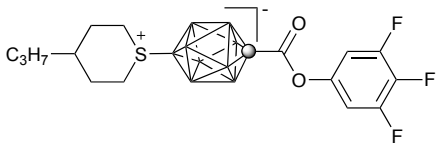
**Ester 4[3]c.**




The ester was obtained in 65% yield, purified by column chromatography ($CH_2Cl_2$/hexane, 1:3) followed by recrystallization from *iso*-octane/toluene (2x) and then methanol/water (2x) to give a white crystalline solid: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.96 (t, $J$ = 5.6 Hz, 3H), 1.39-1.43 (m, 5H), 1.67-1.79 (m, 2H), 2.38 (br d, $J$ = 11.6 Hz, 2H), 3.44 (br t, $J$ = 10.4, 2H), 3.72 (br d, $J$ = 10.0 Hz, 2H), 7.29 (d, $J$ = 6.8 Hz, 2H), 7.37-7.40 (m,

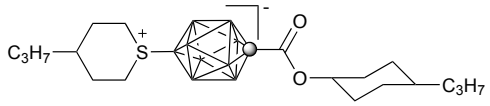
2H); {$^1$H}$^{11}$B NMR (128 MHz, $CDCl_3$) δ -19.6 (4B), -14.0 (4B), 32.0 (1B). Anal. Calcd. for $C_{17}H_{28}B_9F_3O_3S$: C, 43.75; H, 6.05. Found: C, 43.94; H, 6.07.

**Ester 4[3]d.**



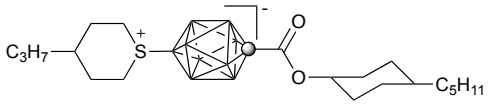

The ester was obtained in 58% yield, purified by column chromatography ($CH_2Cl_2$) followed by recrystallization from *iso*-octane/toluene (2x) and then methanol/water (2x) to give a white crystalline solid: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.96 (t, $J$ = 5.6 Hz, 3H), 1.39-1.43 (m, 5H), 1.67-1.79 (m, 2H), 2.33 (br d, $J$ = 11.2 Hz, 2H), 3.44 (br t, $J$ = 10.4 Hz, 2H), 3.71 (br d, $J$ = 10.8 Hz, 2H), 7.07 (t, $J$ = 5.6 Hz, 2H); {$^1$H}$^{11}$B NMR (128 MHz, $CDCl_3$) δ -19.6 (4B), -13.9 (4B), 32.4 (1B). Anal. Calcd. for $C_{16}H_{26}B_9F_3O_2S$: C, 44.00; H, 6.00. Found: C, 44.03; H, 6.07.

**Ester 4[3]e.**



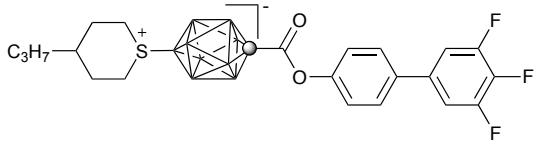

The ester was obtained in 77% yield, purified by column chromatography ($CH_2Cl_2$/hexane, 1:2) followed by recrystallization from *iso*-octane/toluene (2x) to give a white crystalline solid: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.89 (t, $J$ = 5.8 Hz, 3H), 0.96 (t, $J$ = 5.6 Hz, 3H), 1.05-1.12 (m, 2H), 1.18-1.23 (m, 2H), 1.28-1.32 (m, 3H), 1.39-1.43 (m, 5H), 1.47-1.59 (m, 2H), 1.67-1.79 (m, 2H), 1.83 (br d, $J$ = 10.4 Hz, 2H), 2.18 (d, $J$ = 8.4 Hz, 2H), 2.33 (br d, $J$ = 11.2 Hz, 2H), 3.44 (br t, $J$ = 10.4 Hz, 2H), 3.71 (br d, $J$ = 10.8 Hz, 2H), 4.98-5.06 (m, 1H); {$^1$H}$^{11}$B NMR (128 MHz, $CDCl_3$) δ -19.7 (4B), -14.3 (4B), 30.4 (1B). Anal. Calcd. for $C_{19}H_{41}B_9O_2S$: C, 52.96; H, 9.59. Found: C, 53.24; H, 9.72.

**Ester 4[3]f.**



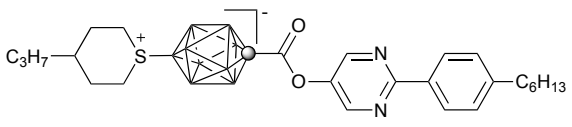
The ester was prepared by method B in 59% yield, purified by column chromatography ($CH_2Cl_2$) followed by recrystallization from *iso*-octane/toluene (2x) to give a white crystalline solid: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.89 (t, *J* = 7.12 Hz, 3H), 0.95 (t, *J* = 6.7 Hz, 3H), 1.04-1.13 (m, 2H), 1.15-1.30 (m, 7H), 1.35-1.43 (m, 5H), 1.45-1.59 (m, 2H), 1.64-1.76 (m, 2H), 1.84 (d, *J* = 12.9 Hz, 2H), 2.18 (d, *J* = 9.0 Hz, 2H), 2.33 (br d, *J* = 12.8 Hz, 2H), 3.41 (br t, *J* = 12.8 Hz, 2H), 3.69 (br d, *J* = 12.9 Hz, 2H), 4.98-5.06 (m, 1H); {$^1$H}$^{11}$B NMR (128 MHz, $CDCl_3$) δ -19.8 (4B), -14.5 (4B), 31.0 (1B). Anal. Calcd. for $C_{21}H_{45}B_9O_2S$: C, 54.96; H, 9.88. Found: C, 55.08; H, 9.82.

**Ester 4[3]g.**



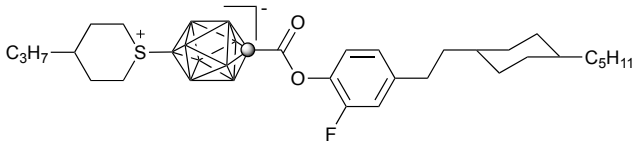
The ester was obtained in 64% yield, purified by column chromatography ($CH_2Cl_2$) followed by recrystallization from *iso*-octane/toluene (2x) and then $CH_3CN$ (2x) to give a white crystalline solid: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.96 (t, *J* = 6.5 Hz, 3H), 1.41-1.42 (m, 5H), 1.67-1.77 (m, 2H), 2.36 (br d, *J* = 14.0 Hz, 2H), 3.44 (br t, *J* = 10.4 Hz, 2H), 3.72 (br d, *J* = 12.7 Hz, 2H), 7.21 (t, *J* = 7.6 Hz Hz, 2H), 7.43 (d, *J* = 8.6 Hz, 2H), 7.58 (d, *J* = 8.6 Hz, 2H); {$^1$H} $^{11}$B NMR (128 MHz, $CDCl_3$) δ -19.6 (4B), -13.9 (4B), 32.0 (1B). Anal. Calcd. for $C_{22}H_{30}B_9F_3O_2S$: C, 51.53; H, 5.90. Found: C, 51.70; H, 6.00.

**Ester 4[3]h.**



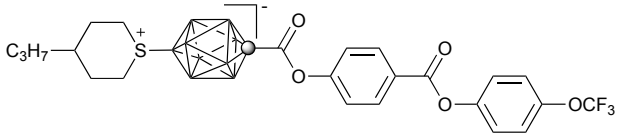
The ester was obtained in 66% yield, purified by column chromatography ($CH_2Cl_2$/hexane, 2:1) followed by recrystallization from *iso*-octane/toluene (2x) to give a white crystalline solid: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.89 (t, *J* = 6.9 Hz, 3H), 0.96 (t, *J* = 6.6 Hz, 3H), 1.25-1.45 (m, 9H), 1.65-1.79 (m, 6H), 2.41 (br d, *J* = 11.2 Hz, 2H), 2.69 (t, *J* = 7.8 Hz, 2H), 3.44 (br t, *J* = 10.4, 2H), 3.71 (br d, *J* = 10.8 Hz, 2H), 7.30 (t, *J* = 8.2 Hz, 2H), 8.36 (s, 2H); {$^1$H}$^{11}$B NMR (128 MHz, $CDCl_3$) δ -19.5 (4B), -13.9 (4B), 32.9 (1B). Anal. Calcd. for $C_{26}H_{43}B_9N_2O_2S$: C, 57.30; H, 7.95; N, 5.14. Found: C, 57.44; H, 8.07; N, 5.19.

**Ester 4[3]i.**




The ester was obtained in 88% yield, purified by column chromatography ($CH_2Cl_2$) followed by recrystallization from *iso*-octane/toluene (2x) and then methanol with few drops of acetone (2x) to give a white crystalline solid: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.88 (t, *J* = 7.2 Hz, 3H), 0.96 (t, *J* = 6.5 Hz, 3H), 1.14-1.16 (m, 4H), 1.21-1.29 (m, 8H), 1.39-1.41 (m, 5H), 1.50-1.54 (m, 2H), 1.69-1.73 (m, 8H), 2.39 (br d, *J* = 12.9 Hz, 2H), 2.63 (t, *J* = 8.1 Hz, 2H), 3.43 (br t, *J* = 11.5 Hz, 2H), 3.73 (br d, *J* = 10.4 Hz, 2H), 6.98 (d, *J* = 8.1 Hz, 1H), 7.03 (d, *J* = 12.6 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 1H); {$^1$H}$^{11}$B NMR (128 MHz, $CDCl_3$) δ -19.6 (4B), -13.9 (4B), 32.0 (1B). Anal. Calcd. for $C_{29}H_{52}B_9FO_2S$: C, 59.94; H, 9.02. Found: C, 59.93; H, 8.91.

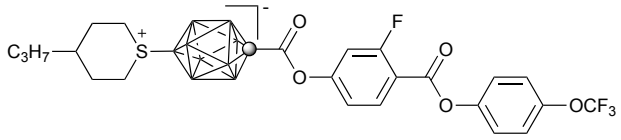
**Ester 4[3]j.**




The ester was obtained in 57% yield, purified by column chromatography ($CH_2Cl_2$) followed by recrystallization from *iso*-octane/toluene (2x) then $CH_3OH$ (2x) to give a white crystalline solid: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.94 (t, *J* = 6.8 Hz, 3H), 1.37-1.43 (m, 5H), 1.65-1.80 (m, 2H), 2.39 (br d, *J* = 12.2 Hz, 2H), 3.44 (br t, *J* = 12.8 Hz, 2H),

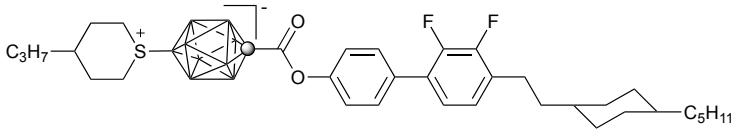
3.72 (br d, $J$ = 12.6 Hz, 2H), 7.27 (s, 4H), 7.52 (d, $J$ = 8.8 Hz, 2H), 8.29 (d, $J$ = 8.8 Hz, 2H); $\{^1H\}^{11}B$ NMR (128 MHz, $CDCl_3$) δ -19.3 (4B), -13.7 (4B), 32.4 (1B). Anal. Calcd. for $C_{24}H_{32}B_9F_3O_5S$: C, 49.12; H, 5.50. Found: C, 49.20; H, 5.51.

**Ester 4[3]k.**




The ester was prepared by method A in 66% yield, purified by column chromatography ($CH_2Cl_2$ then $CH_3CN$) followed by recrystallization from hexane/ethyl acetate (2x) to give a white crystalline solid: $^1H$ NMR ($CD_3CN$, 400 MHz) δ 0.6-2.8 (br m, 8H) 0.94 (t, $J$ = 6.8 Hz, 3H). 1.30-1.43 (m, 5H), 1.62-1.80 (m, 2H), 2.34 (br d, $J$ = 11.9 Hz, 2H), 3.43 (br t, $J$ = 12.0 Hz, 2H), 3.78 (d, $J$ = 12.0 Hz, 2H), 7.36-7.45 (m, 6H), 8.27 (t, $J$ = 8.6 Hz, 1H); $^1H$ NMR ($CDCl_3$, 400 MHz) δ 0.6-2.8 (br m, 8H) 0.96 (t, $J$ = 6.5 Hz, 3H). 1.35-1.46 (m, 5H), 1.63-1.82 (m, 2H), 2.40 (d, $J$ = 11.9 Hz, 2H), 3.44 (t, $J$ = 12.9 Hz, 2H), 3.73 (d, $J$ = 13.0 Hz, 2H), 7.28-7.36 (m, 6H), 8.20 (t, $J$ = 8.4 Hz, 1H); $\{^1H\}^{11}B$ NMR ($CD_3CN$, 128 MHz) δ -20.0 (4B), -14.2 (4B), 34.0 (1B); $\{^1H\}$ $^{11}B$ NMR ($CDCl_3$, 128 MHz) δ -19.5 (4B), -13.8 (4B), 32.6 (1B). Anal. Calcd. for $C_{24}H_{31}B_9F_4O_5S$: C, 47.66; H, 5.17. Found: C, 47.61; H, 5.32.

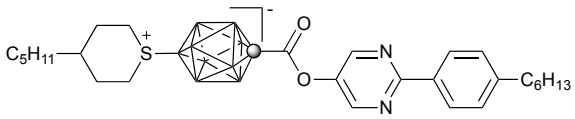
**Ester 4[3]l.**




The ester was obtained in 61% yield, purified by column chromatography ($CH_2Cl_2$) followed by recrystallization from *iso*-octane/toluene (2x) and then $CH_3CN$ (2x) to give a white crystalline solid: $^1H$ NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.88 (t, $J$ = 7.2 Hz, 3H), 0.96 (t, $J$ = 6.5 Hz, 3H), 1.14-1.16 (m, 4H), 1.21-1.29 (m, 8H), 1.39-1.41 (m, 5H), 1.50-1.54 (m, 2H), 1.69-1.73 (m, 8H), 2.39 (br d, $J$ = 12.9 Hz, 2H), 2.63 (t, $J$ = 8.1 Hz, 2H), 3.43 (br t, $J$ = 11.5 Hz, 2H), 3.73 (br d, $J$ = 10.4 Hz, 2H), 6.99 (t, $J$ = 7.4 Hz, 1H), 7.13 (t, $J$ = 6.7 Hz, 1H), 7.42 (d, $J$ =

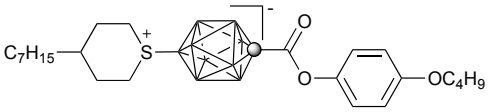
7.6 Hz, 2H), 7.62 (d, $J$ = 8.6 Hz, 2H); $\{^1H\}^{11}B$ NMR (128 MHz, $CDCl_3$) δ -19.5 (4B), -13.9 (4B), 32.1 (1B). Anal. Calcd. for $C_{35}H_{55}B_9F_2O_2S$: C, 62.26; H, 8.21. Found: C, 62.26; H, 8.11.

**Ester 4[5]h.**



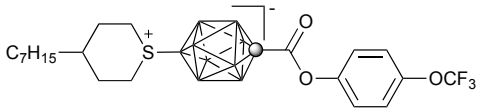

The ester was obtained in 91% yield, purified by column chromatography ($CH_2Cl_2$) followed by recrystallization from hexane (2x) to give a white crystalline solid: $^1H$ NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.90 (t, $J$ = 7.0 Hz, 3H), 0.92 (t, $J$ = 6.7 Hz, 3H), 1.30-1.40 (m, 13H), 1.67-1.77 (m, 6H), 2.40 (br d, $J$ = 12.5 Hz, 2H), 2.69 (t, $J$ = 7.5 Hz, 2H), 3.45 (br t, $J$ = 13.2 Hz, 2H), 3.73 (br d, $J$ = 12.5 Hz, 2H), 7.31 (d, $J$ = 8.2 Hz, 2H), 8.35 (d, $J$ = 8.2 Hz, 2H), 8.86 (s, 2H); $\{^1H\}^{11}B$ NMR (128 MHz, $CDCl_3$) δ -19.5 (4B), -13.8 (4B), 32.9 (1B). Anal. Calcd. for $C_{28}H_{47}B_9N_2O_2S$: C, 58.69; H, 8.27; N, 4.89. Found: C, 58.95; H, 8.19; N, 4.84.

**Ester 4[7]b.**



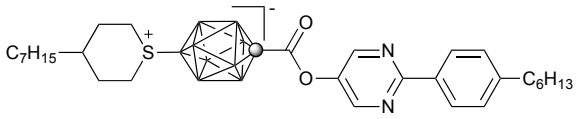

The ester was prepared in 81% yield, purified by column chromatography ($CH_2Cl_2$) followed by recrystallization from *iso*-octane/toluene (2x) and then $CH_3OH$ (2x) to give a white crystalline solid: $^1H$ NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.90 (t, $J$ = 6.5 Hz, 3H), 0.99 (t, $J$ = 7.4 Hz, 3H), 1.25-1.38 (m, 13H), 1.49-1.51 (m, 2H), 1.72-1.80 (m, 4H), 2.37 (br d, $J$ = 12.5 Hz, 2H), 3.43 (br t, $J$ = 11.3 Hz, 2H), 3.71 (br d, $J$ = 12.5 Hz, 2H), 3.98 (t, $J$ = 6.5 Hz, 2H), 6.93 (d, $J$ = 9.0 Hz, 2H), 7.23 (d, $J$ = 9.0 Hz, 2H); $\{^1H\}^{11}B$ NMR (128 MHz, $CDCl_3$) δ -19.7 (4B), -14.2 (4B), 32.5 (1B). Anal. Calcd. for $C_{24}H_{45}B_9O_3S$: C, 56.41; H, 8.88. Found: C, 56.84; H, 8.89.

**Ester 4[7]c.**



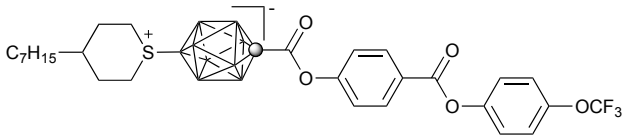
The ester was obtained in 79% yield, purified by column chromatography ($CH_2Cl_2$) followed by recrystallization from *iso*-octane/toluene (2x) and then $CH_3OH$ (2x) to give a white crystalline solid: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.91 (t, *J* = 6.3 Hz, 3H), 1.30-1.39 (m, 11H), 1.70-1.77 (m, 4H), 2.49 (br d, *J* = 13.9 Hz, 2H), 3.44 (br t, *J* = 13.0 Hz, 2H), 3.72 (br d, *J* = 12.4 Hz, 2H), 7.30 (d, *J* = 8.6 Hz, 2H), 7.39 (d, *J* = 9.0 Hz, 2H); {$^1$H} $^{11}$B NMR (128 MHz, $CDCl_3$) δ -19.7 (4B), -14.0 (4B), 32.4 (1B). Anal. Calcd. for $C_{21}H_{36}B_9F_3O_3S$: C, 48.24; H, 6.94. Found: C, 47.39; H, 6.96.

**Ester 4[7]h.**



The ester was obtained in 63% yield, purified by column chromatography ($CH_2Cl_2$) followed by recrystallization from *iso*-octane/toluene (2x) and then $CH_3OH$ (2x) to give a white crystalline solid: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.87-0.92 (m, 6H), 1.25-1.38 (m, 17H), 1.62-1.77 (m, 6H), 2.39 (br d, *J* = 12.6 Hz, 2H), 2.68 (t, *J* = 7.6 Hz, 2H), 3.44 (br t, *J* = 13.1 Hz, 2H), 3.72 (br d, *J* = 12.9 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 8.35 (d, *J* = 8.2 Hz, 2H), 8.86 (s, 2H); {$^1$H} $^{11}$B NMR (128 MHz, $CDCl_3$) δ -19.5 (4B), -13.8 (4B), 32.8 (1B). Anal. Calcd. for $C_{30}H_{51}B_9N_2O_2S$: C, 59.95; H, 8.55; N, 4.66. Found: C, 59.66; H, 8.41; N, 4.59.

**Preparation of ester 4[7]j.**

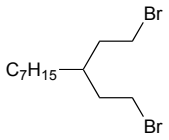


The ester was prepared by method A in 82% yield, purified by column chromatography ($CH_2Cl_2$) followed by recrystallization from *iso*-octane/toluene (2x) and then $CH_3OH$ (2x) to

give a white crystalline solid: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 0.6-2.8 (br m, 8H), 0.90 (t, *J* = 6.6 Hz, 3H), 1.30-1.39 (m, 11H), 1.70-1.77 (m, 4H), 2.49 (br d, *J* = 14.2 Hz, 2H), 3.44 (br t, *J* = 12.7 Hz, 2H), 3.71 (br d, *J* = 12.0 Hz, 2H), 7.29 (s, 4H), 7.52 (d, *J* = 8.7 Hz, 2H). 8.29 (d, *J* = 8.7 Hz, 2H); {$^{1}$H} $^{11}$B NMR (128 MHz, $CDCl_3$) δ -19.4 (4B), -13.7 (4B), 32.0 (1B). Anal. Calcd. for $C_{28}H_{40}B_9F_3O_5S$: C, 52.31; H, 6.27. Found: C, 52.48; H, 6.36.

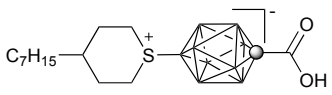
## Intermediates

**Preparation of 1,5-dibromo-3-heptylpentane (8[7]).** [2]




Following a general literature procedure,[3] a biphasic mixture of the 3-heptylpentane-1,5-diol, 47% aqueous HBr (15 eq) and an equal volume of conc. $H_2SO_4$ (relative to HBr) was stirred at 120 °C overnight. The black reaction mixture was cooled to rt, diluted by the addition of half its volume of $H_2O$ and extracted with $CH_2Cl_2$. The organic layers were combined, dried ($MgSO_4$) and evaporated to leave black oil. The oil was passed through a short silica gel plug (hexanes) to give crude dibromide **8[7]** as a slightly brown oil. The dibromide was purified further by short-path distillation (135 °C, 0.7 mmHg) to give 15.4 g (54% yield) of **8[7]** as a colorless oil: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 7.0 Hz, 3H), 1.27 (m, 12H), 1.71-1.74 (m, 1H), 1.77-1.90 (m, 4H), 3.41 (t, *J* = 7.3 Hz, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 14.0, 22.6, 26.0, 29.2, 29.7, 31.2 (2C), 31.8, 32.4, 35.4, 36.6 (2C). Anal. Calcd. for $C_{14}H_{24}Br_2$: C, 43.93; H, 7.37. Found: C, 43.63; H, 7.38.

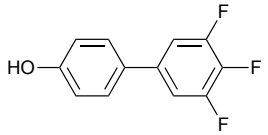
**Preparation of sulfonium acid 9[7].**




The methyl ester **14[7]** (230 mg; 0.61 mmol) was hydrolyzed using KOH (0.17 g, 3.05 mmol) in $CH_3OH$ (3 mL) under reflux overnight. The solvent was evaporated and 10% HCl (5 mL) was added. The solution was extracted with $CH_2Cl_2$ (3x10 mL). The extracts were dried

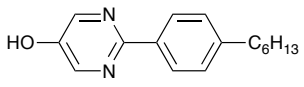
($Na_2SO_4$), evaporated and washed with hot hexane to give 193 mg (87% yield) of a white solid. The crude acid was recrystallized from *iso*-octane/toluene (2x) and then cold $CH_3CN$ (2x) to give acid **9[7]** as a white crystalline solid: mp 175-176 °C; $^1$H NMR (400 MHz, $CDCl_3$) δ major signals 0.5-2.8 (br m, 8H), 0.89 (t, $J$ = 6.7 Hz, 3H), 1.25-1.37 (m, 13H), 1.65-1.78 (m, 2H), 2.38 (br d, $J$ = 14.0 Hz, 2H), 3.42 (br t, $J$ = 12.9 Hz, 2H), 2.69 (br d, $J$ = 12.7 Hz, 2H) (*cis* isomer δ 2.09-2.15 (m), 2.28-2.35 (m), 3.52-3.64 (m)); {$^1$H} $^{11}$B NMR (128 MHz, $CDCl_3$) δ -19.6 (4B), -14.0 (4B), 32.1 (1B). Anal. Calcd. for $C_{14}H_{33}B_9O_2S$: C, 46.35; H, 9.17. Found: C, 46.79; H, 9.15.

**Preparation of phenol 10g**. [4]



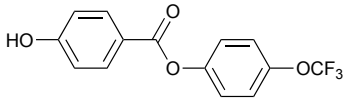

The phenol was prepared via ligand-free Suzuki coupling[5] by reacting 4-hydroxyphenylboronic acid (490 mg, 3.55 mmol) and 1-bromo-3,4,5-trifluorobenzene (500 mg, 2.37 mmol) in 50% EtOH (10 mL) in the presence of $PdCl_2$ (32.5 mg, 0.5 mol %) and $K_2CO_3$ (320 mg, 5.7 mmol). The reaction mixture was stirred for 1 hr at rt. The mixture was washed with brine (15 mL), extracted with diethyl ether (3x10 mL), dried ($MgSO_4$), concentrated under vacuum and the product was purified by column chromatography (EtOAc) to give 420 mg (79% yield) of the product that was further purified by recrystallization (EtOH/$H_2O$) to give **10g** as a white fluffy solid: mp 110.5 °C (lit.[4] mp 237 °C); $^1$H NMR (400 MHz, $CDCl_3$) δ 4.79 (s, 1H), 6.90 (d, $J$ = 8.7 Hz, 2H), 7.08-7.16 (m, 2H), 7.38 (d, $J$ = 8.7 Hz, 2H) [lit.[4] $^1$H NMR ($CDCl_3$) δ 4.90 (s, 1H), 6.91 (d, $J$ = 8.4 Hz, 2H), 7.12 (t, $J$ = 7.96 Hz, 2H), 7.38 (dd, $J$ = 8.44 Hz, 2H)]; $^{13}$C NMR (100 MHz, $CDCl_3$) δ 110.4 (dd, $J_1$ =15.8 Hz, $J_2$ = 5.9 Hz), 115.9, 128.1, 131.0, 136.8 (td, $J_1$ = 7.8 Hz, $J_2$ = 4.6 Hz), 138.8 (dt, $J_1$ = 249 Hz, $J_2$ = 15.4 Hz), 151.3 (ddd, $J_1$ = 247.6 Hz, $J_2$ = 9.9 Hz, $J_3$ = 4.2 Hz), 155.7.

**Phenol 10h.**[6]



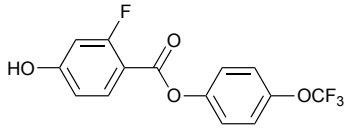
Mp 144-144.5 °C (lit.[6] mp 126-128 °C); $^1$H NMR (400 MHz, $CD_3CN$) δ 0.89 (t, *J* = 7.0 Hz, 3H), 1.28-1.40 (m, 6H), 1.65 (quint, *J* = 7.5 Hz, 2H), 2.67 (t, *J* = 7.7 Hz, 2H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.6 (br s, 1H), 8.22 (d, *J* = 8.3 Hz, 2H), 8.42 (s, 2H); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.87 (t, *J* = 6.9 Hz, 3H), 1.22-1.40 (m, 6H), 1.63 (quint, *J* = 7.5 Hz, 2H), 2.65 (t, *J* = 7.7 Hz, 2H), 7.1 (br s, 1H), 7.27 (d, *J* = 8.6 Hz, 2H), 8.17 (d, *J* = 8.2 Hz, 2H), 8.41 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 14.1, 22.6, 28.9, 31.1, 31.7, 35.8, 127.5, 128.9, 134.0, 144.9, 145.5, 149.9, 157.4. Anal. Calcd. for $C_{16}H_{20}N_2O$: C, 74.97; H, 7.86; N, 10.93. Found: C, 74.71; H, 7.76; N, 10.74.

**Preparation of phenol 10j.**




4-(Trifluoromethoxy)phenyl 4-benzyloxybenzoate (**18j**, 3.20 g, 8.24 mmol) was dissolved in a mixture of ethanol/THF (200 mL). Pd/C (10 %, 0.44 g) was added and $H_2$ was purged through the reaction mixture overnight. The reaction mixture was filtered and the solvent was evaporated to give 2.40 g (97% yield) of phenol **10j** as a white crystalline solid. Analytical sample of **10j** was prepared by recrystallization from *iso*-octane/toluene (2x): mp 146.5 °C; $^1$H NMR (400 MHz, $CDCl_3$) δ 5.41 (br s, 1H), 6.93 (d, *J* = 8.8 Hz, 2H), 7.23-7.29 (m, 4H), 8.11 (d, *J* = 8.8 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 115.5 (2C), 121.3, 122.0 (q), 122.1 (2C), 123.0 (2C), 132.6 (2C), 146.5, 149.1, 160.6, 164.9. Anal. Calcd. for $C_{14}H_9F_3O_4$: C, 56.39; H, 3.04. Found: C, 56.63; H, 3.03.

**Preparation of phenol 10k.**

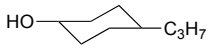



4-(Trifluoromethoxy)phenyl 4-benzyloxy-2-fluorobenzoate (**18k**, 252 mg, 0.62 mmol) was dissolved in a mixture of EtOAc and EtOH. Pd/C (10%, 66 mg) was added and $H_2$ was purged through the reaction for 12 hr. The reaction mixture was filtered and the solvent evaporated to give 190 mg (97% yield) of crude phenol **10k**. Analytical sample of **10k** was prepared by recrystallization from cold methanol to give a white crystalline solid: mp 172.5 °C;

$^1$H NMR (400 MHz, $CD_3CN$) δ 6.72 (dd, $J_1$ = 12.8 Hz, $J_2$ = 2.3 Hz, 1H), 6.80 (dd, $J_1$ = 8.8 Hz, $J_2$ = 2.4 Hz, 1H), 7.32 (d, $J$ = 9.2 Hz, 2H), 7.39 (d, $J$ = 8.7 Hz, 2H), 8.00 (t, $J$ = 8.7 Hz, 1H), 8.1 (br s, 1H). Anal. Calcd. for $C_{14}H_8F_4O_4$: C, 53.18; H, 2.55. Found: C, 53.30; H, 2.54.

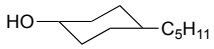
***trans*-4-Alkylcyclohexanol (11)**. 4-Bromobenzoate **19** was hydrolyzed in a solution of KOH in MeOH at 50 °C. Water was added and most MeOH was evaporated. The mixture was extracted with $CH_2Cl_2$ (3x), the extract was dried and evaporated and distilled to give the desired *trans*-alcohol **11**.

***trans*-4-Propylcyclohexanol (11e)**.[7]



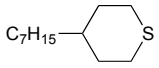

$^1$H NMR (500 MHz, $CDCl_3$) δ 0.87 (t, $J$ = 7.7 Hz, 3H), 0.92-0.97 (m, 2H), 1.13-1.25 (m, 5H), 1.30 (sext, $J$ = 5.9 Hz, 2H), 1.37 (br s, 1H), 1.75 (d, $J$ = 12.0 Hz, 2H), 1.95 (br d, $J$ = 10.2 Hz, 2H), 3.50-3.58 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 14.1, 19.9, 31.1, 35.1, 36.2, 38.8, 70.4.

***trans*-4-Pentylcyclohexanol (11f)**.[7,8]




$^1$H NMR (400 MHz, $CDCl_3$) δ 0.89 (t, $J$ = 7.2 Hz, 3H), 0.89-0.98 (m, 2H), 1.13-1.35 (m, 11H), 1.75 (br d, $J$ = 11.4 Hz, 2H), 1.93 (br d, $J$ = 12.4 Hz, 2H), 3.48-3.58 (m, 1H).

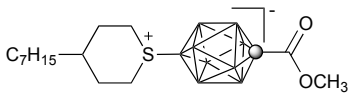
**Preparation of 4-heptylthiane (13[7])**.




Following an analogous procedure for **13[3]**,[1] to a solution of 1,5-dibromo-3-heptylpentane (**8[7]**, 15.4 g, 0.047 mol) in EtOH (100 mL) a solution of $Na_2S \cdot 9H_2O$ (16.9 g, 0.07 mol) in water (50 mL) was added dropwise during 1 h at 50 °C. The mixture was stirred at this temperature for 1 h, then refluxed for 1 h, and diluted with water. The organic product was extracted with hexanes, the extract dried ($Na_2SO_4$) and the solvent evaporated. The yellow oily residue was passed through a silica gel plug (hexanes) to give 8.4 g (89% yield) of thiane **13[7]**

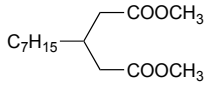
as a colorless oil. Analytical sample of **13[7]** was obtained by short-path distillation (130 °C, 0.7 mm Hg): $^{1}$H NMR (400 MHz, $CDCl_3$) δ 0.86 (t, $J$ = 7.1 Hz, 3H), 1.18-1.35 (m, 15H), 1.96 (br d, $J$ = 12.1 Hz, 2H), 2.54-2.67 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 14.0, 22.6, 26.3, 28.7 (2C), 29.2, 29.7, 31.8, 34.2 (2C), 37.1, 37.3. Anal. Calcd. for $C_{12}H_{24}S$: C, 71.93; H, 12.07. Found: C, 71.85; H, 12.08.

**Preparation of methyl ester 14[7].**




A solution of ester **12**[9,10] (150 mg, 0.73 mmol) in thiane **13[7]** (5 mL) was heated at 120 °C for 1 hr. The solvent was removed under reduced pressure (110 °C, 0.7 mmHg), the residue was washed with hexane, and purified on a short silica gel plug ($CH_2Cl_2$/hexane, 1:1) to give 241 mg (87% yield) of ester **14[7]** as an off-white solid. The ester was recrystallized from *iso*-octane (2x): mp 88 °C (DSC); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 0.5-2.8 (br m, 8H), 0.89 (t, $J$ = 6.6 Hz, 3H), 1.25-1.42 (m, 13H), 1.65-1.77 (m, 2H), 2.37 (br d, $J$ = 12.6 Hz, 2H), 3.40 (br t, $J$ = 13.4 Hz, 2H), 3.69 (br d, $J$ = 12.7 Hz, 2H), 4.02 (s, 3H), (minor signal for the *cis* isomer: δ 2.06-2.12 (m), 2.25-2.32 (m), 3.50-3.60 (m)); $\{^{1}H\}^{11}$B NMR (128 MHz, $CDCl_3$) δ –19.8 (4B), –14.4 (4B), 31.2 (1B) (minor signal for the *cis* isomer: δ 29.4). Anal. Calcd. for $C_{15}H_{35}B_9O_2S$: C, 47.82; H, 9.36. Found: C, 48.09; H, 9.44.

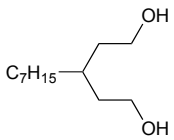
**Preparation of dimethyl 3-heptylglutarate (15[7]).**




Following a procedure for **15[5]**,[1] a mixture of dimethyl malonate (45.8 g, 0.35 mol), octanal (20.5 g, 0.16 mol), benzene (50 mL), piperidine (0.85 mL) and $NEt_3$ (2.5 mL) was stirred at rt for 2 hr and then heated overnight under reflux. A Dean-Stark trap was used to collect water produced in the reaction. The mixture was washed with dilute HCl, dried and excess dimethyl malonate was removed under vacuum (up to 80 °C, 0.05 mmHg). The oily residue was heated overnight under reflux with conc. HCl (250 mL), the aqueous HCl acid was removed under

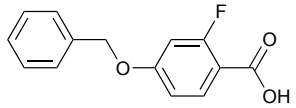
reduced pressure and the oily residue was short-path distilled (150-170 °C, 1 mmHg) to give crude 3-heptylglutaric acid (33.1 g). Without further purification, the diacid was heated with $SOCl_2$ (42 mL) for 2 hr, excess $SOCl_2$ was removed under reduced pressure and the resulting dark acid chloride was heated under reflux with $CH_3OH$ (200 mL) for 2 hr. Excess $CH_3OH$ was evaporated and the crude diester **15[7]** was distilled (135 °C, 1 mmHg) to give 18.7 g (63% overall yield) of dimethyl 3-heptylglutarate (**15[7]**) as a colorless oil: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.86 (t, $J$ = 7.1 Hz, 3H), 1.24-1.35 (m, 12H), 2.30-2.35 (m, 5H), 3.64 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 14.0, 22.5, 26.5, 29.0, 29.4, 31.7, 32.0, 33.5, 38.3(2C), 51.4(2C), 173.0(2C). Anal. Calcd. for $C_{14}H_{26}O_4$: C, 65.09; H, 10.14. Found: C, 64.94; H, 9.95.

**Preparation of 3-heptylpentane-1,5-diol (16[7]).**




Dimethyl 3-heptylglutarate (**15[7]**, 18.7 g, 0.10 mol) was reduced with $LiAlH_4$ (5.7 g, 0.15 mol) in anhydrous THF. The reaction mixture was carefully quenched with $H_2O$ (30 mL) and then 2M KOH (20 mL). After 30 minutes, the white precipitate was removed by filtration and then washed with $Et_2O$ (200 mL). The filtrate was dried ($MgSO_4$), filtered and evaporated to give 17.9 g (86% yield) of 3-heptylpentane-1,5-diol (**16[7]**) as a slightly yellow oil which was used without further purification: $^1$H NMR (400 MHz, $CDCl_3$) δ 0.87 (t, $J$ = 7.0 Hz, 3H), 1.22-1.32 (m, 12 H), 1.48-1.68 (m, 5H), 3.62-3.75 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 14.0, 22.6, 26.5, 29.2, 29.9, 31.1, 31.8, 34.5, 36.5(2C), 60.7(2C).

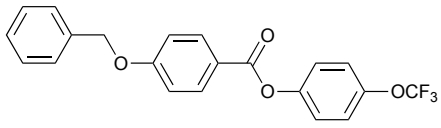
**Preparation of 4-(benzyloxy)-2-fluorobenzoic acid (17k).**




A mixture of 2-fluoro-4-hydroxybenzoic acid (500 mg, 3.20 mmol), potassium hydroxide (395 mg, 7.05 mmol) and benzyl bromide (603 mg, 3.52 mmol) in EtOH/$H_2O$ (22 mL, 10:1) was heated under reflux for 20 hr. Aqueous potassium hydroxide (20%, 10 mL) was added and the mixture was heated under reflux for additional 2 hr. The reaction mixture was cooled, water was

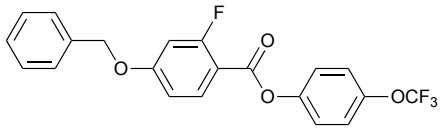
added, and the solution was acidified with 10% HCl. The precipitate was filtered and dried to give 530 mg (67% yield) of acid **17k** as an off-white solid. Analytical sample was prepared by recrystallization from *iso*-octane/toluene (2x) and then cold $CH_3CN$ (2x) to give acid **17k** as colorless crystals: mp 168 °C; $^1$H NMR (400 MHz, CDCl3) δ 5.12 (s, 2H), 6.74 (dd, $J_1$ = 12.7 Hz, $J_2$ = 2.4 Hz, 1H), 6.83 (dd, $J_1$ = 8.8 Hz, $J_2$ = 2.4 Hz, 1H), 7.34-7.42 (m, 5H), 7.98 (t, $J$ = 8.7 Hz, 1H). Anal. Calcd. for $C_{14}H_{11}FO_3$: C, 68.29; H, 4.50. Found: C, 68.28; H, 4.42.

**Preparation of 4-(trifluoromethoxy)phenyl 4-(benzyloxy)benzoate (18j).**




4-Benzyloxybenzoic acid (**17j**, 2.0 g, 8.76 mmol) was suspended in anhydrous $CH_2Cl_2$ (15 mL) and was treated with $(COCl)_2$ (2.25 mL g, 26.3 mmol) and anhydrous DMF (catalytic amounts). The suspension began to bubble and became homogenous and was stirred vigorously for 30 min at rt. The light yellow solution was evaporated to dryness. The residue was redissolved in anhydrous $CH_2Cl_2$ (15 mL) and the 4-trifluoromethoxyphenol (1.64 g, 9.20 mmol) and $NEt_3$ (3.66 mL, 26.3 mmol) were added. The mixture was stirred overnight at rt. The reaction mixture was washed with 5% HCl (15 mL), the organic layer was dried ($Na_2SO_4$) and evaporated to dryness. The product was purified by column chromatography ($CH_2Cl_2$). The eluent was filtered through a cotton plug and evaporated by to give 3.2 g (93% yield) of **18j** as a white crystalline solid. Analytical sample was prepared by recrystallization from *iso*-octane/toluene (2x): mp 174 °C; $^1$H NMR ($CD_3CN$, 400 MHz) δ 5.18 (s, 2H), 7.07 (d, $J$ = 8.9 Hz, 2H), 7.24 and 7.27 (AB, $J$ = 9.2 Hz, 4H), 7.37-7.47 (m, 5H), 8.15 (d, $J$ = 8.8 Hz, 2H). Anal. Calcd. for $C_{21}H_{15}F_3O_4$: C, 64.95; H, 3.89. Found: C, 64.67; H, 3.77.

**Preparation of 4-(trifluoromethoxy)phenyl 4-(benzyloxy)-2-fluorobenzoate (18k).**



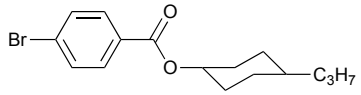

The ester was prepared in 97% yield according to the procedure for **18j**, and purified by column chromatography ($SiO_2$, $CH_2Cl_2$) to give white crystalline solid. Analytical sample of **18k**

was prepared by recrystallization from methanol to give colorless crystals: mp 164 °C; $^1$H NMR (400 MHz, $CD_3CN$) δ 5.21 (s, 2H), 6.92 (dd, $J_1$ = 13.1 Hz, $J_2$ = 2.4 Hz, 1H), 6.97 (dd, $J_1$ = 8.8 Hz, $J_2$ = 2.4 Hz, 1H), 7.33 (d, $J$ = 9.2 Hz, 2H), 7.39-7.51 (m, 7H), 8.08 (t, $J$ = 8.8 Hz, 1H). Anal. Calcd. for $C_{21}H_{14}F_4O_4$: C, 62.08; H, 3.47; Found: C, 62.19; H, 3.59.

**Preparation of *trans*-4-pentylcyclohexyl and *trans*-4-propylcyclohexyl 4-bromobenzoate (19).**

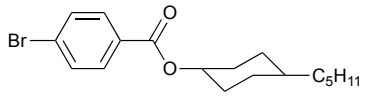
4-Bromobenzoic acid (0.06 mol) was treated with oxalyl chloride (0.18 mol) in $CH_2Cl_2$ in the presence of catalytic amounts of DMF. Volatiles were removed and the crude 4-bromobenzoyl chloride was added to a mixture of isomeric 4-pentylcyclohexanols (obtained from 4-alkylcyclohexanone and $NaBH_4$) and dry pyridine (0.18 mol). The mixture was stirred overnight at 50 °C, cooled and poured into dil. HCl. The organic layer was separated, washed with $NaHCO_3$, dried ($MgSO_4$), and solvent removed. The residue was passed through a short silica gel plug ($CH_2Cl_2$), solvent removed and the residue was crystallized (3x) from pentane at –20 °C (*trans*-4-pentylcyclohexyl 4-bromobenzoate, **19f**) or cold hexanes (2x) (*trans*-4-propylcyclohexyl 4-bromobenzoate, **19e**) to give colorless plates of the desired ester.

***trans*-4-Propylcyclohexyl 4-bromobenzoate (19e)**




Mp 83 °C; $^1$H NMR (400 MHz, $CDCl_3$) δ 0.89 (t, $J$ = 7.3 Hz, 3H), 1.06 (dq, $J_1$ = 3.3 Hz, $J_2$ = 13.4 Hz, 2H), 1.15-1.34 (m, 5H), 1.46 (dq, $J_1$ = 3.5 Hz, $J_2$ = 12.5 Hz, 2H), 1.84 (br d, $J$ = 12.3 Hz, 2H), 2.08 (br d, $J$ = 14.2 Hz, 2H), 4.89 (tt, $J_1$ = 11.0 Hz, $J_2$ = 4.4 Hz, 1H), 7.56 (d, $J$ = 8.6 Hz, 2H), 7.89 (d, $J$ = 8.6 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 14.3, 20.2, 30.9 (2C), 31.7 (2C), 36.3, 31.7, 36.3, 38.8, 74.6, 127.1, 129.8, 131.1 (2C), 131.6 (2C), 165.4.. Anal. Calcd. for $C_{18}H_{25}BrO_2$: C, 59.09; H, 6.51. Found: C, 59.27; H, 6.59.

***trans*-4-Pentylcyclohexyl 4-bromobenzoate (19f)**

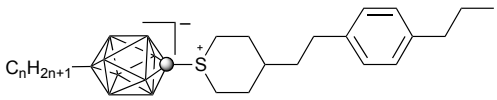



Mp: 69 °C; $^1$H NMR (400 MHz, $CDCl_3$) δ 0.89 (t, $J$ = 7.2 Hz, 3H), 1.06 (dq, $J_1$ = 3.3 Hz, $J_2$ = 13.4 Hz, 2H), 1.15-1.34 (m, 9H), 1.46 (dq, $J_1$ = 3.5 Hz, $J_2$ = 12.5 Hz, 2H), 1.84 (d, $J$ = 13.0 Hz, 2H), 2.07 (br d, $J$ = 12.7 Hz, 2H), 4.89 (tt, $J_1$ = 11.1 Hz, $J$ = 4.4 Hz, 1H), 7.56 (d, $J$ = 8.6 Hz, 2H), 7.89 (d, $J$ = 8.6 Hz, 2H). Anal. Calcd. for $C_{18}H_{25}BrO_2$: C, 61.19; H, 7.13. Found: C, 61.29; H, 7.34.

## 2. Binary mixtures

Preparation of binary mixtures for dielectric studies. Solutions of compounds **3[n]** or **4[n]** in host **ClEster** (15-20 mg) in dry $CH_2Cl_2$ (~0.5 mL) were heated at ~60 $^oC$ for 2 hr in an open vial to assure homogeneity of the sample. The sample was degased under vacuum (0.2 mmHg), left at ambient temperature for 2 hr and analyzed by polarized optical microscopy (POM). After a minimum of several days, the mixtures were inspected again for inhomogeneity and partial crystallization.

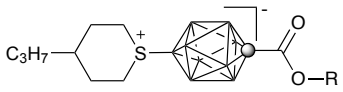
**Table S1. Solubility data for 3[n]b [a]**

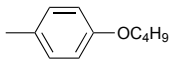
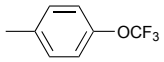
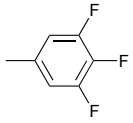
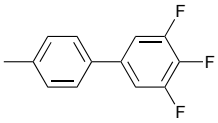
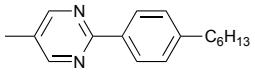
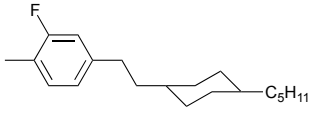
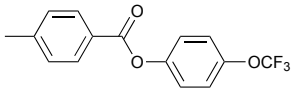
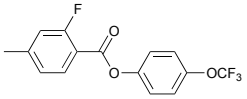
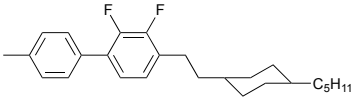



| n | Highest soluble tried [b] | Lowest Insoluble tried [c] |
|---|---|---|
| 3 | 3.67 [d] | 6.52 |
| 5 | 3.26 | 6.19 |

[a] Concentration in mole %. [b] Stable homogenous solution after 24 hrs or longer. [c] Partial crystallization upon cooling to ambient temperature. [d] Partial crystallization after 24 hrs or longer.

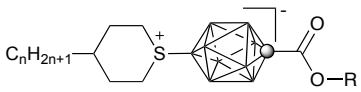
**Table S2. Solubility data for selected esters 4[3] [a]**

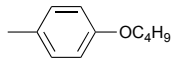
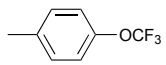
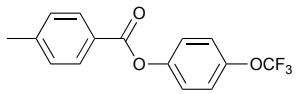



| | R | Highest soluble tried [b] | Lowest insoluble tried [c] |
|---|---|---|---|
| **b** |  | 2.2 | 6.6 |
| **c** |  | 3.6 | ? |
| **d** |  | 3.0 | 6.0 |
| **e** |  | 4.1 | 6.6 |
| **g** |  | ? | 1.1 |
| **h** |  | 4.2 [d] | 5.6 |
| **i** |  | 4.3 | 6.5 |
| **j** |  | 5.6 | 12.1 |
| **k** |  | 4.1 | ? |
| l |  | 3.0 | ? |

[a] concentration in mole %. [b] Stable homogenous solution after 24 hrs or longer. [c] Partial crystallization upon cooling to ambient temperature. [d] Partial crystallization after 24 hrs or longer.

**Table S3. Transition temperatures (°C) and enthalpies (kJ/mol, in italics) for 4[n].** [a]



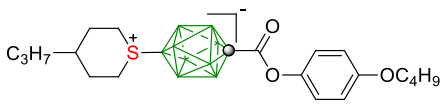

| | R | n = 5 | | n = 7 | |
|---|---|---|---|---|---|
| | | highest soluble tried [b] | lowest insoluble tried [c] | highest soluble tried [b] | lowest insoluble tried [c] |
| b |  | 5.5 | 11.3 | – | – |
| c |  | – | – | 9.9 | ? |
| j |  | – | – | 6.0 | 11.5 |

[a] concentration in mole %. [b] Stable homogenous solution after 24 hrs or longer. [c] Partial crystallization upon cooling to ambient temperature. [d] Partial crystallization after 24 hrs or longer.

Thermal analysis Virtual N-I transition temperatures [$T_{NI}$] were determined for selected compounds in **ClEster** and **CinnCN** hosts. The clearing temperature for each homogenous mixture, prepared as above, was determined by DSC as the peak of the transition using small samples (~0.5 mg) and a heating rate of 5 K·min$^{-1}$. The results are shown in Tables S4-S8. The virtual N-I transition temperatures, [$T_{NI}$], were determined by line extrapolation of the data for peak of the transition to pure substance ($x$ = 1). To minimize the error, the intercept in the fitting function was set as the peak $T_{NI}$ for the pure host.

Results for esters **4[3]c**, **4[3]j**, and **4[3]k** show non-linear dependence of $T_{NI}$ on concentration or scattered data and were not analyzed.

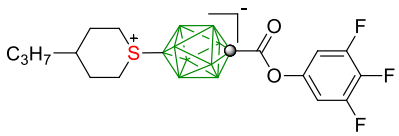
**Table S4**. $T_{NI}$ for solutions of **4[3]b** in **CinnCN**.




| $T_{NI}$/°C | **Mole fraction, *x*** | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0228 | 0.0432 | 0.0689 |
| Onset | | – | 132.89 | 130.57 |
| Peak | 139.5 | – | 133.62 | 131.57 |

$[T_{NI}]$ = 19±6 °C, $r^2$ = 0.983

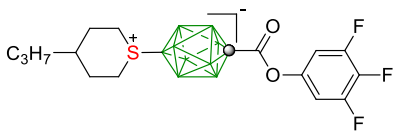
**Table S5**. $T_{NI}$ for solutions of **4[3]d** in **ClEster**.




| $T_{NI}$/°C | **Mole fraction, *x*** | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0108 | 0.02375 | 0.0299<br>not used |
| Onset | | 45.72 | 45.23 | 44.97 |
| Peak | 46.36 | 46.13 | 45.75 | 45.42 |

$[T_{NI}]$ = 21±1 °C, $r^2$ = 0.990

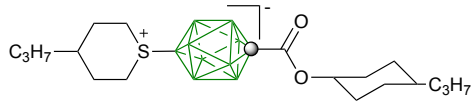
**Table S6**. $T_{NI}$ for solutions of **4[3]d** in **CinnCN**.




| $T_{NI}$/°C | **Mole fraction, *x*** | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0205 | 0.0321 | 0.0895 |
| Onset | | 133.43 | 135.59 | 121.09 |
| Peak | 139.5 | 136.10 | 134.76 | 123.67 |

[$T_{NI}$] = -34±5 °C, $r^2$ = 0.994

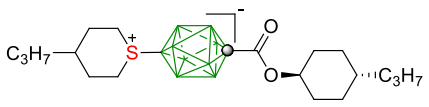
**Table S7**. $T_{NI}$ for solutions of **4[3]e** in **ClEster**.




| $T_{NI}$/°C | **Mole fraction, *x*** | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0368 | 0.0665 | – |
| Onset | | 42.4 | 40.3 | – |
| Peak | 46.36 | 44.29 | 43.13 | – |

[$T_{NI}$] = –4±2 °C, $r^2$ = 0.989

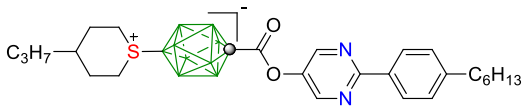
**Table S8**. $T_{NI}$ for solutions of **4[3]e** in **CinnCN**.




| $T_{NI}$/°C | **Mole fraction, *x*** | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0215 | 0.0381 | – |
| Onset | | 135.62 | 133.42 | – |
| Peak | 139.5 | 136.16 | 134.52 | – |

[$T_{NI}$] = 1±6 °C, $r^2$ = 0.987

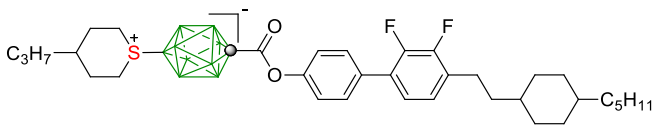
**Table S9**. $T_{NI}$ for solutions of **4[3]h** in **ClEster**.




| $T_{NI}$/°C | **Mole fraction, *x*** | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0161 | 0.0288 | 0.04215 |
| Onset | | 47.62 | 48.81 | 50.00 |
| Peak | 46.36 | 48.3 | 49.59 | 51.23 |

[$T_{NI}$] = 161±3 °C, $r^2$ = 0.999

**Table S10**. $T_{NI}$ for solutions of **4[3]l** in **ClEster**.

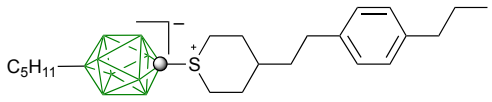



| $T_{NI}$/°C | Mole fraction, $x$ | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0158 | 0.0182 | 0.0301 |
| Onset | | 49.27 | 49.49 | 53.3 |
| Peak | 46.36 | 50.56 | 50.58 | 55.1 |

$[T_{NI}]$ = 331±7 °C, $r^2$ = 0.997

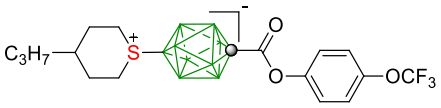
Dielectric measurements. Dielectric properties of solutions of selected esters in **ClEster** were measured by a Liquid Crystal Analytical System (LCAS - Series II, LC Vision, Inc.) using GLCAS software version 0.13.14, which implements literature procedures for dielectric constants.[5] The instrument was calibrated using a series of capacitors (11.30 pF – 3292 pF). The homogenous binary mixtures were loaded into ITO electro-optical cells by capillary forces with moderate heating supplied by a heat gun. The cells (about 10 μm thick, electrode area 1.00 $cm^2$ and anti-parallel rubbed polyimide layer) were obtained from LC Vision, Inc. The filled cells were heated to an isotropic phase and cooled to room temperature before measuring of dielectric properties. Default parameters were used for measurements: triangular shaped voltage bias ranging from 0.1-20 V at 1 kHz frequency. The threshold voltage $V_{th}$ was measured at a 5% change. For each mixture the measurement was repeated 10 times manually for two cells. The results were averaged to calculate the mixture's parameters. Results are shown in Tables S11–S18. All measurements were run at 25 °C. Error in concentration is estimated at about 1.5%. The dielectric values obtained for each concentration were fitted to a linear function in which the intercept was set at the value extrapolated for the pure host. The resulting extrapolated values for pure additives are shown in Table 4 in the main text.

**Table S11**. Dielectric parameters for **3[5]b** in **ClEster** at 25 °C.



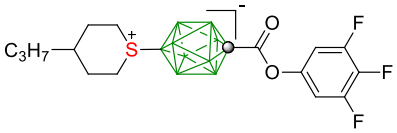

| Parameter | Mole fraction, *x* | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0246 | 0.0374 | – |
| $\varepsilon_{\parallel}$ | 2.86±0.01 | 4.00±0.01 | 4.40±0.01 | – |
| $\varepsilon_{\perp}$ | 3.42±0.01 | 3.55±0.01 | 3.60±0.01 | – |
| $\Delta\varepsilon$ | -0.56±0.01 | 0.45±0.01 | 0.80±0.01 | – |

**Table S12**. Dielectric parameters for **4[3]c** in **ClEster** at 25 °C.



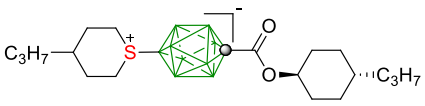

| Parameter | Mole fraction, *x* | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0215 | 0.0478 | 0.0547 |
| $\varepsilon_{\parallel}$ | 2.86±0.01 | 4.37±0.01 | 6.95±0.05 | 7.47±0.1 |
| $\varepsilon_{\perp}$ | 3.42±0.01 | 3.62±0.01 | 4.10±0.05 | 4.20±0.1 |
| $\Delta\varepsilon$ | -0.56±0.01 | 0.75±0.01 | 2.84±0.01 | 3.30±0.1 |

**Table S13**. Dielectric parameters for **4[3]d** in **ClEster** at 25 °C.



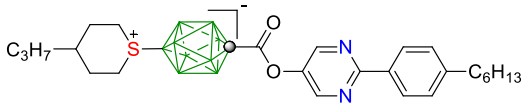
| Parameter | Mole fraction, *x* | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0153 | 0.0279 | 0.0361 |
| $\varepsilon_{\parallel}$ | 2.86±0.01 | 4.01±0.01 | 4.98±0.01 | 5.55±0.02 |
| $\varepsilon_{\perp}$ | 3.42±0.01 | 3.62±0.02 | 3.78±0.01 | 3.96±0.06 |
| $\Delta\varepsilon$ | -0.56±0.01 | 0.40±0.01 | 1.19±0.01 | 1.59±0.06 |

**Table S14**. Dielectric parameters for **4[3]e** in **ClEster** at 25 °C.



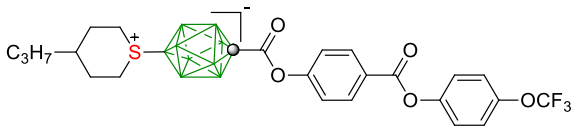
| Parameter | Mole fraction, *x* | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0368 | 0.0665 | – |
| $\varepsilon_{\parallel}$ | 2.86±0.01 | 4.01±0.01 | 4.73±0.04 | – |
| $\varepsilon_{\perp}$ | 3.42±0.01 | 3.71±0.01 | 3.89±0.02 | – |
| $\Delta\varepsilon$ | -0.56±0.01 | 0.31±0.01 | 0.84±0.02 | – |

**Table S15**. Dielectric parameters for **4[3]h** in **ClEster** at 25 °C.



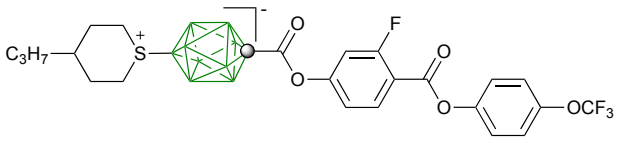
| Parameter | Mole fraction, *x* | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0261 | 0.0353 | – |
| $\varepsilon_{\parallel}$ | 2.86±0.01 | 4.41±0.01 | 4.91±0.04 | – |
| $\varepsilon_{\perp}$ | 3.42±0.01 | 3.63±0.01 | 3.69±0.04 | – |
| $\Delta\varepsilon$ | -0.56±0.01 | 0.78±0.01 | 1.22±0.01 | – |

**Table S16**. Dielectric parameters for **4[3]j** in **ClEster** at 25 °C.



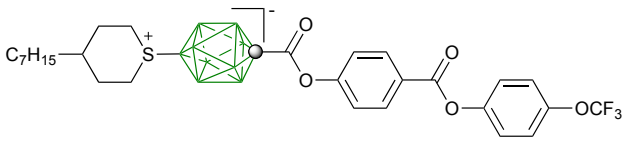
| Parameter | Mole fraction, *x* | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0172 | 0.0278 | 0.0375 |
| $\varepsilon_{\parallel}$ | 2.86±0.01 | 4.36±0.01 | 5.33±0.02 | 5.85±0.05 |
| $\varepsilon_{\perp}$ | 3.42±0.01 | 3.67±0.01 | 3.80±0.01 | 3.90±0.01 |
| $\Delta\varepsilon$ | -0.56±0.01 | 0.69±0.01 | 1.53±0.01 | 1.945±0.06 |

**Table S17**. Dielectric parameters for **4[3]k** in **ClEster** at 25 °C.



| Parameter | Mole fraction, *x* | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.01876 | 0.0231 | 0.0405 |
| $\varepsilon_{\parallel}$ | 2.86±0.01 | 4.57±0.01 | 4.98±0.02 | 6.13±0.06 |
| $\varepsilon_{\perp}$ | 3.42±0.01 | 3.65±0.01 | 3.75±0.01 | 3.92±0.03 |
| $\Delta\varepsilon$ | -0.56±0.01 | 0.92±0.01 | 1.23±0.02 | 2.21±0.04 |

**Table S18**. Dielectric parameters for **4[7]j** in **ClEster** at 25 °C.



| Parameter | Mole fraction, *x* | | | |
|---|---|---|---|---|
| | 0.00 (host) | 0.0165 | 0.0258 | 0.0309 |
| $\varepsilon_{\parallel}$ | 2.86±0.01 | 4.20±0.02 | 5.12±0.01 | 5.52±0.01 |
| $\varepsilon_{\perp}$ | 3.42±0.01 | 3.60±0.01 | 3.73±0.01 | 3.77±0.01 |
| $\Delta\varepsilon$ | -0.56±0.01 | 0.61±0.01 | 1.39±0.01 | 1.75±0.01 |

### 3. Background for calculations in the nematic phase

The equations derived from the Maier-Meier theory[11] used in this work were adopted from literature[12] and had the following form:

$$\Delta\varepsilon = \frac{NFh}{\varepsilon_0}\left\{\Delta\alpha - \frac{F\mu_{eff}^2}{2k_BT}\left(1-3\cos^2\beta\right)\right\}S \qquad (1)$$

$$\varepsilon_{\mathrm{P}} = 1 + \frac{NFh}{\varepsilon_0}\left\{\bar{\alpha} + \frac{2}{3}\Delta\alpha S + \frac{F\mu_{eff}^2}{3k_B T}\left[1 - \left(1 - 3\cos^2\beta\right)S\right]\right\} \qquad (2)$$

$$\varepsilon_{\perp} = 1 + \frac{NFh}{\varepsilon_0}\left\{\bar{\alpha} + \frac{1}{3}\Delta\alpha S + \frac{F\mu_{eff}^2}{3k_B T}\left[1 - \left(1 - 3\cos^2\beta\right)S\right]\right\} \qquad (3)$$

All quantities were in SI units as defined in the ESI in previous publications.[13]

- Dielectric permittivity of vacuum:

$\varepsilon = 1.114 \cdot 10^{-10} / 4\pi = 8.865 \cdot 10^{-12}$ F·m$^{-1}$

- The diagonal values of the electronic polarizibilities tensors matrix $\alpha_{xx}$, $\alpha_{yy}$, $\alpha_{zz}$ expressed in a.u. units were converted to F·m$^2$ units by multiplying with $1.482 \cdot 4\pi\varepsilon \cdot 10^{-31} = 1.651 \cdot 10^{-41}$
- Computed dipole moments $\mu_x$, $\mu_y$, $\mu_z$ in Debye were converted to dipole moments in C·m units using the conversion 1D = $3.3356\ 10^{-30}$ C·m
- Number density *N* is expressed in molecules per m$^3$

Field parameters $F = 1.2090$ and $h = 1.28754$ in equations 1–3 were assummed to be of pure host, **ClEster**, and obtained from literature dielectric and optical data[14] according to equation 4 and 5. Permittivity $\varepsilon_s$ was assumed to be experimental average permittivity ($\varepsilon = 3.07$) for the pure host, **ClEster**. The density of the hosts **ClEster** at 25 °C was taken as 1.02 g/cm$^3$ according to a literature report.[14]

$$F = \frac{1}{1 - \bar{\alpha} \cdot f} \text{ where } f = \frac{2\left(\bar{\varepsilon}_s - 1\right)}{2\bar{\varepsilon}_s + 1} \cdot \frac{N}{3\varepsilon_0} \qquad (4)$$

$$h = \frac{3\varepsilon_s}{(2\varepsilon_s + 1)} \qquad (5)$$

**4. Procedures for Maier-Meier analysis.**

The order parameter *S* and the Kirkwood factor *g* for the additives were obtained by solving simultaneously equations for $\Delta\varepsilon$ and $\varepsilon_{\parallel}$ (equation 1 and 2). The unknown *g* from the expression

for Δε (equation 1) was substituted into the expression for $\varepsilon_{\parallel}$ (equation 2) and solved for *S* (equation 6). In this form, order parameter *S* does not depend on the dipole moment μ, but depends on the dielectric permittivity components $\varepsilon_{\parallel}$ and $\varepsilon_{\perp}$. The obtained value *S* was substituted to the expression for parameter *g* (equation 7).

$$S = \frac{\Delta\varepsilon\varepsilon_0}{\Delta\alpha NFh + (1-3\cos^2\beta)[\Delta\varepsilon\varepsilon_0 - \frac{3}{2}(\varepsilon_P\varepsilon_0 - \varepsilon_0 - \bar{\alpha}NFh)]} \qquad (6)$$

$$g = \frac{2(\Delta\alpha NFhS - \Delta\varepsilon\varepsilon_0)k_BT}{NF^2h\mu^2(1-3\cos^2\beta)S} \qquad (7)$$

The protocol was verified by substituting the computed parameters *S* and *g* into equation 1–3 and calculating back the dielectric parameters.

## 5. Quantum mechanical calculation

Quantum-mechanical calculations were carried out using Gaussian 09 suite of programs.[15] Geometry optimizations for unconstrained conformers of with the most extended molecular shapes were undertaken at the B3LYP/6-31G(d,p) level of theory using default convergence limits. The alkyl groups were set in all-*trans* conformation in the input structures. No conformational search was attempted. The nature of the stationary point was verified by frequency calculations.

Calculations in solvent media using the PCM model[16] were requested with the SCRF(Solvent=Generic,Read) keyword and eps=3.07 and epsinf=2.286 input parameters. Exact polarizabilities were obtained with the POLAR keyword.

Dipole moment components and polarizability tensors for selected molecules in **vacuum**
All molecules are in Gaussian standard orientation with their long molecular axes oriented along the x axis. Dipole moments in Debye and polarizability in au (1Å$^3$ = 0.1482 au)

**3[5]b**

```
Dipole moment (field-independent basis, Debye):
X= 14.8261    Y=  -0.2155    Z=  1.9707  Tot=   14.9580
  Exact polarizability: 545.009  -5.008 298.764  18.419   4.173 263.534
```

**3[6]a**

```
Dipole moment (field-independent basis, Debye):
```

```
 X= 14.3783    Y=   1.0547    Z=  2.2309  Tot= 14.5885
  Exact polarizability: 437.478   2.589 250.632   7.877   5.079 254.336
```

**4[3]a-*trans*** PhC5-trans

```
Dipole moment (field-independent basis, Debye):
X=  9.5951    Y=  1.7984    Z=   0.6690  Tot= 9.7850
  Exact polarizability: 542.873   5.322 258.807  -2.808   3.843 287.918 Sum
of electronic and thermal Enthalpies=          -1595.618506
```

**4[3]a-*cis*** PhC5-cis

```
Dipole moment (field-independent basis, Debye):
X= 8.5701    Y=  -2.2973    Z -0.5574  Tot=   8.8902
Exact polarizability: 513.734  -7.083 283.507  -5.775 -14.759 278.849
Sum of electronic and thermal Enthalpies=          -1595.616554
```

**4[3]c-*trans*** PhOCF3-trans

```
Dipole moment (field-independent basis, Debye):
X=   13.0013    Y=   1.2407    Z=   0.6028  Tot=    13.0743
Exact polarizability: 475.403  -1.708 258.259  -6.147  -2.394 219.485
Sum of electronic and thermal Enthalpies=          -1811.421272
```

**4[3]c-*cis*** PhOCF3-cis

```
Dipole moment (field-independent basis, Debye):
X=  11.6958    Y=  -2.2702    Z=   0.3757  Tot=   11.9200
Exact polarizability: 453.318  -1.913 270.215  -2.745   9.778 221.946
Sum of electronic and thermal Enthalpies=          -1811.418907
```

**4[3]d-*trans*** PhF3 trans

```
Dipole moment (field-independent basis, Debye):
X=   13.5129    Y=  -1.4305    Z=  -0.5496  Tot=  13.5995
Exact polarizability: 448.431   1.303 250.967   1.726  -0.469 208.532
Sum of electronic and thermal Enthalpies=          -1696.881706
```

**4[3]d-*cis*** PhF3 cis:

```
Dipole moment (field-independent basis, Debye):
X= 12.4745    Y=    -2.5310    Z=   0.5468  Tot=  12.7404
Exact polarizability: 421.813  -1.692 263.900   1.070   7.558 210.884
Sum of electronic and thermal Enthalpies=          -1696.879845
```

**4[3]e-*trans*** ChxC3 trans

```
Dipole moment (field-independent basis, Debye):
X=   8.8854    Y=  1.7939    Z=  1.0248  Tot=   9.1224
Exact polarizability: 473.787  -0.690 264.472   1.099  -2.077 266.403
Sum of electronic and thermal Enthalpies=          -1520.614372
```

**4[3]e-*cis*** ChxC3 cis

```
Dipole moment (field-independent basis, Debye):
 X= -7.8686    Y= -2.4241    Z=  0.7395  Tot=  8.2667
Exact polarizability: 448.441   0.973 279.973  -1.736   0.942 265.504
Sum of electronic and thermal Enthalpies=          -1520.611632
```

**4[3]g-*trans*** PhPhF3 trans

```
Dipole moment (field-independent basis, Debye):
 X=  -13.7100    Y=  -0.7254    Z=  1.2056  Tot=  13.7820
Exact polarizability: 601.332  -0.705 301.646   0.492  -1.636 235.350
Sum of electronic and thermal Enthalpies=          -1927.861744
```

**4[3]g-*cis*** PhPhF3 cis

```
Dipole moment (field-independent basis, Debye):
 X=  12.7668    Y=   -1.8294    Z= 0.8253  Tot=  12.9236
Exact polarizability: 574.597  -4.954 299.636   4.882  22.561 253.552
Sum of electronic and thermal Enthalpies=           -1927.859749
```

**4[3]h-*trans*** PyrimPhC6 trans

```
Dipole moment (field-independent basis, Debye):
 X=   12.0631    Y=   -1.2976    Z=  1.4399  Tot=   12.2178
 Exact polarizability: 724.524 -11.556 298.768   3.855  23.478 332.713
Sum of electronic and thermal Enthalpies=           -1897.984226
```

**4[3]h-*cis*** PyrimPhC6 cis

```
Dipole moment (field-independent basis, Debye):
X=   11.1362    Y=   -1.5491    Z=  1.4716  Tot=  11.3393
Exact polarizability: 697.490  -6.726 353.460  14.762  16.838 294.170
Sum of electronic and thermal Enthalpies=           -1897.982292
```

**4[3]j-*trans*** COOPhCOOPhOCF3 trans

```
Dipole moment (field-independent basis, Debye):
X=  -15.0098    Y=  -0.9454    Z=  1.0565  Tot=   15.0766
Exact polarizability: 650.791   7.170 321.287  -0.263  12.528 262.597
Sum of electronic and thermal Enthalpies=           -2230.942505
```

**4[3]j-*cis*** COOPhCOOPhOCF3 cis

```
Dipole moment (field-independent basis, Debye):
X= 14.1369    Y=   0.6195    Z=  1.4687  Tot=   14.2265
Exact polarizability: 619.633   4.211 343.423   1.970 -12.084 260.182
Sum of electronic and thermal Enthalpies=           -2230.940586
```

**4[3]k-*trans*** COOPhFCOOPhOCF3 trans

```
Dipole moment (field-independent basis, Debye):
X= -16.0030    Y= 0.3116    Z=  0.2352  Tot=  16.0078
  Exact polarizability: 664.913   6.165 330.587  -3.977   4.402 251.466
Sum of electronic and thermal Enthalpies=           -2330.176220
```

**4[3]k-*cis*** COOPhFCOOPhOCF3 cis

```
Dipole moment (field-independent basis, Debye):
X= 15.1283    Y=  -0.8144    Z=  -0.0546  Tot= 15.1503
Exact polarizability: 637.127   3.900 341.851   1.463 -24.289 257.608
Sum of electronic and thermal Enthalpies=           -2330.174275
```

**4[3]l-*trans*** PhPhF2CH2CH2Chx trans

```
Dipole moment (field-independent basis, Debye):
 X=  -9.8733    Y=   -3.2580    Z=  0.9272  Tot=  10.4383
Exact polarizability: 836.074   2.449 409.840 -13.023  12.198 357.153
Sum of electronic and thermal Enthalpies=           -2338.176176
```

**4[3]l-*cis*** PhPhF2CH2CH2Chx cis

```
Dipole moment (field-independent basis, Debye):
 X=  -8.9542    Y= -3.6559    Z=  -0.6221  Tot=   9.6917
Exact polarizability: 809.658   8.497 405.194 -10.082  17.899 377.089
Sum of electronic and thermal Enthalpies=           -2338.173978
```

**4[3]m-*trans*** PhCN trans

```
Dipole moment (field-independent basis, Debye):
 X=   15.7576    Y= -1.4756    Z=  0.5586  Tot=  15.8364
Exact polarizability: 502.588   1.023 244.002   2.758  14.145 219.959
Sum of electronic and thermal Enthalpies=           -1491.423098
```

**4[3]m-*cis*** PhCN cis

```
Dipole moment (field-independent basis, Debye):
X=  14.7299    Y= -2.7633    Z=  0.5740  Tot=    14.9978
Exact polarizability: 476.119  -7.256 265.070  -0.308  10.005 214.577
Sum of electronic and thermal Enthalpies=           -1491.421207
```

**4[5]a-*trans*** PhC5 trans

```
Dipole moment (field-independent basis, Debye):
X=   9.6186    Y=  2.2847    Z=    0.3644  Tot=    9.8929
Exact polarizability: 574.338   7.824 279.659  -1.832   3.157 304.909
Sum of electronic and thermal Enthalpies=           -1674.191858
```

**4[5]a-*cis*** PhC5-cis

```
Dipole moment (field-independent basis, Debye):
X=  8.4943    Y=  -3.0202    Z=    0.0324  Tot=  9.0153
Exact polarizability: 543.187 -15.283 308.925  -6.012 -14.580 296.373
Sum of electronic and thermal Enthalpies=           -1674.189825
```

**4[7]j-*trans*** COOPhCOOPhOCF3 trans

```
Dipole moment (field-independent basis, Debye):
X=   15.1534    Y=   -0.6646    Z=  1.5556  Tot=   15.2476
Exact polarizability: 713.281  -5.030 356.354   8.734  18.500 305.667
```

**4[7]j-*cis*** COOPhCOOPhOCF3 cis

```
Dipole moment (field-independent basis, Debye):
X=  14.1953    Y=   -1.5275    Z=  1.0129  Tot=   14.3132
Exact polarizability: 670.869 -14.396 399.504   4.164  -3.045 293.155
```

**Table S19**. Calculated molecular parameters for selected compounds in vacuum.[a]

| | $\mu_{\|\|}$ /D | $\mu_{\perp}$ /D | $\mu$ /D | $\beta$ [b] /° | $\Delta\alpha$ /Å$^3$ | $\alpha_{avrg}$ /Å$^3$ |
|---|---|---|---|---|---|---|
| **3[5]b** | 14.83 | 1.98 | 14.96 | 7.6 | 39.10 | 54.70 |
| **3[6]a** | 14.38 | 2.47 | 14.59 | 9.7 | 27.42 | 46.56 |
| ***4[3]*** | | | | | | |
| **a-*trans*** | 9.60 | 1.92 | 9.79 | 11.3 | 39.94 | 53.83 |
| **a-*cis*** | 8.57 | 2.36 | 8.89 | 15.4 | 34.46 | 53.16 |
| **a** | 9.38 | 2.01 | 9.59 | 12.1 | 38.79 | 53.69 |
| **c-*trans*** | 13.00 | 1.38 | 13.07 | 6.1 | 35.05 | 47.09 |
| **c-*cis*** | 11.70 | 2.30 | 11.92 | 11.13 | 30.71 | 46.71 |
| **c** | 12.73 | 1.56 | 12.82 | 7.0 | 34.14 | 47.01 |
| **d-*trans*** | 13.51 | 1.53 | 13.60 | 6.5 | 32.41 | 44.85 |

| | | | | | | |
|---|---|---|---|---|---|---|
| **d-*cis*** | 12.47 | 2.59 | 12.74 | 11.7 | 27.33 | 44.29 |
| **d** | 13.29 | 1.75 | 13.41 | 7.5 | 31.34 | 44.73 |
| **e-*trans*** | 8.89 | 2.07 | 9.12 | 13.1 | 30.88 | 49.63 |
| **e-*cis*** | 7.87 | 2.53 | 8.27 | 17.9 | 26.04 | 49.10 |
| **e** | 8.67 | 2.15 | 8.94 | 14.0 | 29.86 | 49.52 |
| **g-*trans*** | 13.71 | 1.41 | 13.78 | 5.9 | 49.33 | 56.23 |
| **g-*cis*** | 12.77 | 2.01 | 12.92 | 8.9 | 44.16 | 55.71 |
| **g** | 13.51 | 1.48 | 13.59 | 6.2 | 48.24 | 56.12 |
| **h-*trans*** | 12.06 | 1.94 | 12.2 | 9.1 | 60.58 | 66.99 |
| **h-*cis*** | 11.14 | 2.14 | 11.3 | 10.9 | 55.38 | 66.45 |
| **h** | 11.87 | 1.98 | 12.0 | 9.5 | 59.49 | 66.87 |
| **j-*trans*** | 15.01 | 1.42 | 15.08 | 5.4 | 53.18 | 60.99 |
| **j-*cis*** | 14.14 | 1.59 | 14.23 | 6.4 | 47.10 | 60.43 |
| **j** | 14.83 | 1.44 | 14.90 | 5.6 | 51.90 | 60.87 |
| **k-*trans*** | 16.00 | 0.39 | 16.01 | 1.4 | 55.41 | 61.60 |
| **k-*cis*** | 15.13 | 0.82 | 15.15 | 3.1 | 50.00 | 61.09 |
| **k** | 15.82 | 0.46 | 15.83 | 1.7 | 54.27 | 61.49 |
| **l-*trans*** | 9.87 | 3.39 | 10.44 | 18.9 | 67.07 | 79.19 |
| **l-*cis*** | 8.95 | 3.71 | 9.69 | 22.5 | 62.02 | 78.64 |
| **l** | 9.68 | 3.45 | 10.28 | 19.6 | 79.08 | 79.08 |
| **m-*trans*** | 15.76 | 1.58 | 15.84 | 5.7 | 40.10 | 47.75 |
| **m-*cis*** | 14.73 | 2.82 | 10.00 | 10.9 | 35.02 | 47.21 |
| **m** | 15.54 | 1.83 | 15.65 | 6.7 | 39.04 | 47.64 |
| **4[5]a-*trans*** | 9.62 | 2.31 | 9.89 | 13.5 | 41.80 | 57.25 |
| **4[5]a-*cis*** | 8.49 | 3.02 | 9.02 | 19.57 | 35.65 | 56.74 |
| **4[5]a** | 9.38 | 2.46 | 9.70 | 14.7 | 40.51 | 57.14 |
| **4[7]j-*trans*** | 15.15 | 1.69 | 15.25 | 6.4 | 56.65 | 67.94 |
| **4[7]j-*cis*** | 14.20 | 1.83 | 14.31 | 7.4 | 48.10 | 67.36 |
| **4[7]j** | 14.95 | 1.67 | 15.05 | 6.4 | 54.86 | 67.82 |

[a] Vacuum dipole moments and polarizabilities obtained at the B3LYP/6-31G(d,p) level of theory. Polarizability values calculated from diagonal polarizability tensors were converted from a.u. to Å$^3$ using the factor 0.1482. [b] Angle between the net dipole vector m and $m_{||}$.

Dipole moment components and polarizability tensors for selected molecules in **ClEster** dielectric medium

All molecules are in Gaussian standard orientation with their long molecular axes oriented along the x axis. Dipole moments in Debye and polarizability in au (1Å$^3$ = 0.1482 au).

**3[5]b**

```
Dipole moment (field-independent basis, Debye):
X=  16.3932    Y= -0.2907    Z= 2.3645  Tot= 16.5654
Exact polarizability: 583.784  -4.169 362.400  21.864   5.223 316.933
```

**3[6]a**

```
Dipole moment (field-independent basis, Debye):
X=  16.1039    Y= 1.1720    Z=  2.7095  Tot=  16.3722
Exact polarizability: 471.669   3.522 300.575   9.564   6.460 307.605
```

**4[3]a-*trans*** PhC5 trans

```
Dipole moment (field-independent basis, Debye):
X=  10.5763    Y= 2.1194    Z=  0.8608  Tot= 10.8209
Exact polarizability: 583.242   8.402 309.429  -3.131   6.193 350.581
```

**4[3]a-*cis*** PhC5 cis

```
Dipole moment (field-independent basis, Debye):
X=  -9.6831    Y=  -2.8849    Z= 0.5998  Tot= 10.1216
Exact polarizability: 557.527  11.750 338.839  -7.757  20.783 337.461
```

**4[3]c-*trans*** PhOCF3 trans

Dipole moment (field-independent basis, Debye):

```
X=  14.2478    Y=   -1.5437    Z=   -0.6871  Tot=   14.3476
Exact polarizability: 515.733   0.636 313.308   6.627  -2.598 263.151
```

**4[3]c-*cis*** PhOCF3 cis

```
Dipole moment (field-independent basis, Debye):
X=  -13.0415    Y=  -2.8787    Z=   -0.4305  Tot= 13.3624
Exact polarizability: 497.964   4.617 324.762  -2.774 -12.508 266.513
```

**4[3]d-*trans*** PhF3 trans

```
Dipole moment (field-independent basis, Debye):
X=  14.8538    Y= -1.7611    Z= -0.6376  Tot=  14.9714
Exact polarizability: 489.846   0.237 304.062   2.184  -0.013 250.881
```

**4[3]d-*cis*** PhF3, cis

```
Dipole moment (field-independent basis, Debye):
X=   13.9302    Y= -3.1609    Z=  0.6567  Tot=  14.2994
Exact polarizability: 466.997  -4.553 316.862   1.574   9.698 253.963
```

**4[3]e-*trans*** ChxC3, trans

```
Dipole moment (field-independent basis, Debye):
 X=  -9.9665    Y=  -2.1679    Z=  1.2165  Tot=  10.2719
```

```
 Exact polarizability: 509.645   0.801 320.118  -1.962   2.156 321.973
```

**4[3]e-*cis*** ChxC3, cis

```
Dipole moment (field-independent basis, Debye):
X=  -9.0511    Y= -3.0629    Z= 0.8753  Tot=  9.5953
Exact polarizability: 487.956   3.809 336.116  -2.310   0.958 321.050
```

**4[3]g-*trans*** PhPhF3 trans

```
Dipole moment (field-independent basis, Debye):
X=  14.9447    Y=  0.9330    Z= 1.4503  Tot=  15.0439
 Exact polarizability: 652.010   0.375 366.465   0.112   3.326 282.133
```

**4[3]g-*cis*** PhPhF3 cis

```
Dipole moment (field-independent basis, Debye):
 X=  14.1445    Y=  -2.3465    Z= 1.0057  Tot= 14.3731
Exact polarizability: 629.774  -8.669 361.072   6.854  29.620 304.044
```

**4[3]h-*trans*** PyrimPhC6 trans

```
Dipole moment (field-independent basis, Debye):
 X=   13.1012    Y=  1.4057    Z=  -1.7541  Tot=  13.2926
Exact polarizability: 776.494  14.998 355.930  -6.836  31.675 404.462
```

**4[3]h-*cis*** PyrimPhC6 cis

```
Dipole moment (field-independent basis, Debye):
 X=   12.3343    Y=   -2.0322    Z=  1.6799  Tot=  12.6130
 Exact polarizability: 753.798 -11.443 426.729  20.033  22.892 350.544
```

**4[3]j-*trans*** COOPhCOOPhOCF3 trans

```
Dipole moment (field-independent basis, Debye):
X=  -16.2947    Y=   -1.0515    Z=  1.2505  Tot=   16.3764
  Exact polarizability: 697.567   6.289 389.698  -0.797  16.160 312.408
```

**4[3]j-*cis*** COOPhCOOPhOCF3 cis

```
Dipole moment (field-independent basis, Debye):
X=  15.6185    Y=    0.5377    Z=    1.7460  Tot=   15.7250
  Exact polarizability: 672.083   1.006 411.340   1.689 -15.300 310.106
```

**4[3]k-*trans*** COOPhFCOOPhOCF3 trans

```
Dipole moment (field-independent basis, Debye):
X=  -17.3124    Y=  0.4403    Z= 0.2979  Tot=  17.3205
Exact polarizability: 712.831   5.637 402.343  -5.343   5.114 298.280
```

**4[3]k-*cis*** COOPhFCOOPhOCF3 cis

```
Dipole moment (field-independent basis, Debye):
 X=  16.6184    Y=  -1.1571    Z= -0.0554  Tot= 16.6587
Exact polarizability: 690.422   1.195 410.834   0.940 -32.359 307.259
```

**4[3]l-*trans*** PhPhF2CH2CH2Chx trans

```
Dipole moment (field-independent basis, Debye):
X=  -10.7218    Y=  -3.8838    Z= 1.0455  Tot= 11.4514
  Exact polarizability: 883.264   5.364 497.088 -14.675  14.618 426.890
```

**4[3]l-*cis*** PhPhF2CH2CH2Chx cis

```
Dipole moment (field-independent basis, Debye):
 X=  9.9531    Y=  -4.4683    Z=  0.6527  Tot=  10.9296
```

```
  Exact polarizability: 861.071 -13.610 489.781 -13.429 -25.340 450.180
```

**4[3]m-*trans*** PhCN trans

```
Dipole moment (field-independent basis, Debye):
X=    17.3751    Y= -1.8013    Z=   0.6498  Tot= 17.4803
  Exact polarizability: 551.071   0.148 296.400   3.897  18.450 264.393
```

**4[3]m-*cis*** PhCN cis

```
Dipole moment (field-independent basis, Debye):
 X=    16.4615    Y=  -3.4179    Z 0.6770  Tot=   16.8262
Exact polarizability: 528.508 -10.828 318.837  -0.323  12.723 258.276
```

**4[5]a-*trans*** PhC5 trans

```
Dipole moment (field-independent basis, Debye):
X=   10.5185    Y=   2.7036    Z=   0.5030  Tot=  10.8721
Exact polarizability: 613.334  11.643 333.778  -2.235   5.296 370.754
```

**4[5]a-*cis*** PhC5 cis

```
Dipole moment (field-independent basis, Debye):
 X=   9.5022    Y=  -3.7470    Z=   0.1092  Tot= 10.2149
Exact polarizability: 586.754 -21.213 367.287  -8.388 -20.748 358.79
```

**4[7]j-*trans*** COOPhCOOPhOCF3 trans

```
Dipole moment (field-independent basis, Debye):
X=   16.3183    Y=  -0.8183    Z=   1.8067  Tot=  16.4384
Exact polarizability: 758.690  -7.916 428.048  10.668  25.859 364.968
```

**4[7]j-*cis*** COOPhCOOPhOCF3 cis

```
Dipole moment (field-independent basis, Debye):
X=  15.5672    Y=  -1.9445    Z=   1.2039  Tot=  15.7343
Exact polarizability: 724.236 -19.471 472.140   4.513  -3.303 349.462
```

**Table S20**. Calculated molecular parameters for selected compounds in **ClEster** dielectric medium.[a]

| | $\mu_{\parallel}$ /D | $\mu_{\perp}$ /D | $\mu$ /D | $\beta$ [b] /° | $\Delta\alpha$ /Å$^3$ | $\alpha_{avrg}$ /Å$^3$ |
|---|---|---|---|---|---|---|
| **3[5]b** | 16.39 | 2.38 | 16.57 | 8.3 | 36.18 | 62.40 |
| **3[6]a** | 16.10 | 2.95 | 16.37 | 10.4 | 24.84 | 53.34 |
| ***4[3]*** | | | | | | |
| **a-*trans*** | 10.58 | 2.29 | 10.82 | 12.2 | 37.53 | 61.42 |
| **a-*cis*** | 9.68 | 2.95 | 10.12 | 16.9 | 32.51 | 60.95 |
| **a** | 10.39 | 2.43 | 10.66 | 13.2 | 36.45 | 61.32 |
| **c-*trans*** | 14.25 | 1.69 | 14.35 | 6.8 | 33.72 | 53.95 |
| **c-*cis*** | 13.04 | 2.91 | 13.36 | 12.6 | 29.98 | 53.81 |
| **c** | 13.99 | 1.95 | 14.12 | 7.9 | 32.91 | 53.92 |
| **d-*trans*** | 14.85 | 1.87 | 14.97 | 7.2 | 31.47 | 51.61 |

| | | | | | | |
|---|---|---|---|---|---|---|
| **d-*cis*** | 13.93 | 3.23 | 14.30 | 13.1 | 26.91 | 51.27 |
| **d** | 14.66 | 2.16 | 14.81 | 8.4 | 30.49 | 51.54 |
| **e-*trans*** | 9.97 | 2.49 | 10.27 | 14.0 | 27.95 | 56.90 |
| **e-*cis*** | 9.05 | 3.19 | 9.60 | 19.4 | 23.62 | 56.57 |
| **e** | 9.77 | 2.64 | 10.12 | 15.1 | 27.02 | 56.83 |
| **g-*trans*** | 14.94 | 1.72 | 15.04 | 6.6 | 48.57 | 64.25 |
| **g-*cis*** | 14.14 | 2.55 | 14.37 | 10.2 | 44.05 | 63.97 |
| **g** | 14.77 | 1.90 | 14.89 | 7.3 | 47.60 | 64.19 |
| **h-*trans*** | 13.10 | 2.25 | 13.29 | 9.7 | 58.73 | 75.92 |
| **h-*cis*** | 12.33 | 2.64 | 12.61 | 12.1 | 54.12 | 75.63 |
| **h** | 12.94 | 2.33 | 13.14 | 10.2 | 57.74 | 75.86 |
| **j-*trans*** | 16.29 | 1.63 | 16.38 | 5.7 | 51.35 | 69.14 |
| **j-*cis*** | 15.62 | 1.83 | 15.72 | 6.7 | 46.14 | 68.84 |
| **j** | 16.15 | 1.68 | 16.24 | 5.9 | 50.23 | 69.08 |
| **k-*trans*** | 17.31 | 0.53 | 17.32 | 1.8 | 53.73 | 69.82 |
| **k-*cis*** | 16.62 | 1.16 | 16.66 | 4.0 | 49.11 | 69.58 |
| **k** | 17.16 | 0.67 | 17.18 | 2.2 | 52.73 | 69.77 |
| **l-*trans*** | 10.72 | 4.02 | 11.45 | 20.6 | 62.43 | 89.28 |
| **l-*cis*** | 9.95 | 4.52 | 10.93 | 24.4 | 57.96 | 88.97 |
| **l** | 10.56 | 4.13 | 11.34 | 21.4 | 61.47 | 89.21 |
| **m-*trans*** | 17.38 | 1.91 | 17.48 | 6.3 | 40.11 | 54.93 |
| **m-*cis*** | 16.46 | 3.48 | 16.83 | 12.0 | 35.56 | 54.62 |
| **m** | 17.18 | 2.25 | 17.33 | 7.5 | 39.14 | 54.86 |
| **4[5]a-*trans*** | 10.52 | 2.75 | 10.87 | 14.7 | 38.69 | 65.10 |
| **4[5]a-*cis*** | 9.50 | 3.75 | 10.21 | 21.5 | 33.15 | 64.85 |
| **4[5]a** | 10.30 | 2.96 | 10.72 | 16.1 | 37.50 | 65.05 |
| **4[7]j-*trans*** | 16.32 | 1.98 | 16.44 | 6.9 | 53.68 | 76.65 |
| **4[7]j-*cis*** | 15.57 | 2.29 | 15.73 | 8.4 | 46.45 | 76.36 |
| **4[7]j** | 16.16 | 2.05 | 16.29 | 7.2 | 52.12 | 76.59 |

[a] Dipole moments and polarizabilities obtained at the B3LYP/6-31G(d,p) level of theory in **ClEster** dielectric medium. Polarizability values calculated from diagonal polarizability tensors were converted from a.u. to Å$^3$ using the factor 0.1482. [b] Angle between the net dipole vector μ and $\mu_{||}$.

## 6. Archive for DFT calculations

### 3[5]b


```
1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C22H43B9S1\PIOTR\18-Oct-2013\0
 \\#P B3LYP/6-31G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fcheck
  freq=noraman\\10-C5-1-(SC5-CH2CH2-PhC3)-CB9, C1\\0,1\B,-0.2060989755,
 -1.6499257015,-2.0300929206\B,-1.9084779378,-1.0687807627,-2.463938974
 1\B,-1.2408960262,0.6060443391,-2.8503710467\B,0.4650481091,0.02408179
 05,-2.4155096476\B,-0.5572404839,-0.8286100242,-3.493150227\C,-0.32445
 99118,-1.2816785916,-5.0010069045\C,0.2271379985,-0.1894235612,-5.9357
 126435\C,0.4389562928,-0.6619636366,-7.3796029832\C,0.9843343295,0.426
 167517,-8.3126729474\C,1.1935164943,-0.0539140791,-9.7522432713\H,0.29
 55572079,-2.7290750608,-2.0643768418\H,-2.8596463633,-1.6537798149,-2.
 8756988603\H,-1.6193699753,1.4625729302,-3.5851930405\H,1.5417981574,0
 .38578411,-2.772388653\H,-1.2708502908,-1.6570798711,-5.4164607998\H,0
 .3607872047,-2.1416125447,-5.019402498\H,-0.4562851278,0.6706431179,-5
 .9349012329\H,1.1792238089,0.1863280635,-5.5362915065\H,1.1271065912,-
 1.520263475,-7.3838896536\H,-0.5128953339,-1.0392034481,-7.7817821566\
 H,0.2960640215,1.282619761,-8.3094817122\H,1.9351439319,0.8030050268,-
 7.9111430571\H,0.252978932,-0.4036463975,-10.193565533\H,1.9038564543,
 -0.8879209147,-9.7922503225\B,0.2709234552,-0.5259985364,-0.71891413\B
 ,-1.4271845362,-1.3047424146,-0.7536809358\B,-2.1570209409,0.303708261
 9,-1.3369436551\B,-0.4703989475,1.0892614011,-1.3063236395\C,-1.072585
 1378,0.1467765805,-0.1452852335\S,-1.3835835272,0.6696384297,1.5173162
 189\C,0.082493074,1.6888910542,1.969951474\C,0.1480293089,1.8811679363
 ,3.4866483581\C,0.3221411464,0.5759253723,4.2883769818\C,-0.8449122306
 ,-0.3958371539,4.023587631\C,-1.0017399783,-0.8027651191,2.5560723571\
 C,0.4873888303,0.8960078428,5.7861746317\C,0.8645631861,-0.3063743923,
 6.6762761523\H,1.1801719087,-0.7187080269,0.0268781751\H,-1.891091276,
 -2.131820873,-0.0370204991\H,-3.2099037735,0.7853448019,-1.0736665844\
 H,-0.1578212288,2.203960812,-1.0365481482\H,0.9573035763,1.1708085907,
 1.5686751262\H,-0.0453150774,2.6306634274,1.4337496636\H,-0.7476028941
 ,2.4130589426,3.8342128806\H,0.9955378984,2.5478908454,3.683930418\H,1
 .2471219657,0.0908508072,3.9400428362\H,-0.6973966939,-1.3242809006,4.
 5847785723\H,-1.7818966654,0.0425781388,4.3926863174\H,-0.0949736035,-
 1.2505855203,2.1409073279\H,-1.8354885548,-1.4889647324,2.3990338646\H
 ,1.2665356227,1.6607365572,5.8938389503\H,-0.4369053235,1.3518573585,6
 .1671133794\H,0.0638303067,-1.0545155616,6.6542773747\H,1.7580901208,-
 0.7910552243,6.2624694261\H,1.5833932529,0.7451485591,-10.3921522495\C
 ,1.1260455735,0.0989459869,8.1118940952\C,0.0819247992,0.1723680486,9.
 0423140775\C,0.3159441557,0.5854045877,10.3529575661\C,1.602184432,0.9
 38009543,10.7822779903\C,2.6453164326,0.863311978,9.8503467112\C,2.412
 1776317,0.4515227712,8.5389389787\H,-0.926904249,-0.0984874641,8.73837
 55075\H,-0.5128705053,0.6337609128,11.0553363195\H,3.6541472371,1.1300
 89168,10.1563445097\H,3.242266687,0.4007760426,7.8377768711\C,1.863742
 6408,1.3391589743,12.2173981309\C,2.1872745067,0.1405969565,13.1321678
 473\H,0.9883889817,1.8663286054,12.6178248935\H,2.6983076654,2.0507406
 541,12.2548157724\C,2.4510351171,0.5526441513,14.582745274\H,1.3547949
 862,-0.573165841,13.0920280241\H,3.0601218919,-0.3891381114,12.7300967
 629\H,2.6790095115,-0.3167225282,15.2075028436\H,3.2991402239,1.243265
 049,14.6516347211\H,1.5801169087,1.0557744785,15.0179014951\\Version=E
 M64L-G09RevC.01\State=1-A\HF=-1486.2779151\RMSD=4.591e-09\RMSF=3.599e-
 06\Dipole=0.3434633,1.0547672,5.7794559\Quadrupole=13.5229908,11.68422
 56,-25.2072164,0.5778162,-6.4760831,-5.0070228\PG=C01 [X(C22H43B9S1)]\
 \@
```


### 3[6]a

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C17H41B9S1\PIOTR\17-Aug-2013\0
\\#P B3LYP/6-31G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fcheck
freq=noraman\\10-hexyl-1-(4-Pentyl-thiaChx-1-yl)-CB9, C1\\0,1\B,-2.05
88067395,-0.2683637348,-1.581492845\B,-2.4404806286,-2.0200800338,-1.1
189786494\B,-2.8096817945,-1.4843613712,0.6077240997\B,-2.4275706288,0
.2683907417,0.1427942678\B,-3.4969659362,-0.7180054403,-0.7627728466\C
,-5.0212443673,-0.508016485,-1.1699962751\C,-5.8476119092,0.3601954414
,-0.2037491636\C,-7.3166266337,0.5152774384,-0.6181100334\C,-8.1403879
832,1.3863943911,0.3380800656\C,-9.610054296,1.5372527807,-0.073635386
4\C,-10.4236688061,2.4110983538,0.8859318286\B,-0.7369093856,0.1582766
159,-0.4494036032\B,-0.7477021349,-1.4788908802,-1.349704537\B,-1.2823
324194,-2.3381712962,0.2122893178\B,-1.2751845814,-0.712269056,1.11716
20103\C,-0.1193431294,-1.2166799087,0.1125887332\S,1.5607174506,-1.526
2703067,0.5765182526\C,2.0018694609,-0.1391649216,1.7050628246\C,3.520
5297184,-0.0585427143,1.8758808272\C,4.2921471604,0.243806049,0.575933
6328\C,4.0312480751,-0.8421199744,-0.4867906221\C,2.5594591093,-0.9982
434398,-0.8780205728\C,5.7939762747,0.414277538,0.8756643401\C,6.64327
39655,0.9276904282,-0.295340226\C,8.1024897871,1.1934969025,0.09747568
99\C,8.9647125817,1.7023984714,-1.0643566261\C,10.4183405419,1.9700449
755,-0.6636183247\H,-2.1280380517,0.3068454157,-2.6215911799\H,-2.8400
522688,-2.9375796929,-1.7633249569\H,-3.52077456,-1.9426183804,1.44518
59085\H,-2.8017719825,1.3063648662,0.5896397561\H,-5.5060956304,-1.490
5034672,-1.2638209174\H,-5.0708989375,-0.0634832992,-2.1746165162\H,-5
.8018235699,-0.071517484,0.8056979666\H,-5.3893735583,1.3551281931,-0.
1226945375\H,-7.3642332696,0.9432105821,-1.6302794619\H,-7.7790980932,
-0.4799852376,-0.6913402897\H,-8.0912627788,0.961161363,1.3510863259\H
,-7.681036855,2.383187625,0.4084078187\H,-10.0703091543,0.5418986107,-
0.1409874527\H,-9.6602556456,1.9613010438,-1.0859499853\H,-11.46770488
98,2.4974348121,0.5662411689\H,-10.4201047767,1.9949303017,1.900015214
2\H,-10.0097542981,3.4243481358,0.9461132775\H,-0.0163307279,1.0970634
366,-0.5874961276\H,-0.0373435073,-1.864294419,-2.221164742\H,-0.98500
68376,-3.4162580673,0.6113266139\H,-0.9905156423,-0.4736981376,2.24637
02304\H,1.5751387122,0.766768498,1.2666579699\H,1.4849279113,-0.353925
6974,2.6417325061\H,3.8959550055,-0.9888381551,2.3226053056\H,3.714178
4519,0.7329936465,2.6092596908\H,3.9144153819,1.1986932031,0.179131225
4\H,4.5712715384,-0.6036134023,-1.4087031986\H,4.4289880024,-1.8042344
135,-0.1366475272\H,2.1155502799,-0.0672175735,-1.2405526534\H,2.40663
69787,-1.7753027351,-1.6287055957\H,5.8964172839,1.1156663603,1.714598
1821\H,6.2004096412,-0.5432333383,1.2324853314\H,6.6269661654,0.206577
8899,-1.1229851216\H,6.1990114338,1.8536231937,-0.6871542685\H,8.12974
38332,1.9252616824,0.9172219322\H,8.5445145957,0.2711184824,0.50028571
01\H,8.9390245431,0.9692634565,-1.8819123311\H,8.5204114558,2.62223829
21,-1.4679424785\H,11.0060904681,2.3317502956,-1.5130524217\H,10.47885
32898,2.7253453453,0.1279251013\H,10.9007746286,1.0602447911,-0.289054
2402\\Version=EM64L-G09RevC.01\State=1-A\HF=-1294.5342952\RMSD=3.581e-
09\RMSF=5.824e-06\Dipole=5.6566814,0.3455093,0.9084133\Quadrupole=3.49
34144,-3.6539856,0.1605712,-3.7899295,0.1611281,-0.4209951\PG=C01 [X(C
17H41B9S1)]\\@

**4[3]a-trans**

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C21H39B9O2S1\PIOTR\17-Oct-2013
\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)\\
C3_C5S_CB9COOPhC5 trans\\0,1\B,0.1669625483,0.0138527677,-0.0441105428
\B,0.0816420252,0.0118175047,1.8245408168\B,1.9244635245,-0.0359171016
,1.9089064017\B,2.0093880185,-0.0348841017,0.0395166321\C,1.0704314703
,0.9150059442,0.9338675704\C,1.105962201,2.4068769385,0.8814065071\O,1
.0850526569,2.9241326074,2.1435715325\C,1.0757868249,4.3023402774,2.37
27274661\C,1.8619986714,5.2099697111,1.6633785578\C,1.8220635627,6.556

085741,2.0256504259\C,1.0238698979,7.0153780234,3.0815495064\C,1.02628
20423,8.4751246176,3.4805597128\C,2.1521987309,8.834507542,4.470474944
5\C,2.1615340437,10.3166807524,4.8611791981\C,3.2863094827,10.68586729
44,5.8364268562\C,3.2926211902,12.1691391907,6.2179957954\H,2.35184748
62,12.458678394,6.6999412593\H,4.1065783509,12.4011871298,6.9125286353
\H,3.4185161341,12.8048916002,5.3341448885\H,3.1934169858,10.074165009
3,6.7440090019\H,4.2533666807,10.4184000651,5.3894940434\H,2.253508253
1,10.9310595955,3.9538236132\H,1.1925809394,10.5824249259,5.3079512366
\H,2.049172193,8.2141188366,5.3708393962\H,3.1191845601,8.5636964317,4
.0258913107\H,1.1284095792,9.100302363,2.5842564548\H,0.0594372773,8.7
349178292,3.9297791318\C,0.2528403877,6.0752367359,3.7773997443\C,0.27
38651002,4.7261861287,3.4301675086\H,-0.3231281523,3.9948142022,3.9645
861003\H,-0.3783287439,6.4022463456,4.5999644447\H,2.4261753889,7.2665
619471,1.4667088248\H,2.4743372442,4.8768129717,0.8367621217\O,1.14443
92372,3.0586223819,-0.1337381514\H,-0.5457689456,0.5452210896,-0.82538
09277\H,-0.7017743946,0.5391243086,2.5388204939\H,2.6660393961,0.45020
03856,2.6931420711\H,2.816634611,0.456202169,-0.6736109715\B,1.0651343
33,-1.5041271453,-0.3904706636\B,-0.3098552564,-1.4720339759,0.8702653
411\B,0.9449842855,-1.5085530874,2.2522528152\B,2.3222871075,-1.541288
4434,0.9909924029\B,0.9792518218,-2.542349446,0.9275907841\S,0.9377090
531,-4.4251663585,0.938298436\C,2.3339262546,-4.9211932164,-0.15851867
5\C,2.1884516323,-6.3806095768,-0.5912236532\C,0.9190870595,-6.6787696
631,-1.4153024235\C,-0.3580035461,-6.329521919,-0.6244787967\C,-0.4468
747545,-4.8634816269,-0.1970774649\C,0.9272774807,-8.1460427935,-1.885
7826549\C,-0.1642832208,-8.521306716,-2.8980217128\C,-0.0264337547,-9.
9609544635,-3.4035669411\H,1.1055001142,-1.9302716363,-1.5046502012\H,
-1.4364498685,-1.8553515994,0.814575466\H,0.8831678969,-1.940032403,3.
3591503903\H,3.4278435313,-1.9830264479,1.0364194585\H,2.3337431819,-4
.228409066,-1.0041544358\H,3.2375384244,-4.7485280125,0.4295820415\H,2
.2164313779,-7.0325268794,0.2919408828\H,3.0741159618,-6.6302468086,-1
.1879634307\H,0.9442848381,-6.036302287,-2.3093431687\H,-1.24296656,-6
.5341158965,-1.2362633717\H,-0.4329145435,-6.978642771,0.2583075477\H,
-0.3925492434,-4.1754204481,-1.0447853025\H,-1.3582201917,-4.647947785
2,0.3643204821\H,1.9063965497,-8.3551208605,-2.3377926269\H,0.85444643
64,-8.8054146545,-1.008424806\H,-1.1574258691,-8.3944012656,-2.4499013
086\H,-0.1213182106,-7.8285208446,-3.7493174878\H,0.93863138,-10.11643
27556,-3.8984897522\H,-0.0944783731,-10.6792780008,-2.5789648198\H,-0.
8130687881,-10.2063207013,-4.1235159621\\Version=EM64L-G09RevC.01\Stat
e=1-A\HF=-1596.2534288\RMSD=6.425e-09\RMSF=3.358e-06\Dipole=-0.0755766
,-3.8029699,-0.5934673\Quadrupole=-19.9073708,40.1489168,-20.241546,3.
9295557,-1.535657,23.7949828\PG=C01 [X(C21H39B9O2S1)]\\@

**4[3]a-cis**

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C21H39B9O2S1\PIOTR\17-Oct-2013
\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)\\
C3_C5S_CB9COOPhC5 cis\\0,1\B,-0.0323029582,-0.037148301,0.0387072569\B
,-0.1386000821,-0.0801409613,1.8773529215\B,1.7277878052,-0.0524049222
,1.9882079815\B,1.8345690402,-0.0097662677,0.1461077465\C,0.8337321884
,0.8821552244,1.0335469238\C,0.8757738315,2.3741933879,1.06456588\O,-0
.3868598527,2.889349998,0.9925979926\C,-0.5861360231,4.273184487,0.988
7772712\C,-1.5755929979,4.7574169623,1.8397823848\C,-1.8795670062,6.11
76652817,1.8302342138\C,-1.2069402835,7.0060726425,0.9810835537\C,-1.5
648878043,8.4761604632,0.947943678\C,-2.6892762215,8.8065102154,-0.053
7058509\C,-3.048001534,10.2963714313,-0.0893807544\C,-4.1724109259,10.
6321737341,-1.076892602\C,-4.5233959315,12.1226859349,-1.1090388153\C,
-0.2179243804,6.4855203547,0.1357395386\C,0.0989313834,5.1280379125,0.
1274256688\O,1.8837355868,3.0327704567,1.1409922371\H,-0.7438945921,0.
4734210967,-0.7576690902\H,-0.9395121709,0.3934409524,2.6094776565\H,2

.4245582399,0.4515414431,2.8014387696\H,2.6182551326,0.5305987818,-0.5
574381786\H,-2.0924862599,4.0663861952,2.4972246747\H,-2.6494038965,6.
4941873869,2.4991703515\H,-1.8730107546,8.8021917615,1.949477623\H,-0.
6746407959,9.0643815243,0.6917254078\H,-2.3849546465,8.4751747952,-1.0
555204631\H,-3.5803311716,8.2174843006,0.2017293478\H,-3.3414296399,10
.6247622772,0.9182047946\H,-2.1526435073,10.8801007878,-0.3477698255\H
,-3.8802940484,10.302679352,-2.0831557614\H,-5.0673259476,10.050881916
8,-0.8164759265\H,-3.657932335,12.7275186106,-1.4028641652\H,-5.329740
1989,12.3295290294,-1.8202053184\H,-4.8508498695,12.473978084,-0.12386
81934\H,0.3215194695,7.155309266,-0.5293747217\H,0.8735606344,4.743022
5018,-0.5232970138\B,0.9522877018,-1.5124045542,-0.3353467303\B,-0.439
8601873,-1.5587230294,0.9020674684\B,0.8002157649,-1.5743423971,2.2921
534518\B,2.1985839181,-1.5165823751,1.055607529\B,0.9010291817,-2.5836
992523,0.9549042135\S,0.715945416,-4.4611654486,0.9036883774\C,1.77133
43445,-5.0769107088,-0.4792056083\C,3.2725152038,-4.9072979011,-0.2569
631553\C,3.808908483,-5.5779920427,1.0226751899\C,3.1564800607,-4.9676
652988,2.2782896233\C,1.6405383744,-5.1428721016,2.3482258134\C,5.3461
547795,-5.4774801418,1.0647700838\C,6.0309152161,-6.2958947479,2.16803
94019\C,7.5593680625,-6.2411726172,2.0764389814\H,1.022890649,-1.89590
62006,-1.4616342171\H,-1.5348618646,-2.017663479,0.8281169113\H,0.7424
459959,-2.0114779576,3.3996147474\H,3.3270926288,-1.8903450101,1.11262
12975\H,1.4917216202,-6.1289969582,-0.5956278747\H,1.4194721813,-4.526
9499055,-1.3548034459\H,3.5213326664,-3.8412103322,-0.2482442429\H,3.7
711388767,-5.3421546431,-1.1325741867\H,3.5424311013,-6.6474773936,0.9
835916914\H,3.5620445159,-5.4409797157,3.1796499224\H,3.4030548122,-3.
9028423013,2.3401728091\H,1.3527916556,-6.1983485031,2.390035048\H,1.2
071016933,-4.6318124733,3.2108128886\H,5.7368441979,-5.8096061822,0.09
31127996\H,5.6339025529,-4.4209277579,1.1597146754\H,5.7208981516,-5.9
358855457,3.1567070984\H,5.6975524269,-7.3409180947,2.1037140998\H,7.9
133298642,-6.6359461876,1.1175338935\H,7.9245754154,-5.2120837393,2.16
48297305\H,8.0271700632,-6.8293091009,2.8719305208\\Version=EM64L-G09R
evC.01\State=1-A\HF=-1596.2518279\RMSD=6.676e-09\RMSF=6.501e-06\Dipole
=0.5988731,-3.4446771,-0.0954129\Quadrupole=-19.1051407,38.1360438,-19
.0309032,-20.796261,-2.3423107,-2.6109513\PG=C01 [X(C21H39B9O2S1)]\\@

**4[3]c-trans** PhOCF3-trans

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C17H28B9F3O3S1\PIOTR\31-Jul-20
12\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3-C5S-CB9-COO-PhOCF3, trans\\0,1\B,0.2053617461,-1.1191190413,0.174
3949166\B,-0.3752662034,0.1750065038,1.3946636987\B,-0.5234965583,1.40
2356376,0.0234530418\B,0.0576785401,0.1073531475,-1.197288266\C,-1.036
3372177,-0.1207617249,-0.0413660665\C,-2.431465613,-0.5767648575,-0.30
22680048\O,-3.3079281369,0.1067387178,0.496395117\C,-4.6810746524,-0.1
152375448,0.4501097423\C,-5.4664000297,1.0160299704,0.6759560017\C,-6.
8527975439,0.8985277949,0.7290324577\C,-7.4284855991,-0.355874744,0.54
90967583\O,-8.821943856,-0.5081678248,0.6692173331\C,-9.5703502751,-0.
2430793673,-0.4293040816\F,-10.8421007226,-0.5055032732,-0.1261768235\
F,-9.4827524134,1.047247686,-0.8147787246\F,-9.2151453559,-0.995375501
1,-1.4881004892\C,-6.6506826251,-1.4871240655,0.3281699881\C,-5.261521
3186,-1.3743141494,0.2812305407\O,-2.746704055,-1.423637856,-1.1012990
557\H,0.0134846918,-2.2872919471,0.1742457543\H,-1.0279941364,0.041399
0337,2.3730716021\H,-1.2991699011,2.2835130223,-0.1317428218\H,-0.2550
820311,-0.0497549913,-2.3276895887\H,-4.9790439051,1.9746205912,0.8148
479916\H,-7.4820073945,1.7620140188,0.9094771329\H,-7.13315449,-2.4494
564192,0.1997700365\H,-4.645739782,-2.2440512628,0.1028719996\B,1.6658
806918,-0.349833451,-0.5366257039\B,1.3622615879,-0.3094030244,1.30563
4577\B,0.8470308063,1.4803306274,1.1890547151\B,1.1517779583,1.4417886
464,-0.6535200171\B,2.2389689876,0.857797289,0.4812734231\S,4.01678429

01,1.4001495072,0.783368363\C,4.7101765061,1.6880760586,-0.9006026276\
C,6.2378502274,1.7333965927,-0.8516239379\C,6.8980018222,0.4219336449,
-0.3791620347\C,6.4280740326,0.0354788772,1.0385440709\C,4.9166723203,
-0.1630397199,1.164352485\C,8.4317074275,0.5376335104,-0.4692813677\C,
9.2055022532,-0.7708366977,-0.2558503008\C,10.7137675558,-0.6030714302
,-0.466710808\H,2.4150458885,-1.0003504143,-1.1992330736\H,1.844174866
1,-0.9377755724,2.1953661306\H,0.9113256823,2.3687890541,1.9772845669\
H,1.4550249545,2.2986508393,-1.4231773473\H,4.3342782844,0.8859056329,
-1.5411918274\H,4.2746088891,2.6317485374,-1.2351620813\H,6.5626555782
,2.56324959,-0.2101751007\H,6.5864327491,1.970289877,-1.8641530785\H,6
.5778193114,-0.3768394251,-1.0663065131\H,6.8957201162,-0.9071621904,1
.3423447232\H,6.7638278611,0.7950795518,1.7571813717\H,4.5354568366,-0
.9238591833,0.4780492977\H,4.6139920078,-0.4294251353,2.178977539\H,8.
6877597458,0.9336339309,-1.4615366626\H,8.7789667066,1.2904563419,0.25
34475743\H,9.028560054,-1.1568425491,0.7554853921\H,8.821892245,-1.533
8267509,-0.9465920209\H,11.2439913434,-1.5471573302,-0.3091063003\H,10
.936522745,-0.2615125047,-1.4835973811\H,11.1320815062,0.1333139776,0.
2284827641\\Version=EM64L-G09RevC.01\State=1-A\HF=-1811.9208462\RMSD=4
.123e-09\RMSF=5.630e-06\Dipole=5.0903321,0.6528748,0.348235\Quadrupole
=26.3115222,-10.3551364,-15.9563858,1.4783507,-3.8346056,-3.3691363\PG
=C01 [X(C17H28B9F3O3S1)]\\@

**4[3]c-cis** PhOCF3-cis

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C17H28B9F3O3S1\PIOTR\31-Jul-20
12\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3-C5S-CB9-COO-PhOCF3, cis, start at the HF/6-31G* geom\\0,1\B,-0.22
52090911,-1.6365131419,-0.737889988\B,-0.055330422,-1.3551836074,1.076
5001303\B,0.7469154304,0.3020293804,0.7438751878\B,0.5772251028,0.0190
661665,-1.0724700993\C,-0.5718732612,-0.2610763897,0.017246516\C,-1.88
91974216,0.4380750853,0.0300950982\O,-2.8876179496,-0.4485732431,0.322
869992\C,-4.2267831906,-0.0720633986,0.3846988576\C,-4.6770372314,1.15
23759247,0.8825661391\C,-6.0492988368,1.3839500646,0.9580639795\C,-6.9
474473802,0.3995379481,0.5574841497\O,-8.3035113311,0.7123091284,0.735
2858455\C,-9.2161896969,0.3182652183,-0.1830482138\F,-10.3575083108,0.
953022984,0.0849659771\C,-6.5016770221,-0.8314451224,0.079032189\C,-5.
1302142572,-1.0564417075,-0.0137314496\O,-2.0526878791,1.6138012558,-0
.1862113728\F,-8.8436264295,0.6034885109,-1.4427956196\F,-9.4629804195
,-1.0122244968,-0.1342628135\H,-1.0712695254,-2.1951768248,-1.34956088
63\H,-0.7601467909,-1.6789069412,1.9705819339\H,0.678878017,1.30643861
88,1.3667470652\H,0.3697511383,0.7903341975,-1.9457193817\H,-3.9749472
154,1.9158334156,1.1849447118\H,-6.4322088362,2.3276048303,1.330358610
6\H,-7.2033509542,-1.6014223722,-0.2133969653\H,-4.7474212988,-2.00164
52296,-0.3823949822\B,1.4877495566,-1.5240842519,-1.3164811627\B,1.038
0372208,-2.4891581578,0.2127606959\B,1.7297860202,-1.121646291,1.27362
12447\B,2.1704939045,-0.1473647544,-0.2563064627\B,2.546816602,-1.7744
541177,-0.0389533234\S,4.135309726,-2.7917734095,-0.0519128446\C,5.055
6823482,-2.3602372635,-1.5930537533\C,5.599526826,-0.9336328699,-1.632
4142786\C,6.5273095078,-0.5679169685,-0.4572962184\C,5.7779095408,-0.6
666695903,0.8858562169\C,5.2640289213,-2.0666101779,1.2156647289\C,7.1
289793215,0.8339219427,-0.6772878249\C,8.2491313684,1.2300924185,0.294
5026164\C,8.8627876801,2.5934857604,-0.0402192747\H,1.7542254881,-1.87
44891415,-2.4238559242\H,0.9595918511,-3.6608867637,0.401610058\H,2.20
00852814,-1.1303541023,2.3685365543\H,3.0061968235,0.6749245444,-0.460
7163639\H,5.8558094503,-3.104863105,-1.6545923767\H,4.342714002,-2.552
29225,-2.3979846862\H,4.7647169168,-0.2272851117,-1.6781408453\H,6.150
9353401,-0.8338198315,-2.5760736741\H,7.3578554989,-1.292921788,-0.440
0622026\H,6.4429447661,-0.3815962989,1.7088747803\H,4.9426788084,0.041
3151407,0.8941755874\H,6.0808841995,-2.789833452,1.3061189095\H,4.6822

861549,-2.0853301829,2.1399070003\H,7.5251339337,0.8804790528,-1.70095
15252\H,6.3229590382,1.5799967933,-0.6323159941\H,7.8692376039,1.25450
24271,1.3232111417\H,9.0334128211,0.460808822,0.2755963447\H,9.6602032
39,2.853965677,0.6625633087\H,9.29198549,2.5987983874,-1.0483475854\H,
8.1094538122,3.3877316596,0.002301522\\Version=EM64L-G09RevC.01\State=
1-A\HF=-1811.9185626\RMSD=5.417e-09\RMSF=4.107e-06\Dipole=4.5501334,-1
.1355629,-0.0078478\Quadrupole=24.0617564,-12.1850019,-11.8767544,-7.4
535526,-2.3867635,3.7191933\PG=C01 [X(C17H28B9F3O3S1)]\\@

**4[3]d-trans** PhF3 trans:

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C16H26B9F3O2S1\PIOTR\31-Jul-20
12\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3-C5S-CB9-COO-PhF3, trans\\0,1\B,0.7384634292,-1.27235222,0.3956933
504\B,0.2148296923,0.2591452819,1.3375379837\B,0.0964237284,1.19451132
89,-0.2498689053\B,0.6191769572,-0.3373386363,-1.1910174553\C,-0.47015
21227,-0.2915526227,-0.0088996046\C,-1.8812049842,-0.7420782732,-0.168
1240665\O,-2.7294418151,0.1556682226,0.4242276079\C,-4.1098785904,0.01
64435054,0.4235381017\C,-4.8007728331,1.2237273584,0.5526222001\C,-6.1
851998554,1.1975676813,0.6257393305\C,-6.8909517724,-0.0024347836,0.57
40401855\F,-8.2292822016,-0.0148948507,0.6423859819\C,-6.1713277728,-1
.1872546952,0.4479031243\C,-4.7834236141,-1.2063561086,0.3740202235\O,
-2.2294905737,-1.7482743432,-0.7347763525\F,-6.8755119339,2.3420048903
,0.7491364232\F,-6.8545562048,-2.3416818241,0.3994472673\B,2.217297599
4,-0.7134446424,-0.4582947635\B,1.934729687,-0.2992365804,1.3405464644
\B,1.4802521152,1.451423355,0.8716719922\B,1.7645053107,1.0371509324,-
0.9256407945\B,2.8427765298,0.650142455,0.2989557332\S,4.6400155002,1.
18145945,0.4815176653\C,5.3297235144,1.0890541311,-1.2254130142\C,6.85
85039533,1.0931618672,-1.187645432\C,7.4817336157,-0.1097170723,-0.450
0087492\C,7.0075240144,-0.1769104998,1.0164487733\C,5.4914807428,-0.29
68892531,1.1797427782\C,9.0178901876,-0.0599034335,-0.5592095187\C,9.7
555809742,-1.3120624063,-0.0648055036\C,11.267536124,-1.2353539721,-0.
2998584882\H,0.504749314,-2.4092389899,0.6278155708\H,-0.4324315405,0.
3461981119,2.3249728836\H,-0.6490138986,2.0550200786,-0.5749375224\H,0
.2883040413,-0.7038468576,-2.2665823134\H,-4.2669724809,2.1645902804,0
.5989505912\H,-4.2652946559,-2.1459500596,0.2599859335\H,2.9356185816,
-1.5089027233,-0.9820821646\H,2.4022184649,-0.7555723408,2.336399929\H
,1.5850579185,2.4753686156,1.4676421117\H,2.0899445282,1.712663486,-1.
8510544042\H,4.9221787027,0.1845148161,-1.6847113343\H,4.9227475562,1.
9565701043,-1.7488491568\H,7.2138146059,2.0285547742,-0.7355382821\H,7
.2068868795,1.1004754796,-2.227538049\H,7.1354145493,-1.0250297315,-0.
9549513543\H,7.4473437584,-1.0498320065,1.5103396633\H,7.370928889,0.7
047954172,1.5610986984\H,5.0827201465,-1.1713979917,0.6667621329\H,5.1
868197169,-0.3367626413,2.2274163943\H,9.2816111998,0.1046309636,-1.61
28757137\H,9.3884308671,0.8214075733,-0.0153764848\H,9.5695184053,-1.4
648290426,1.0054085823\H,9.3496941384,-2.1956410916,-0.5756507873\H,11
.7714110347,-2.1371058696,0.0610279013\H,11.4987920292,-1.1284866561,-
1.3654362861\H,11.7069668467,-0.377701941,0.2215409221\\Version=EM64L-
G09RevC.01\State=1-A\HF=-1697.3457885\RMSD=4.667e-09\RMSF=4.001e-06\Di
pole=5.3237896,0.533553,0.0099169\Quadrupole=16.6443111,-10.5075247,-6
.1367864,-1.5851652,-2.5916752,-3.8262067\PG=C01 [X(C16H26B9F3O2S1)]\\
@

**4[3]d-cis** PhF3, Cis:

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C16H26B9F3O2S1\PIOTR\31-Jul-20
12\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3-C5S-CB9-COO-PhF3, cis\\0,1\B,0.3221835456,-1.2824470932,-0.595835
2696\B,0.4204343552,-0.9124949935,1.2083684818\B,1.1548633465,0.764496
1827,0.8250542886\B,1.0554560215,0.395296188,-0.9812372382\C,-0.112759

6795,0.1070382276,0.0855786666\C,-1.4588403589,0.7435045866,0.03374927
68\O,-2.4283165951,-0.1912642375,0.2872287756\C,-3.7830172077,0.109138
0552,0.3014488628\C,-4.3110871924,1.3402590538,0.6965799594\C,-5.69402
844,1.4731758088,0.731460662\C,-6.5471609569,0.4258425893,0.3947396077
\F,-7.8772119919,0.5828678444,0.4377966923\C,-5.9847122261,-0.78923594
65,0.0105436626\C,-4.609723206,-0.9631766636,-0.0406376934\O,-1.670144
6342,1.908464746,-0.1951835905\F,-6.2409773297,2.6413635245,1.10269127
31\F,-6.8052103258,-1.8010507715,-0.3125573642\B,2.0451736351,-1.11192
45309,-1.1278100517\B,1.59305614,-2.029624534,0.4298882504\B,2.1853492
871,-0.5838401585,1.4470040109\B,2.6284662257,0.3417914923,-0.11284093
08\B,3.0737264649,-1.2537503153,0.1911439197\S,4.7096870182,-2.1868858
59,0.2955742142\C,5.6194477848,-1.8808277537,-1.2808142664\C,6.0892772
882,-0.4404361095,-1.4725372164\C,6.9982374262,0.0911593355,-0.3468966
89\C,6.2529731014,0.1008271564,1.0022557402\C,5.7938418532,-1.27603227
94,1.479553301\C,7.5325274742,1.4888508314,-0.7165861511\C,8.631246332
2,2.039510346,0.2033537856\C,9.1792579234,3.3870529068,-0.2774174962\H
,-0.4769966516,-1.907429354,-1.2061653346\H,-0.2969050503,-1.229963701
6,2.0948706176\H,1.0190946601,1.7906502951,1.3991017315\H,0.8387915462
,1.1168338062,-1.8939709523\H,-3.6848093217,2.1818109293,0.95023739\H,
-4.1877689944,-1.9156191546,-0.335818187\H,2.3625630692,-1.4973472302,
-2.209715524\H,1.5641770888,-3.1940295955,0.6701308483\H,2.6202497967,
-0.521102156,2.5544003385\H,3.4305089837,1.1930589623,-0.3317746046\H,
6.4575425878,-2.58475157,-1.2588370312\H,4.9240837702,-2.1957002336,-2
.062094605\H,5.2194747097,0.2146341487,-1.5858491195\H,6.6336235484,-0
.4112391031,-2.4249867634\H,7.8619961003,-0.5882094274,-0.2570865736\H
,6.9054021504,0.4957213375,1.7891304567\H,5.3903433012,0.7719699149,0.
9392052505\H,6.6385918962,-1.9502083064,1.6535760585\H,5.2049324097,-1
.2175735549,2.3975858691\H,7.9275070329,1.4454584052,-1.7408444107\H,6
.6916804574,2.1961364325,-0.7476508277\H,8.2489643791,2.1553748128,1.2
249176977\H,9.4512614021,1.3107099191,0.2634899407\H,9.96107324,3.7596
097562,0.3915422217\H,9.6107339568,3.3046293778,-1.2811904969\H,8.3884
028517,4.1440056604,-0.3189054641\\Version=EM64L-G09RevC.01\State=1-A\
HF=-1697.3440059\RMSD=5.852e-09\RMSF=4.205e-06\Dipole=4.9067477,-1.023
6532,-0.0297298\Quadrupole=14.810504,-9.8267683,-4.9837357,-3.6901596,
-0.7321489,1.8635072\PG=C01 [X(C16H26B9F3O2S1)]\\@

**4[3]e-trans** ChxC3

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C19H41B9O2S1\PIOTR\18-Oct-2013
\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)\\
C3_C5S_CB9COOChxC5 trans\\0,1\B,0.1662946001,-0.0276819247,-0.32181885
52\B,-0.0789497798,0.0738769861,1.5299723638\B,1.7496653128,0.07023147
,1.7713047501\B,1.9942794263,-0.0322137146,-0.0785074839\C,0.966141091
7,0.9467136215,0.6745352786\C,0.9848919659,2.4370839076,0.544912081\O,
0.832756763,3.0343984096,1.7442527348\O,1.1221120307,3.0278078912,-0.5
051032521\H,-0.4856571264,0.4413823969,-1.1914160071\H,-0.9300619391,0
.6224453238,2.1436537843\H,2.4137683831,0.6152100279,2.5860602246\H,2.
8525524501,0.4332461784,-0.7478961737\B,1.116462552,-1.5434038162,-0.5
016821506\B,-0.362691218,-1.4705655165,0.6334616068\B,0.7704142038,-1.
4018651404,2.1166555878\B,2.2496057072,-1.4763765315,0.9814569906\B,0.
93385954,-2.5079852923,0.8616484927\S,0.9179419122,-4.3878138644,0.976
9211002\C,2.3824079037,-4.9209477245,-0.007689285\C,2.2881539699,-6.40
46037384,-0.3680496791\C,1.0731492403,-6.7646135216,-1.2473793354\C,-0
.2521024978,-6.3936384826,-0.551263104\C,-0.3910988892,-4.9093275652,-
0.2110422517\C,1.0659032552,-8.2534587582,-1.6440375372\C,2.2208877344
,-8.6994687705,-2.551481631\C,2.0946196034,-10.1624271147,-2.988600131
4\H,1.2585148211,-2.0284244952,-1.5829501534\H,-1.4737830599,-1.881469
9401,0.5047485707\H,0.6209012601,-1.7721691932,3.2374711871\H,3.354243
9682,-1.8911732166,1.1469629928\H,2.4217475966,-4.2763608931,-0.889654

5819\H,3.2473366642,-4.6993574805,0.6208472253\H,2.2700170985,-7.00951
11293,0.5484931575\H,3.2158216702,-6.6614001884,-0.8905660158\H,1.1406
504992,-6.1685352835,-2.1709784055\H,-1.0914519211,-6.6545205008,-1.20
73017431\H,-0.3729243783,-6.9950314144,0.3596319143\H,-0.2970558191,-4
.2664751168,-1.0902365741\H,-1.3371581858,-4.6809630266,0.2837773469\H
,1.0578994269,-8.8688183279,-0.7324269753\H,0.1188326648,-8.466638841,
-2.1583057823\H,2.2521979601,-8.0534473867,-3.4392261236\H,3.181283733
2,-8.5623806638,-2.0394758643\H,2.0909227897,-10.8358723861,-2.1242606
024\H,1.1651977566,-10.3319023665,-3.5435243561\H,2.9267145442,-10.456
9038509,-3.6353547902\C,-0.6088068512,6.5513312101,1.6184855716\C,-0.5
638475373,5.0242013506,1.4553114971\C,0.8339161322,4.4882548745,1.7646
271497\C,1.3050860399,4.9087304728,3.1530101417\C,1.2549241783,6.43685
53925,3.3122446786\C,-0.1434443068,7.0124676049,3.0130673281\H,-1.2758
540898,4.5515029922,2.1446655849\H,-0.8491073561,4.7355806765,0.439154
2667\H,0.0320353441,7.0182673741,0.8562116505\H,-1.6264411444,6.911996
563,1.42567272\H,0.6567734027,4.433353506,3.9004051898\H,2.319370107,4
.5336411004,3.3280548232\H,1.5726604349,6.7021986487,4.3261778238\H,1.
9817259745,6.9011088817,2.6288967149\H,-0.8430412259,6.5897641669,3.75
25889774\H,1.5357600437,4.8312967098,0.9970752528\C,-0.2003896226,8.54
59096864,3.1338361612\C,0.0414211779,9.1049896651,4.5424231105\H,-1.18
7979434,8.884665356,2.7894177759\H,0.527728791,8.9883345796,2.43761600
86\C,-0.1217761624,10.626715424,4.61390905\H,-0.657140302,8.6289678289
,5.2442378545\H,1.0478377421,8.8367427871,4.8866916085\H,0.0585549428,
11.0020718523,5.6265151289\H,0.5814392347,11.1323104939,3.9422393568\H
,-1.1328897984,10.9316587667,4.3209740296\\Version=EM64L-G09RevC.01\St
ate=1-A\HF=-1521.2606692\RMSD=5.442e-09\RMSF=4.133e-06\Dipole=-0.04212
37,-3.5786724,-0.2691417\Quadrupole=-15.5894449,35.338805,-19.7493601,
-3.3811452,0.2148778,18.710522\PG=C01 [X(C19H41B9O2S1)]\\@

**4[3]e-cis** ChxC3

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C19H41B9O2S1\PIOTR\18-Oct-2013
\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)\\
C3_C5S_CB9COOChxC5 cis\\0,1\B,0.2132220714,0.0630443204,0.0382459461\B
,0.1027730095,0.0425312405,1.8767636614\B,1.9662425832,-0.0480406836,1
.9891140514\B,2.0763263376,-0.0255288058,0.1474261208\C,1.1341307008,0
.9342402543,1.0266687975\C,1.260662957,2.4249079646,1.0545392288\O,0.0
61824786,3.0222834186,0.9004380558\O,2.3095733198,3.0156509705,1.20031
19956\H,-0.4645524206,0.6100626115,-0.7634187331\H,-0.6667626341,0.573
1110198,2.6037853187\H,2.6931333301,0.4156788825,2.7998085934\H,2.8938
300471,0.4560293705,-0.5607086148\B,1.100137167,-1.4755192465,-0.32169
06074\B,-0.2934810971,-1.4219374357,0.9137311004\B,0.9435092664,-1.505
8832322,2.3053945267\B,2.3417159528,-1.5460245361,1.0697648673\B,0.978
4710458,-2.530460031,0.9772892974\S,0.6767758814,-4.3928482712,0.95746
44331\C,1.6651587801,-5.0953323298,-0.4333057053\C,3.1773718113,-5.005
9747149,-0.2421559298\C,3.7018149095,-5.6882072428,1.0364901344\C,3.10
92822511,-5.0264666181,2.2958516459\C,1.5868225336,-5.1090136114,2.394
3632737\C,5.2428111165,-5.6705676922,1.0487105744\C,5.9031677696,-6.51
01070261,2.1513350689\C,7.4306051285,-6.5371401826,2.0342505146\H,1.14
78102616,-1.8718411922,-1.444946967\H,-1.4162325102,-1.8091456974,0.84
22990066\H,0.858598419,-1.9285537111,3.4168358226\H,3.443487357,-1.993
4008019,1.1292367802\H,1.3245039918,-6.1319959842,-0.5226098808\H,1.32
7909114,-4.5432735173,-1.313343291\H,3.4826643516,-3.9548059843,-0.253
2850793\H,3.6347554351,-5.4783358294,-1.1208245991\H,3.3767758882,-6.7
419304165,1.0174989966\H,3.501565237,-5.5138061891,3.1955820605\H,3.42
07809036,-3.9778635137,2.3400180391\H,1.2369713025,-6.1445609753,2.456
8721363\H,1.2013122352,-4.5613911416,3.2572268203\H,5.5972965609,-6.03
61271624,0.0751015587\H,5.5886416202,-4.6300112647,1.123937012\H,5.629
5700568,-6.1216648362,3.1399173573\H,5.5140825186,-7.5367115001,2.1065

300397\H,7.7474234146,-6.9633213813,1.0758335737\H,7.8506271982,-5.527
5564619,2.1017683142\H,7.8799391017,-7.1380008733,2.8309438084\C,0.230
0842145,6.5488917447,-0.5147320235\C,0.3820365902,5.0205277498,-0.4797
178441\C,0.0439797509,4.4766345261,0.9082314723\C,-1.3521686557,4.8985
326721,1.3543146991\C,-1.5019823497,6.427953381,1.3140982288\C,-1.1703
408583,7.0153595127,-0.0721700276\H,-0.297579675,4.5584117212,-1.20781
32232\H,1.4012408236,4.727269309,-0.748246184\H,0.9827952116,7.0041526
088,0.1455154572\H,0.4454629198,6.9174235673,-1.5249414672\H,-2.087868
9655,4.4329103935,0.6858530041\H,-1.5500589726,4.5155224833,2.36135474
23\H,-2.5209632128,6.6962638904,1.6125663347\H,-0.83159844,6.881176701
3,2.0595646882\H,-1.8987930599,6.6056752832,-0.7908557906\H,0.79848975
23,4.8138916965,1.6270177182\C,-1.2778444688,8.550191257,-0.115455377\
C,-2.6867301258,9.1186958573,0.1026065316\H,-0.9104767834,8.8965256493
,-1.0919848779\H,-0.5931682811,8.978967099,0.6314976776\C,-2.741762695
5,10.6427408968,-0.0445117771\H,-3.3770338428,8.6569810814,-0.61670414
65\H,-3.0547316733,8.8416134422,1.0980974709\H,-3.7556076977,11.024419
7421,0.1141889443\H,-2.0843279464,11.1347718209,0.6813265148\H,-2.4205
716209,10.9565199538,-1.0442918697\\Version=EM64L-G09RevC.01\State=1-A
\HF=-1521.2591008\RMSD=3.263e-09\RMSF=2.558e-06\Dipole=0.2666975,-3.23
97074,-0.1055914\Quadrupole=-18.1890479,33.4319773,-15.2429295,-15.519
3561,0.0958547,-2.1934419\PG=C01 [X(C19H41B9O2S1)]\\@

**4[3]g-trans** PhPhF3-trans

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C22H30B9F3O2S1\PIOTR\02-Aug-20
12\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3-C5S-CB9-COO-PhPhF3, trans\\0,1\B,3.3509220821,-0.287648221,-1.179
9079863\B,2.727453561,-0.9867305592,0.4406210116\B,2.8016589686,0.6956
803745,1.1947125212\B,3.4247250606,1.3951643491,-0.4256051059\C,2.2035
608748,0.3625027184,-0.2604660564\C,0.8176108642,0.638326142,-0.736273
5126\O,-0.0929829603,0.2459136004,0.2070977515\C,-1.4627294713,0.40023
25072,0.0124718974\C,-2.1911604013,0.7565673015,1.1465966034\C,-3.5760
303614,0.8613402964,1.0713298364\C,-4.2558582418,0.6145914599,-0.13273
16109\C,-5.7332463592,0.7295075437,-0.2136495483\C,-3.4953939705,0.253
8205672,-1.2567019869\C,-2.1084052429,0.1406015158,-1.1969852337\O,0.5
349902439,1.1382861312,-1.796946505\B,4.9229930727,0.4428298966,-0.704
564244\B,4.4318461132,-1.2527655149,-0.0971534705\B,4.0447996529,-0.54
53231098,1.5868182714\B,4.5372035257,1.1506935409,0.9806462059\B,5.461
4587019,-0.2269254254,0.7394971732\S,7.229699783,-0.5560032009,1.29752
98906\C,8.1094741534,1.0382663966,1.0088973425\C,9.6240258503,0.826906
5686,1.0129602197\C,10.1378827586,-0.1072403597,-0.1018534543\C,9.5036
789927,-1.5092013934,0.0058337959\C,7.9770609242,-1.5143836286,-0.0886
528379\C,11.677566885,-0.165250444,-0.08071691\C,12.3252086882,-0.8651
885319,-1.2836501242\C,13.8555140401,-0.7992276975,-1.2498589035\C,-7.
7952035489,1.8259451173,0.4178406777\C,-6.4136800629,1.7308239436,0.49
93550133\C,-6.478629801,-0.1612474441,-1.0041527904\C,-7.8588716244,-0
.0418436524,-1.0734064884\F,-9.8719136219,1.0504257025,-0.4389889664\C
,-8.5383241627,0.9472225771,-0.3664858966\F,-8.4488223287,2.7881780221
,1.0899583782\F,-8.5763519483,-0.8977199432,-1.8200467177\H,3.08790430
23,-0.6146652247,-2.2867407392\H,1.9688592938,-1.875594822,0.630129924
3\H,2.1035398211,1.198732819,2.0080242238\H,3.2224573201,2.4556678304,
-0.9104887977\H,-1.6627570993,0.9332457541,2.0771610976\H,-4.137465828
2,1.11163664,1.9660182231\H,-3.9923923024,0.0818379509,-2.2064075441\H
,-1.5386967734,-0.1206045075,-2.0778877252\H,5.6949707834,0.7853944657
,-1.5472564232\H,4.7784795226,-2.3404341904,-0.4375212064\H,4.08206119
71,-1.0329216587,2.6710865498\H,4.9708279033,2.1010292991,1.552952493\
H,7.7445183157,1.4348487411,0.0578043567\H,7.7777611546,1.700631113,1.
811034643\H,9.942708296,0.4455402525,1.9921004608\H,10.0874821215,1.81
4477534,0.9003170131\H,9.828901199,0.3262483486,-1.0659470902\H,9.8710

424752,-2.1485438198,-0.8038652274\H,9.8192632959,-1.9839822005,0.9445
260084\H,7.6126276187,-1.0659810917,-1.0166584522\H,7.5576351045,-2.51
87464205,-0.0024631113\H,12.0591994617,0.8636910213,-0.0315083093\H,12
.0068331046,-0.6530373077,0.8483974535\H,12.0150852085,-1.9166096795,-
1.3238126594\H,11.9589409624,-0.4022340977,-2.2098646223\H,14.29363447
59,-1.3031038972,-2.116739182\H,14.2082855856,0.2380466757,-1.25408084
99\H,14.2537239123,-1.2801781114,-0.3495058941\H,-5.8801212335,2.46059
99365,1.0968167663\H,-6.0022288884,-0.9688184991,-1.5472906196\\Versio
n=EM64L-G09RevC.01\State=1-A\HF=-1928.4114123\RMSD=5.560e-09\RMSF=1.95
1e-06\Dipole=5.3535663,-0.6122647,0.6046919\Quadrupole=30.5798285,-14.
8268279,-15.7530006,-2.4613997,0.3714047,4.407083\PG=C01 [X(C22H30B9F3
O2S1)]\\@

**4[3]g-cis** PhPhF3-cis

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C22H30B9F3O2S1\PIOTR\02-Aug-20
12\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3-C5S-CB9-COO-PhPhF3, cis\\0,1\B,0.2877115579,-1.293910152,-0.49261
90152\B,0.4655261234,-0.8695998993,1.2923888721\B,1.1933743823,0.78981
26763,0.8258657732\B,1.0151252785,0.3644585586,-0.9607511918\C,-0.1089
665162,0.1189828007,0.1629656367\C,-1.4505596227,0.7693009933,0.137371
0895\O,-2.4242920579,-0.1408753313,0.4466634762\C,-3.7728633419,0.2054
589743,0.4630261415\C,-4.2614199139,1.4055255338,0.9810035756\C,-5.638
2736597,1.6151916936,1.0074605609\C,-6.5418617445,0.6497872454,0.53520
92823\C,-8.0056522878,0.8922184366,0.5658256263\C,-8.8299298998,0.4238
242352,-0.4712057783\C,-8.5942966486,1.595786749,1.6300867982\C,-6.017
8546332,-0.5520959841,0.0313205842\C,-4.645629836,-0.77516915,-0.00680
73212\O,-1.6524585962,1.929500539,-0.1237203049\C,-10.196971643,0.6558
526058,-0.4322690256\C,-9.9631459811,1.8199104556,1.6429999728\B,1.987
9655203,-1.1523251797,-1.1028809515\B,1.5982887457,-2.016707021,0.5001
481206\B,2.2438553042,-0.5445920944,1.445837132\B,2.6239278246,0.32861
7464,-0.1589263563\B,3.0720501078,-1.260356,0.1736960936\S,4.704355127
3,-2.2053197597,0.2284539644\C,5.5895453955,-1.8697700424,-1.357008783
5\C,6.0610220391,-0.4275791309,-1.5279429328\C,6.9850611335,0.08050998
34,-0.4041866452\C,6.2558896777,0.0680281068,0.9532913759\C,5.80789095
99,-1.3182806888,1.412637259\C,7.5246716496,1.4805854474,-0.7562753343
\C,8.6315670471,2.0107118574,0.1655107946\C,9.200626273,3.3514756031,-
0.3100058252\C,-10.7846127098,1.3554379863,0.6187437583\F,-10.98705642
98,0.2188248074,-1.4271116357\F,-12.1054302389,1.5762728292,0.64392825
94\F,-10.5315210121,2.4836387052,2.6633964309\H,-0.5393958669,-1.93259
11366,-1.0490462003\H,-0.2137042237,-1.1554427483,2.2188797734\H,1.088
4030896,1.8344418012,1.3726284298\H,0.7636834054,1.0587666979,-1.88561
0351\H,-3.5813221667,2.1693564549,1.3310602009\H,-6.0139144109,2.56325
44799,1.3795797211\H,-8.4189732393,-0.0955695077,-1.328868684\H,-8.005
3384014,1.9503032798,2.467772946\H,-6.6905637515,-1.3320076658,-0.3113
613355\H,-4.2366134548,-1.7058423873,-0.3848842894\H,2.2552569505,-1.5
746046704,-2.1846506748\H,1.5741227262,-3.1730741947,0.7778145973\H,2.
726656115,-0.4510592613,2.5312904817\H,3.41974304,1.168380678,-0.43778
65416\H,6.4250766063,-2.5771350388,-1.3628154897\H,4.8797717772,-2.166
9941349,-2.1321540074\H,5.1904486836,0.2295410394,-1.6174988242\H,6.59
33916073,-0.382335975,-2.4865112023\H,7.8461294982,-0.6050755398,-0.33
5800484\H,6.9174795771,0.4517796865,1.7380092042\H,5.3905054484,0.7378
705781,0.9128198265\H,6.6568293248,-1.9934478745,1.5606302474\H,5.2324
085284,-1.2787961485,2.340160992\H,7.9139127049,1.4486480248,-1.783186
7832\H,6.6885330077,2.1936946638,-0.7731386007\H,8.2513687582,2.128541
3378,1.1876534704\H,9.4407430932,1.2695278323,0.2227074972\H,9.9868337
975,3.7103942887,0.3612940436\H,9.6324462331,3.2653280245,-1.313334810
7\H,8.4214321683,4.120534562,-0.350742629\\Version=EM64L-G09RevC.01\St
ate=1-A\HF=-1928.4097144\RMSD=6.679e-09\RMSF=2.620e-06\Dipole=4.962410

6,-1.1047652,-0.0800205\Quadrupole=26.0746856,-13.3782937,-12.6963918,
-6.3158092,-1.9534748,3.9441229\PG=C01 [X(C22H30B9F3O2S1)]\\@

**4[3]h-trans** PyrimPhC6-trans

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C26H43B9N2O2S1\PIOTR\01-Aug-20
12\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3-C5S-CB9-COO-PyrimidPhC6, trans\\0,1\B,0.3691378187,1.3931692586,-
0.6228154029\B,-0.0887824089,-0.046998163,-1.730463848\B,-0.464723804,
-1.0716232507,-0.2414530326\B,-0.0073751532,0.3675357889,0.8647259722\
C,-0.9258060727,0.454868639,-0.4521266892\C,-2.3222240742,0.9694785933
,-0.4522644676\O,-3.126632219,0.171584757,-1.2301818139\C,-4.475938509
5,0.4541107281,-1.3634253939\C,-5.3568081509,-0.6245111083,-1.36836222
05\N,-6.6637533252,-0.4682516167,-1.5623746973\C,-7.110113096,0.788322
5652,-1.7546112115\C,-8.5640871669,0.9771311264,-1.9698554605\N,-6.328
1384357,1.8838925559,-1.7715513133\C,-5.0198954562,1.7215062535,-1.578
3443403\O,-2.7110617088,1.945403489,0.1383950318\B,1.6907660621,0.7017
892301,0.3793033148\B,1.6379955469,0.4167586767,-1.4647384201\B,1.0466
031609,-1.3328666806,-1.1841119627\B,1.1003046386,-1.0477557603,0.6602
836865\B,2.3519731136,-0.6436673314,-0.3798895545\S,4.1332164989,-1.25
56070493,-0.3487207566\C,4.5865375178,-1.2661643828,1.43816553\C,6.104
6527322,-1.3362194841,1.6078147762\C,6.8677889089,-0.1321057486,1.0187
756589\C,6.6045626966,0.0152214841,-0.4936810096\C,5.1311284167,0.2088
904326,-0.8564286126\C,8.3704432338,-0.2517173798,1.338276715\C,9.2176
014032,0.9840901148,1.0045468261\C,10.6744469953,0.8363764894,1.455271
563\C,-10.8002429068,0.0603327855,-2.1755868636\C,-9.4361147947,-0.122
4692242,-1.9728486848\C,-9.0969803575,2.2595953219,-2.1718330585\C,-10
.4626278318,2.431399073,-2.3743144248\C,-12.8168128443,1.5257450218,-2
.649373319\C,-11.3401580635,1.3378480673,-2.3825127362\C,-13.173977884
,1.4393215023,-4.1472775446\C,-14.6696532396,1.6296899194,-4.424268284
6\C,-15.0303282285,1.5433515655,-5.912303711\C,-16.5260535465,1.731287
0538,-6.194055129\C,-16.8772303887,1.6427844047,-7.6822333208\H,0.2208
795236,2.5533414041,-0.8043633311\H,-0.5984063573,-0.036463636,-2.7988
545502\H,-1.2857178916,-1.9091371962,-0.0792383351\H,-0.46483693,0.682
5546669,1.9097188689\H,-4.9794608508,-1.6339903344,-1.2160569908\H,-4.
3973684878,2.609611148,-1.5899529422\H,2.3666428685,1.4235318501,1.046
9190866\H,2.2582841089,0.9090915616,-2.3543628648\H,1.1841449201,-2.32
16904385,-1.8305178681\H,1.2639691021,-1.7964163791,1.5719085436\H,4.1
553893623,-0.3640208487,1.8799779249\H,4.0785769255,-2.1357830231,1.86
00116341\H,6.4842810597,-2.2667466128,1.1654112856\H,6.3059841586,-1.4
011665486,2.6839704302\H,6.4880591256,0.7757165189,1.5133839035\H,7.14
13111102,0.8871711852,-0.8823632878\H,7.0050798107,-0.8588061582,-1.02
47184692\H,4.6893325399,1.0802635425,-0.3658356431\H,4.9761755803,0.30
30580888,-1.9330763915\H,8.475728581,-0.4645393781,2.4108965457\H,8.78
10912822,-1.1284593331,0.8163881948\H,9.1972489851,1.1789175061,-0.074
6568318\H,8.7736832244,1.866887675,1.4841854566\H,11.259275722,1.72706
45552,1.2064532775\H,10.7410360707,0.6857601255,2.5384162684\H,11.1540
599225,-0.0220728585,0.9719813255\H,-11.4613766814,-0.8031565419,-2.16
9804542\H,-9.027984891,-1.1135684776,-1.8111325666\H,-8.4264253907,3.1
111889741,-2.1631087975\H,-10.8583100378,3.4331316428,-2.5247839966\H,
-13.139865621,2.5000526305,-2.2613705805\H,-13.3894951984,0.7662147763
,-2.1021391952\H,-12.8464978036,0.4662593614,-4.5367975156\H,-12.59675
54756,2.1950103597,-4.6963378603\H,-14.9916992204,2.6036168397,-4.0284
781622\H,-15.2414357478,0.8734467354,-3.8674649183\H,-14.7071414664,0.
570035445,-6.3084898921\H,-14.459400689,2.3001179285,-6.4690911875\H,-
16.849047435,2.7042126681,-5.7991848232\H,-17.0963974872,0.9749427744,
-5.637766731\H,-17.9504075247,1.7804160665,-7.8500601598\H,-16.5981857
292,0.6678810488,-8.098050841\H,-16.349448145,2.409882968,-8.260306260
5\\Version=EM64L-G09RevC.01\State=1-A\HF=-1898.7109257\RMSD=4.620e-09\

RMSF=1.543e-06\Dipole=4.7216836,-0.7528238,0.4948476\Quadrupole=68.679
1303,-35.1193883,-33.5597421,-8.941543,22.0149516,-6.6853051\PG=C01 [X
(C26H43B9N2O2S1)]\\@

**4[3]h-cis** PyrimPhC6-cis

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C26H43B9N2O2S1\PIOTR\02-Aug-20
12\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3-C5S-CB9-COO-PyrimPhC6, cis\\0,1\B,11.137507327,-0.5895336472,-3.3
000103101\B,11.140234092,0.1258405555,-1.6005314889\B,11.7485842377,1.
7572249895,-2.2863950644\B,11.7455879077,1.0413219409,-3.988000579\C,1
0.5667102807,0.8620560412,-2.9094303767\C,9.1797412375,1.3595670769,-3
.119266872\O,8.2664176913,0.4412797087,-2.6606985708\C,6.9076245557,0.
687725177,-2.7698721454\C,6.2796950431,1.9041937032,-2.4969084515\N,4.
9541385422,2.0224352649,-2.5615003557\C,4.2376832318,0.9330646049,-2.8
959071791\C,2.7646423539,1.0753833264,-2.9720294422\C,1.9541182803,-0.
0243180189,-3.2925453\C,2.1527305219,2.3153336141,-2.7309806361\N,4.76
48385961,-0.277975873,-3.1620094021\C,6.0889959187,-0.3901374217,-3.09
81632488\O,8.8816221968,2.415288148,-3.6184425359\C,0.5718653889,0.116
7289547,-3.3672524652\C,0.7701376365,2.4458841989,-2.8096374377\B,12.8
592712077,-0.3738066159,-3.8226374429\B,12.4282951069,-1.0112806841,-2
.12470437\B,12.8634040967,0.6476305274,-1.3959817055\B,13.2850833808,1
.2931792116,-3.0966982502\B,13.8480874415,-0.169960513,-2.4818316827\S
,15.5516143891,-0.9132055718,-2.1554844666\C,16.5102314355,-0.81684025
49,-3.7298822122\C,16.8601055612,0.6015654545,-4.1744977742\C,17.65380
128,1.4204980585,-3.1379983457\C,16.8402534637,1.6057533579,-1.8423104
767\C,16.4873575756,0.302027058,-1.1286015045\C,18.0776381063,2.769956
7369,-3.7499962837\C,19.049273933,3.6043148729,-2.9037819582\C,19.5181
626773,4.8709703168,-3.6271033797\C,-0.0473232582,1.3516053595,-3.1276
236971\C,-1.5521951112,1.4925299433,-3.1728532536\C,-2.2217515942,1.28
49365287,-1.7990828485\C,-3.7469740863,1.4329599514,-1.8447477246\C,-4
.4219973076,1.2314724905,-0.482606042\C,-5.9479299533,1.3794293373,-0.
5267958591\C,-6.6150252233,1.17977969,0.8373350647\H,10.4143383943,-1.
3869291838,-3.7929824403\H,10.4208737262,-0.0777239708,-0.6828921986\H
,11.5086086688,2.8586731963,-1.9252425066\H,11.5029178496,1.5530350865
,-5.0270065759\H,6.8490670712,2.7877844298,-2.2301480353\H,2.424305509
2,-0.981984656,-3.4845172644\H,2.7771345751,3.1676028743,-2.4888051185
\H,6.5304560401,-1.3629279961,-3.3066031751\H,-0.0398884431,-0.7457214
21,-3.6214094456\H,0.3144326149,3.4162419572,-2.6265758758\H,13.243634
3027,-0.9308233605,-4.8031356041\H,12.4865419863,-2.1059471738,-1.6634
492893\H,13.2535036957,0.958434845,-0.3136800548\H,14.0210225253,2.154
9488734,-3.4600283017\H,17.4050565579,-1.4203589475,-3.546551163\H,15.
8871484539,-1.3369522673,-4.4608396751\H,15.9432016921,1.1356503569,-4
.4438288633\H,17.4520841569,0.5060992208,-5.0936386919\H,18.5700324356
,0.8596839635,-2.8893583895\H,17.4110790626,2.204088957,-1.1232682639\
H,15.9225220331,2.1613887226,-2.0600605424\H,17.380536339,-0.240139482
8,-0.8019992335\H,15.8476416875,0.4695420021,-0.2593879283\H,18.547476
349,2.5712164288,-4.7230401715\H,17.1777290475,3.3631203338,-3.9657586
902\H,18.577882408,3.8904210183,-1.955616831\H,19.9208797164,2.9894527
648,-2.6399619474\H,20.2063649625,5.4519373658,-3.0055144251\H,20.0377
887446,4.6255096689,-4.5599690638\H,18.6717435365,5.5185550769,-3.8808
763069\H,-1.8169595178,2.488690268,-3.5497963288\H,-1.9678644152,0.769
064269,-3.885460308\H,-1.9571852575,0.2896006999,-1.4181618923\H,-1.80
14665548,2.0044157353,-1.0838697423\H,-4.1602526598,0.7124471648,-2.56
51441575\H,-4.0036594784,2.4289473937,-2.2333444532\H,-4.0094064359,1.
9521566124,0.2378825131\H,-4.1657545127,0.2357505923,-0.0933798905\H,-
6.3601330728,0.6577800411,-1.2452286137\H,-6.2032207837,2.3739294873,-
0.9175173764\H,-7.7023926004,1.2903513647,0.7723573088\H,-6.2498206337
,1.9105965599,1.5678869456\H,-6.4057859377,0.181511529,1.2382691421\\V

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=2.121e-06\Dipole=4.4150126,-0.5339061,0.3537618\Quadrupole=68.2493727
,-33.3077812,-34.9415915,-7.0617802,-0.0454239,3.8877676\PG=C01 [X(C26
H43B9N2O2S1)]\\@

**4[3]j-trans** COOPhCOOPhOCF3


1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C24H32B9F3O5S1\PIOTR\15-Oct-20
13\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3_C5S_CB9COOPhCOOPhOCF3, trans\\0,1\B,-0.1711219546,-1.1971392271,-
3.7156210352\B,1.4347245845,-0.3234486657,-3.3134881817\B,0.5223761197
,1.2700609419,-3.1294425853\B,-1.0837874566,0.3975853096,-3.5341973805
\C,0.0453725486,-0.1406526373,-2.5234145309\C,-0.2093798214,-0.4475915
077,-1.0881158143\O,0.8196262896,0.0269885706,-0.3143334886\C,0.834964
4382,-0.1124405279,1.0659240922\C,-0.298574008,0.0172301095,1.87322112
\C,-0.1513830008,-0.0659021875,3.2548651532\C,1.1103328025,-0.27048073
17,3.831171599\C,2.2358366362,-0.3909226856,3.0024029409\C,2.100612388
3,-0.3123683611,1.6235241329\H,2.9566427891,-0.399424264,0.9636194118\
H,3.2071131671,-0.5455694863,3.4587875327\H,-1.0218372125,0.03199682,3
.8922670565\H,-1.2727513148,0.1670360991,1.4300666781\O,-1.1728410298,
-1.0324652608,-0.6607059705\H,-0.5090604068,-2.3010799004,-3.455019784
5\H,2.3832451414,-0.7308722283,-2.7338134979\H,0.7169312932,2.18025317
13,-2.3977755209\H,-2.1736551753,0.6072832964,-3.1229413326\B,-0.74758
75664,-0.2937598879,-5.1593329831\B,1.0381890681,-0.8142652155,-5.0057
016386\B,1.5215868178,0.9410993865,-4.5913933219\B,-0.2633995073,1.462
8177246,-4.7450328688\B,0.5308317635,0.5217605876,-5.8830845799\S,0.80
66498928,0.8940978598,-7.7088503398\C,-0.805135479,1.5773022477,-8.288
1746573\C,-0.8903875982,1.5393080242,-9.8145904298\C,-0.8290281018,0.1
217705612,-10.4189628871\C,0.4842648242,-0.5926824197,-10.0396571294\C
,0.6992587058,-0.750944577,-8.5334992237\C,-1.0343304891,0.1850133819,
-11.9449041282\C,-1.2234251734,-1.1700086513,-12.6415349973\C,-1.52747
78134,-1.025027955,-14.1361203777\H,-1.6444581576,-0.7325008719,-5.812
7134139\H,1.6450811522,-1.7021934316,-5.5171799887\H,2.5333890956,1.54
01676715,-4.7700623638\H,-0.7610220389,2.5047352033,-5.0371485745\H,-1
.5900745088,0.9864688054,-7.8089730515\H,-0.8458492656,2.5942650312,-7
.8926986307\H,-0.0943831931,2.1605740335,-10.2459685506\H,-1.838724235
,2.0125828978,-10.0963368377\H,-1.6607027088,-0.4583175482,-9.98932930
89\H,0.4965246057,-1.6011869212,-10.4662038888\H,1.3352985748,-0.05759
48235,-10.4818678737\H,-0.1142750862,-1.2968788716,-8.0486796884\H,1.6
399531384,-1.2525669982,-8.2978860127\H,-1.9188086961,0.8046844696,-12
.1459701864\H,-0.1856638318,0.715694997,-12.4008289623\H,-0.3260397311
,-1.7887053685,-12.5187049987\H,-2.0415581352,-1.7159730896,-12.152622
5976\H,-2.4438293897,-0.4472321156,-14.2998976963\H,-0.7138668631,-0.5
096391046,-14.6585252182\H,-1.6606001652,-2.0018731747,-14.6108076407\
C,1.3237692668,-0.361131314,5.2962333543\O,2.3973112264,-0.5183272409,
5.8337537436\O,0.1377907014,-0.2452239726,5.9829420172\C,0.1007054829,
-0.2963786567,7.3722385563\C,0.9978902477,0.3996833235,8.1848822905\C,
0.8341436661,0.3520770287,9.5682573268\C,-0.2173697773,-0.3790211791,1
0.111668833\C,-1.1159549284,-1.0706451655,9.3054998594\C,-0.9520821692
,-1.0271574898,7.9228015467\H,1.8154065932,0.9557041252,7.7472552154\H
,1.5167496731,0.8767266405,10.2268931918\H,-1.9237904233,-1.6341257134
,9.7575166214\H,-1.632147979,-1.553626079,7.2622731963\O,-0.3269387386
,-0.4768496116,11.5105017238\C,-1.1360972685,0.4173971505,12.129403115
\F,-1.0788081797,0.1777114038,13.4392784212\F,-0.7587455614,1.69214230
24,11.9085374326\F,-2.4204155548,0.3116599436,11.7306600069\\Version=E
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06\Dipole=-0.3662102,0.4266686,-5.9048754\Quadrupole=-24.969498,-24.00
8424,48.9779221,-0.2585253,2.0013604,-2.2924128\PG=C01 [X(C24H32B9F3O5
S1)]\\@

**4[3]j-cis** COOPhCOOPhOCF3


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1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C24H32B9F3O5S1\PIOTR\15-Oct-20
 13\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
 \\C3_C5S_CB9COOPhCOOPhOCF3, cis\\0,1\B,-0.1549919847,0.4041653307,-0.0
 857903698\B,-0.0375939934,0.292552443,1.7781283099\B,1.8020370717,0.34
 39411995,1.6673813532\B,1.6868793066,0.4562069525,-0.1966693378\C,0.80
 1287632,1.2990395123,0.8474115223\C,0.7663621123,2.7880523761,0.880074
 5378\O,0.8430750023,3.2350444616,2.1750390313\C,0.8575718119,4.5865701
 723,2.4896727815\C,1.5440506637,5.548668847,1.7437743173\C,1.556166711
 1,6.8650357286,2.1953148565\C,0.8974746637,7.2234427626,3.3800721806\C
 ,0.2204592311,6.2404490529,4.117160752\C,0.1993537142,4.9249966865,3.6
 747696244\H,-0.3147127254,4.1481568066,4.2298366938\H,-0.2827600766,6.
 5277162834,5.0336004131\H,2.0836377263,7.6208735202,1.6261555033\H,2.0
 458159644,5.2758392171,0.8263153957\O,0.6786209833,3.5036797758,-0.085
 9321799\H,-0.9718191824,0.9383423555,-0.755133124\H,-0.7671744484,0.73
 02500129,2.6013985595\H,2.5991520625,0.8254251031,2.3982381694\H,2.385
 9842902,1.0337138907,-0.9574694299\B,0.7788445555,-1.0343567339,-0.622
 4552619\B,-0.4527668556,-1.1583909109,0.775132234\B,0.9421059054,-1.19
 55177525,2.010319905\B,2.1742832719,-1.0836817422,0.6157985038\B,0.885
 7972446,-2.1598054127,0.6254829799\S,0.9334439614,-4.0437821751,0.7234
 177962\C,-0.4616770719,-4.6882867828,-0.2996291674\C,-0.3167494054,-4.
 4505370659,-1.8013364406\C,0.9752598507,-5.0197233222,-2.419588422\C,2
 .2202903227,-4.3624884296,-1.7924363818\C,2.3687453807,-4.6049614998,-
 0.2918494789\C,0.9456821683,-4.8511585985,-3.9511941414\C,2.0620124964
 ,-5.5770183429,-4.7149423221\C,1.9109428622,-5.4533909126,-6.234604801
 8\H,0.7202331871,-1.3584082706,-1.7658836601\H,-1.5587838313,-1.599504
 4831,0.816458746\H,1.0210353392,-1.701221453,3.0838577465\H,3.30082174
 37,-1.4604387857,0.5224882861\H,-0.5108483487,-5.754903267,-0.05793345
 76\H,-1.3482725163,-4.2005064767,0.1116626131\H,-0.3833192949,-3.37784
 03454,-2.0083753162\H,-1.1864626526,-4.920004685,-2.2783926922\H,1.011
 6421297,-6.0997324402,-2.200001139\H,3.1294307417,-4.7578239531,-2.259
 3527374\H,2.2056933815,-3.2851071196,-1.9882058236\H,2.4755206755,-5.6
 691162383,-0.0582204844\H,3.223752081,-4.0712547082,0.1288493364\H,-0.
 0221866797,-5.2194424559,-4.31804133\H,0.9721760292,-3.7794870826,-4.1
 942434006\H,3.0422531223,-5.1810934078,-4.422425241\H,2.0630659626,-6.
 6385961239,-4.4317724762\H,0.9621336713,-5.8824674085,-6.5753782341\H,
 1.9314762727,-4.4044905164,-6.5501364217\H,2.7188225129,-5.9738636427,
 -6.7580455401\C,0.8842191685,8.610200499,3.9069002684\O,0.3438113373,8
 .9595234395,4.9326018089\O,1.5689973755,9.4654037245,3.0761220107\C,1.
 6934078993,10.8190722475,3.368940454\C,2.003791469,11.3015119114,4.642
 1082249\C,2.1882008718,12.6719288412,4.8199533914\C,2.0680861043,13.52
 88401702,3.7304032911\C,1.7625732778,13.051689191,2.4598663172\C,1.572
 4014986,11.6836464581,2.2808573678\H,2.0852983828,10.6233427186,5.4800
 835404\H,2.4236317045,13.0774948148,5.7970985422\H,1.6733796825,13.744
 5546542,1.631188452\H,1.3334441521,11.2748540288,1.3052993039\O,2.1885
 20814,14.9164412966,3.9268728557\C,3.4326187046,15.4456556798,3.826373
 6323\F,3.3316298206,16.7607604438,4.0187247217\F,4.2819120227,14.94235
 78663,4.7447941074\F,3.9872619637,15.2294810692,2.6168243754\\Version=
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 -06\Dipole=0.1938526,-5.3353846,-1.6804487\Quadrupole=-22.7439099,40.3
 473129,-17.603403,0.9147979,0.4990775,15.5966705\PG=C01 [X(C24H32B9F3O
 5S1)]\\@
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**4[3]k-trans** COOPhFCOOPhOCF3


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1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C24H31B9F4O5S1\PIOTR\16-Oct-20
 13\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
 \\C3_C5S_CB9COOPhFCOOPhOCF3, trans\\0,1\B,0.0836980992,0.0087659937,-0
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.0016088303\B,0.1162778729,-0.0000494765,1.8708768371\B,1.9627424038,0
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0184496376,0.9354429231,0.9222281619\C,1.0111962926,2.4239210205,0.873
7583813\O,0.9629266766,2.9320783887,2.1469309063\C,0.9193950164,4.2771
070237,2.4616315674\C,1.1857901659,5.3255813929,1.5807840464\C,1.12344
67077,6.6279998782,2.0678656505\C,0.808005169,6.9277118085,3.401363515
8\C,0.5502015502,5.8372138306,4.2536354588\C,0.6043580005,4.5305827341
,3.8036637268\H,0.407025836,3.6941272054,4.4637455862\H,0.3030804189,6
.0576503712,5.2857363756\F,1.3820156938,7.6022614949,1.1811630779\H,1.
4218918797,5.1561094954,0.5421758434\O,1.0393593872,3.0852926052,-0.13
43158249\H,-0.6917950876,0.5212205821,-0.7343845409\H,-0.6359514841,0.
5019432109,2.6348360748\H,2.7358463709,0.5207537523,2.5756993597\H,2.6
740720276,0.5366832556,-0.7927895672\B,1.005943515,-1.478732504,-0.408
2848131\B,-0.2880540857,-1.4925159223,0.9375980798\B,1.0531302658,-1.4
920618767,2.2366242473\B,2.347771196,-1.4791629202,0.8906031747\B,1.03
49846961,-2.5226319666,0.9080937899\S,1.0520256261,-4.4059908925,0.919
1828592\C,2.3610504592,-4.8608846225,-0.2966657282\C,2.2246948447,-6.3
262027199,-0.7118643837\C,0.8980958236,-6.6637893568,-1.4232918863\C,-
0.3161466939,-6.3508398662,-0.524988571\C,-0.4131852325,-4.8872670213,
-0.09055374\C,0.9067198757,-8.1308530603,-1.894234698\C,-0.2552402427,
-8.5347852164,-2.812638367\C,-0.1251070171,-9.9718785467,-3.3276133576
\H,0.9873095433,-1.8994540186,-1.5244672622\H,-1.4031342514,-1.9103590
901,0.9513694666\H,1.0749874631,-1.9273500719,3.3432039099\H,3.4665759
225,-1.8867842838,0.8650561142\H,2.2613964795,-4.1745473031,-1.1416762
651\H,3.3073669899,-4.6551335643,0.2076744653\H,2.3492130297,-6.973633
862,0.1661030459\H,3.0627773054,-6.5504214324,-1.3827881075\H,0.827609
6029,-6.0219121558,-2.3152931363\H,-1.2441921069,-6.5828464224,-1.0581
089254\H,-0.2955140484,-7.0000416009,0.3605689805\H,-0.4545207414,-4.1
995773998,-0.9394122442\H,-1.2779596587,-4.6991695462,0.548848921\H,1.
8498925102,-8.3143815393,-2.4267191736\H,0.9246593693,-8.7912603311,-1
.0148610921\H,-1.2108676266,-8.4313357813,-2.2841235453\H,-0.299546011
5,-7.8427907747,-3.6644628618\H,0.7977321911,-10.1049316132,-3.9029491
879\H,-0.1050883065,-10.6894651856,-2.4998592187\H,-0.9639702682,-10.2
38094858,-3.9777605955\C,0.7046337577,8.2821378786,4.005685161\O,0.376
2179245,8.4763572814,5.1572841741\O,1.020644168,9.2665770173,3.1192557
214\C,0.9590477241,10.6233184654,3.4176782054\C,1.1511148312,11.176341
4151,4.6865400623\C,1.1210735269,12.5646563588,4.8264387182\C,0.910895
3166,13.3684283274,3.7116400846\C,0.7258070885,12.8202968784,2.4458178
416\C,0.7511266344,11.436989642,2.3011085885\H,1.3025446643,10.5406714
165,5.5457928179\H,1.2589779926,13.0229405301,5.7988958004\H,0.5631468
622,13.4717128568,1.5949106955\H,0.6158787434,10.9692078008,1.33236250
7\O,0.8107136666,14.7627952972,3.8690137306\C,1.9660518291,15.47091441
09,3.8335326853\F,1.6553802028,16.7616836292,3.9542908603\F,2.80564832
69,15.1382089835,4.8352479553\F,2.6406344812,15.2967960499,2.679966350
6\\Version=EM64L-G09RevC.01\State=1-A\HF=-2330.7710604\RMSD=7.056e-09\
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9891599,45.793556,-21.8043962,0.474985,1.7364603,18.1706727\PG=C01 [X(
C24H31B9F4O5S1)]\\@

**4[3]k-cis** COOPhFCOOPhOCF3

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C24H31B9F4O5S1\PIOTR\16-Oct-20
13\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3_C5S_CB9COOPhFCOOPhOCF3, cis\\0,1\B,0.0807288131,0.4705565757,-0.2
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0402408,1.7140740223\B,1.9256543122,0.41961353,-0.1532890448\C,0.99850
62973,1.3204159169,0.8039236466\C,1.0379610779,2.8092332487,0.82711138
94\O,0.9805402718,3.2563289893,2.1217121181\C,0.9814230025,4.582922428
9,2.5093596055\C,0.9314865309,5.6833702035,1.6530703625\C,0.9226470207

,6.956572236,2.2158718648\C,0.96231532,7.1778857143,3.6002624979\C,1.0
076520586,6.0373498817,4.4244260313\C,1.0183093762,4.7579576674,3.8998
140536\H,1.0532278759,3.8830260049,4.5382199704\H,1.0332793898,6.19652
66509,5.4962933528\F,0.8678295019,7.9822742269,1.3513279323\H,0.903968
6917,5.5746240887,0.5804823478\O,1.1099561017,3.5154650732,-0.14794956
67\H,-0.6422670009,1.0434714696,-0.9489046056\H,-0.748609581,0.8560194
6,2.4141793575\H,2.6221359028,0.7649957541,2.5108530133\H,2.7209367139
,0.950705735,-0.8504251992\B,0.9766150858,-1.0226018583,-0.6525087552\
B,-0.3788403834,-1.0639848452,0.6318926039\B,0.8960871379,-1.165520858
9,1.9865343741\B,2.25140675,-1.1364665235,0.7073172378\B,0.9093485353,
-2.1393187228,0.606981537\S,0.8479206334,-4.0214039454,0.7217890077\C,
-0.5522576643,-4.5910114389,-0.3371771261\C,-0.3464316578,-4.371069313
6,-1.8344030752\C,0.9217641341,-5.0320887581,-2.409485752\C,2.19033600
02,-4.4552748688,-1.7511659263\C,2.2757811799,-4.6826542568,-0.2431923
144\C,0.9486348376,-4.8780324895,-3.9427336148\C,2.0403800303,-5.67894
68552,-4.6661648799\C,1.9396109017,-5.5656594422,-6.1907583102\H,0.999
7725431,-1.3569931123,-1.7943146696\H,-1.5075393423,-1.4416014994,0.57
78788636\H,0.8512097359,-1.6642286073,3.0652733078\H,3.358798529,-1.57
53214738,0.7181781072\H,-0.6710061074,-5.6514009491,-0.0924139098\H,-1
.4202533961,-4.0490062722,0.0447813165\H,-0.3331192549,-3.2972025944,-
2.0463885425\H,-1.2312241449,-4.7820180154,-2.3369806265\H,0.877270397
3,-6.1096590893,-2.1798532716\H,3.0824412417,-4.9234303799,-2.18207141
96\H,2.2612686864,-3.3835192483,-1.9637331329\H,2.3081950317,-5.747741
0806,0.0077943692\H,3.150089219,-4.1983774381,0.1973125302\H,-0.028760
3858,-5.190351882,-4.3353667051\H,1.0480848543,-3.8126318084,-4.194193
7169\H,3.0339763769,-5.3387066193,-4.3496614624\H,1.9694884968,-6.7351
82918,-4.3718234948\H,0.9764196963,-5.9411834504,-6.5536778122\H,2.032
4491419,-4.5240891058,-6.5174142985\H,2.7287402945,-6.1405688442,-6.68
50011334\C,0.9517336432,8.4955750206,4.2887465206\O,0.9256450648,8.618
379425,5.4954856698\O,0.9787512279,9.5343872268,3.409163703\C,0.940221
789,10.8721512588,3.7862527994\C,1.4086443009,11.3806755514,5.00077911
01\C,1.3613392201,12.7590449036,5.2148765138\C,0.8605625507,13.5972276
954,4.2253839865\C,0.3980210982,13.0936989716,3.0129713119\C,0.4403698
766,11.7205472095,2.7948897821\H,1.7847857465,10.7180045181,5.76534419
63\H,1.7108229168,13.1833407013,6.1490865777\H,0.0120108336,13.7706476
247,2.2596540924\H,0.0954835031,11.2870827407,1.8628227327\O,0.7515689
758,14.9769258667,4.4775240464\C,1.8245759813,15.7451089252,4.16738237
65\F,1.5170452262,17.0092439474,4.4583673987\F,2.9243206243,15.4000205
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Dipole=-0.1509553,-5.7436301,-1.5863707\Quadrupole=-21.2945972,40.6633
229,-19.3687257,-0.7703345,2.7455558,17.7524162\PG=C01 [X(C24H31B9F4O5
S1)]\\@

**4[3]l-trans** PhPhF2CH2CH2Chx-trans

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C35H55B9F2O2S1\PIOTR\17-Oct-20
13\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3_C5S_CB9COOPhPhF2CH2CH2ChxC5 trans\\0,1\B,0.579594419,1.3459473513
,-0.8343567266\B,-0.081441713,-0.3083603505,-1.4072186044\B,-0.3774136
513,-0.7977109493,0.3472950697\B,0.2835903669,0.8566932141,0.920491147
8\C,-0.7526421964,0.6308887863,-0.2876968458\C,-2.1090522517,1.2503289
331,-0.3422274637\O,-3.0207967808,0.3461991938,-0.8099837521\C,-4.3679
069612,0.6661795082,-0.9660960842\C,-5.2592960299,-0.369679959,-0.6919
869932\C,-6.6215659038,-0.1755591957,-0.8934720694\C,-7.1178738648,1.0
503989877,-1.3676724755\C,-8.5792242284,1.2421025409,-1.5417467335\C,-
6.1940473418,2.0721205818,-1.6445878823\C,-4.8266635842,1.8919229175,-
1.449586155\O,-2.3651777943,2.3838106356,-0.017920854\B,1.945489063,0.
8684864743,0.2329838949\B,1.6905423169,0.0461907889,-1.4246684031\B,1.

013487481,-1.4719345936,-0.5763792855\B,1.268160594,-0.6521536723,1.08
08110742\B,2.4354024514,-0.6992381622,-0.121144599\S,4.1619426865,-1.4
44942145,-0.03736191\C,4.777788998,-0.9985231869,1.6417574963\C,6.2961
24361,-1.1619482392,1.7201935176\C,7.0857230648,-0.2499373268,0.758870
6774\C,6.6954670695,-0.5098722165,-0.7104523984\C,5.2128501035,-0.2868
108824,-1.0134337827\C,8.5991152649,-0.4178026514,0.9948074863\C,9.498
0095156,0.5881248188,0.2617984166\C,10.9774617882,0.4273457996,0.62595
6332\C,-10.8780522244,0.8461625097,-0.8028461343\C,-9.5047701745,0.690
9979045,-0.6368849433\C,-9.1188189823,1.9592767165,-2.6162516087\C,-10
.4928996014,2.1106159855,-2.7756329088\C,-12.8958224762,1.7301095636,-
2.1063066411\C,-11.4110852877,1.5623467834,-1.8824548676\C,-13.4419836
271,0.8085629259,-3.2172961702\H,0.4942461027,2.4066714776,-1.35298029
27\H,-0.6907897617,-0.572262422,-2.3870126305\H,-1.2326494613,-1.46690
55723,0.8192750449\H,-0.045310864,1.5133678826,1.8484776473\H,-4.87141
11601,-1.3186688471,-0.3378255202\H,-4.1328040008,2.6953382988,-1.6537
139058\H,2.7308944772,1.6909503655,0.5943977992\H,2.2520917646,0.18572
70685,-2.4658315285\H,1.0205955149,-2.6180898003,-0.8948871136\H,1.471
7392126,-1.1049434595,2.1636334514\H,4.454734279,0.0272881579,1.837516
7708\H,4.2501931321,-1.6638485676,2.3281637592\H,6.5651219345,-2.21106
31471,1.5392628482\H,6.591579376,-0.9409712496,2.7529693776\H,6.818779
5437,0.7919426262,0.9953765494\H,7.255866245,0.1623344223,-1.368774911
6\H,6.9822520484,-1.5318527237,-0.992400382\H,4.8821516817,0.725992367
3,-0.7686532678\H,4.9665385277,-0.4869510556,-2.0581197662\H,8.7894769
591,-0.3313547265,2.0732118711\H,8.8941419558,-1.4407824297,0.71861167
94\H,9.3839292399,0.4784876714,-0.823586289\H,9.1702480057,1.608334943
3,0.5031650581\H,11.5986171592,1.1555145136,0.0956316224\H,11.13896717
69,0.5710129296,1.7000824132\H,11.3432061363,-0.5726584203,0.367604447
1\H,-11.5579624952,0.4142058374,-0.0740160908\H,-9.1281552649,0.153085
4899,0.2266949871\H,-13.1098242373,2.7716611349,-2.3752804248\H,-13.41
30032821,1.5330670592,-1.1620735781\H,-13.2393717382,-0.2375267435,-2.
9492008282\H,-12.8758079633,1.0079304591,-4.1350355217\H,-7.3071775435
,-0.9947446025,-0.7013025752\H,-6.5469628918,3.0272984684,-2.014358091
4\F,-8.3209699522,2.5190904883,-3.5488496565\F,-10.9341118496,2.807282
2968,-3.8461308388\C,-16.8355380901,0.3105615897,-5.0981517622\C,-15.3
417944263,0.1816483563,-4.7707070166\C,-14.94249947,0.9776079472,-3.51
39283034\C,-15.8428623305,0.5683832813,-2.3335229488\C,-17.3388118825,
0.6932932164,-2.6628282309\C,-17.7353462254,-0.1039722162,-3.919553864
4\H,-15.0959219556,-0.8787956757,-4.6113505898\H,-14.7392780634,0.5123
23414,-5.6260304344\H,-17.059668126,1.3537481782,-5.3664673773\H,-17.0
780354055,-0.2931206658,-5.9819780142\H,-15.6166200556,-0.4741855012,-
2.063310143\H,-15.6167307036,1.1728793175,-1.4473151217\H,-17.92902746
26,0.3674207971,-1.798815126\H,-17.5871088297,1.7529981396,-2.82550316
29\H,-17.5416445621,-1.1696224655,-3.7136497944\H,-15.1273364261,2.043
9445183,-3.7235717569\C,-19.2243973049,0.042027118,-4.2817646516\C,-20
.2096821265,-0.5461739796,-3.2626593605\H,-19.3944210796,-0.4439663293
,-5.2530327919\H,-19.4521970984,1.1073605582,-4.4350135381\C,-21.67299
83287,-0.4545705392,-3.7135945649\H,-19.9534818058,-1.5994870749,-3.07
79422237\H,-20.1035165,-0.0343975899,-2.297346666\C,-22.6654909506,-1.
0373757434,-2.7000639887\H,-21.9290744511,0.5972260083,-3.9064382353\H
,-21.7908361148,-0.9743500367,-4.6754118218\H,-22.4091176678,-2.087963
4134,-2.5066701809\H,-22.5491884958,-0.5164780226,-1.7398055252\C,-24.
1240642789,-0.9435369743,-3.1576625639\H,-24.4203399065,0.0981783971,-
3.3257799913\H,-24.2803630826,-1.4853721334,-4.0974585186\H,-24.806410
6689,-1.3667130581,-2.4132476636\\Version=EM64L-G09RevC.01\State=1-A\H
F=-2339.098847\RMSD=4.764e-09\RMSF=2.577e-06\Dipole=3.7607878,-1.37080
3,0.9178706\Quadrupole=103.9150648,-54.3503889,-49.564676,-12.7903849,
15.6717685,-4.7527732\PG=C01 [X(C35H55B9F2O2S1)]\\@

**4[3]l-cis** PhPhF2CH2CH2Chx-cis


```
1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C35H55B9F2O2S1\PIOTR\17-Oct-20
 13\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
 \\C3_C5S_CB9COOPhPhF2CH2CH2ChxC5 cis\\0,1\B,-0.1382878068,0.3352395011
 ,-0.2093454319\B,-0.0724952775,0.2832979259,1.65990069\B,1.7665576144,
 0.3665538551,1.5984458422\B,1.7044425036,0.4198799891,-0.2694777726\C,
 0.7731254048,1.2770348084,0.7217872979\C,0.7104999572,2.7680397902,0.7
 113381471\O,0.7050846282,3.2470245664,1.9907802166\C,0.6741747667,4.61
 16236291,2.2719803402\C,1.4027123439,5.0001254467,3.3949928836\C,1.378
 4852723,6.3288608018,3.8041351461\C,0.6328161978,7.2912914368,3.102632
 9253\C,0.6571263002,8.7100164522,3.5377951001\C,-0.1013693871,6.867018
 0356,1.9823842794\C,-0.0887675307,5.5389863468,1.5616480266\O,0.675164
 386,3.4513714153,-0.2823432892\B,0.836557022,-1.1015408524,-0.67599018
 81\B,-0.4321552177,-1.2058113445,0.6913659604\B,0.9272368655,-1.178202
 1802,1.964998748\B,2.196271306,-1.085461164,0.6038161321\B,0.928254585
 9,-2.1848489773,0.6098978665\S,1.0068124884,-4.0635305285,0.7700678226
 \C,-0.3834392656,-4.7583254807,-0.2263783594\C,-0.2471004651,-4.556518
 2857,-1.7337163284\C,1.0460941394,-5.1340392294,-2.3414122318\C,2.2893
 515525,-4.4497960012,-1.7403791469\C,2.4448412714,-4.6397042575,-0.232
 6507381\C,1.0106114782,-5.0104863226,-3.877208083\C,2.1148316502,-5.77
 2646443,-4.623173507\C,1.9751792036,-5.668991612,-6.1453374199\C,1.861
 7054401,10.6275622761,4.4647862674\C,1.8315549034,9.304239979,4.034601
 7249\C,-0.4782778139,9.5280903056,3.4966026651\C,-0.4406450298,10.8508
 003125,3.9276830079\C,0.713156153,12.8715498514,4.9049161363\C,0.72086
 12139,11.4394341666,4.4237329245\C,0.0570538327,13.0331205334,6.292502
 3194\H,-0.945749957,0.8319826463,-0.9181967524\H,-0.8333971182,0.73049
 94411,2.4486534677\H,2.5338851688,0.8846956832,2.3364148043\H,2.415392
 3589,0.9859224493,-1.0276329295\H,1.9685405315,4.2525944484,3.94042512
 74\H,-0.6469580006,5.2352126377,0.6872225743\H,0.8162914644,-1.4625274
 345,-1.8100896447\H,-1.5310689682,-1.6662876356,0.7159201402\H,0.98466
 56783,-1.6494790026,3.0557032034\H,3.3322160962,-1.4428583905,0.555234
 4949\H,-0.4145551192,-5.8190766081,0.0428725152\H,-1.274968894,-4.2728
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 896972768\H,3.1990257945,-4.8563924129,-2.1965491033\H,2.2689108711,-3
 .3801930647,-1.9735525559\H,2.5662138484,-5.6941430683,0.0356858387\H,
 3.2944663112,-4.0814471059,0.1666317746\H,0.0368560527,-5.3774711822,-
 4.2294533071\H,1.04872083,-3.9468945685,-4.1519598199\H,3.1022223391,-
 5.3952714887,-4.3298240083\H,2.0892854879,-6.829438506,-4.3238286261\H
 ,2.7692857536,-6.2220080883,-6.6563755013\H,1.0152099392,-6.074276965,
 -6.4841715443\H,2.0289880999,-4.6263470409,-6.4773760724\H,2.792993218
 6,11.0506079451,4.8306409308\H,2.7424510063,8.7153145974,4.0551103863\
 H,0.1725035121,13.4968964377,4.184176877\H,1.7456065828,13.2338650793,
 4.9288569477\H,0.593519835,12.4069333173,7.0188176205\H,-0.9630085441,
 12.6345492452,6.2351813482\H,1.9290169604,6.6189670422,4.6933463488\H,
 -0.6889760117,7.5855012647,1.4237354406\F,-1.6595203924,9.054871407,3.
 0489551272\F,-1.5824421279,11.5708053733,3.8662407232\C,-0.949983277,1
 5.990931612,8.6448441207\C,-0.8710579364,14.5653297278,8.0822276849\C,
 -0.0038227633,14.4799269291,6.8126023206\C,1.3856230812,15.0820815579,
 7.0930857237\C,1.3059969635,16.5086630468,7.6595557304\C,0.4392359544,
 16.5907819458,8.9295693219\H,-0.4474343206,13.8966893873,8.8464555505\
 H,-1.8794536766,14.1891121702,7.8688009118\H,-1.4744069992,16.63663922
 25,7.9246812546\H,-1.5537258356,15.9984986428,9.5612403283\H,1.9103622
 428,14.4354207108,7.8126084851\H,1.995199691,15.087955456,6.1817614591
 \H,2.3185743593,16.8763690789,7.8608584714\H,0.8791021341,17.178320177
 7,6.8976317782\H,0.9180860588,15.9652381825,9.7010590836\H,-0.48749266
 17,15.0980705336,6.038422006\C,0.3208514551,18.019898105,9.4890637331\
 C,1.6287548501,18.6363640462,10.0036877465\H,-0.4083008863,18.01095348
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18,10.3117906683\H,-0.1089496211,18.6729236389,8.7148758588\C,1.437467
2048,20.0246989461,10.6274216027\H,2.0773417563,17.9637143277,10.74902
19911\H,2.3573536331,18.7125209673,9.1862190753\C,2.7383001865,20.6501
794843,11.1456122807\H,0.9838924793,20.6971269995,9.884996619\H,0.7145
939175,19.9566528167,11.4531354292\H,3.1905458442,19.9796454056,11.889
0590354\H,3.4606891015,20.7174399022,10.3206647667\C,2.539064944,22.03
71900005,11.7638952447\H,2.120297812,22.7397379428,11.0343239997\H,1.8
490614038,21.9966278488,12.6144581468\H,3.4846295969,22.4561594771,12.
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PG=C01 [X(C35H55B9F2O2S1)]\\@

**4[3]m-trans** PhCN

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C17H28B9N1O2S1\PIOTR\16-Oct-20
13\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3-C5S-CB9-COO-PhOCF3, trans\\0,1\B,0.013698561,0.0316941419,-0.0420
351218\B,-0.0446824268,0.0225639039,1.8303790887\B,1.8000514033,0.0096
664061,1.887832309\B,1.8595199106,0.0177327641,0.0174186039\C,0.913234
0724,0.9466980521,0.927533648\C,0.9231497993,2.4348360033,0.8786831223
\O,0.9095717384,2.9493899766,2.1514554296\C,0.9067393259,4.31153733,2.
40852712\C,1.5741547006,5.2614590115,1.6293928338\C,1.553715059,6.5935
413105,2.0309418101\C,0.880031627,6.9806714178,3.2006827477\C,0.221208
5212,6.0104965836,3.9753950616\C,0.2365590437,4.6805821632,3.577996727
8\H,-0.262001538,3.9135050843,4.1598574167\H,-0.297485612,6.3049639423
,4.8810564678\H,2.0647367864,7.3423975319,1.435643473\H,2.0846700575,4
.9683298677,0.7238052219\O,0.9345575166,3.0992695833,-0.1270985989\H,-
0.7187118166,0.5534348783,-0.811282802\H,-0.8272663425,0.5333619481,2.
5574700074\H,2.5426701173,0.5089267754,2.6629081106\H,2.6468491571,0.5
287139151,-0.7037729939\B,0.9377547292,-1.4666302944,-0.4051270644\B,-
0.4209422956,-1.4649655595,0.8758840388\B,0.8545242036,-1.481673493,2.
2389759343\B,2.2135728417,-1.4843588501,0.9587732406\B,0.8886113804,-2
.5114686596,0.9100204158\S,0.8771928855,-4.3945667434,0.9247005278\C,2
.2882792302,-4.8728955028,-0.1606792017\C,2.169872226,-6.3381597597,-0
.5813692009\C,0.9124050934,-6.660920741,-1.4144872501\C,-0.3772712995,
-6.3251456825,-0.6377316724\C,-0.4933707832,-4.8587911889,-0.217139448
\C,0.9447258776,-8.1315449488,-1.873313442\C,-0.1310068545,-8.52850789
45,-2.893979302\C,0.025629486,-9.9727778728,-3.3807122708\H,0.96831737
67,-1.8859592452,-1.521508046\H,-1.5405668063,-1.8688650018,0.83483651
38\H,0.8168969855,-1.9183441474,3.3446199152\H,3.3272047712,-1.9056756
556,0.9882887285\H,2.2799685617,-4.1891501083,-1.0135998881\H,3.185798
0395,-4.6790172396,0.430136153\H,2.199887493,-6.9820168295,0.307540773
7\H,3.0647948303,-6.5788311845,-1.1678707494\H,0.9370563379,-6.0245767
715,-2.3129592203\H,-1.2533044868,-6.5448696112,-1.257105754\H,-0.4522
900798,-6.9717062215,0.2469485399\H,-0.446120059,-4.1725666631,-1.0667
897249\H,-1.4112464636,-4.6571751683,0.3387392941\H,1.9311632171,-8.33
13062908,-2.3135159952\H,0.8713680489,-8.7847178812,-0.99145996\H,-1.1
308413784,-8.405741527,-2.4597135679\H,-0.0838526619,-7.8451685755,-3.
7525905708\H,0.9971945735,-10.1255931378,-3.8635047279\H,-0.0448771671
,-10.681626923,-2.5481682081\H,-0.7510845615,-10.2338291125,-4.1058324
858\C,0.8662225704,8.3558198476,3.6038100334\N,0.8547754764,9.47194404
77,3.9327679585\\Version=EM64L-G09RevC.01\State=1-A\HF=-1491.9095138\R
MSD=5.525e-09\RMSF=3.429e-06\Dipole=-0.0061247,-6.0903007,-1.3143079\Q
uadrupole=8.9873014,-12.2174435,3.230142,1.1875887,-2.6483569,-1.68586
63\PG=C01 [X(C17H28B9N1O2S1)]\\@

**4[3]m-cis** PhCN

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C17H28B9N1O2S1\PIOTR\16-Oct-20

13\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)
\\C3-C5S-CB9-COO-PhOCF3, cis\\0,1\B,-0.0971488419,0.5018034995,-0.0093
397266\B,-0.0677192552,0.3144976483,1.8522781324\B,1.7762550732,0.3505
767364,1.8284911007\B,1.748382027,0.538092609,-0.0329672438\C,0.822844
8279,1.3481038735,1.002798404\C,0.7995235457,2.8338885881,1.1006663454
\O,0.8529296555,3.2182566442,2.4175249271\C,0.8648473185,4.546877928,2
.8121572405\C,1.4884076294,5.5743175294,2.0978597176\C,1.4978651661,6.
8569954274,2.6369786576\C,0.8964712644,7.1183949825,3.8787982893\C,0.2
793691224,6.0716404778,4.5850971551\C,0.2654963685,4.7905294479,4.0507
855324\H,-0.2003816748,3.9656862769,4.578174327\H,-0.1836091007,6.2688
938961,5.5456782765\H,1.9767778568,7.664816917,2.0944245658\H,1.943703
2829,5.3782689856,1.1381381506\O,0.7396146011,3.5949917594,0.167890488
4\H,-0.8772377471,1.0709809707,-0.6934238825\H,-0.8307788132,0.7277855
242,2.6578099269\H,2.5430775117,0.7946463377,2.6132639799\H,2.48754938
03,1.137828809,-0.7366433764\B,0.8477397197,-0.9248472838,-0.559988879
7\B,-0.4481667211,-1.0904604982,0.7734279335\B,0.8869546916,-1.1913917
908,2.0700159763\B,2.1831839706,-1.0373955017,0.7394270601\B,0.8872383
765,-2.0994932777,0.646316204\S,0.9188773348,-3.9852596174,0.675774244
1\C,-0.4754802288,-4.5793688894,-0.3787854184\C,-0.3129271271,-4.29133
34778,-1.869868882\C,0.9743390078,-4.8628551882,-2.4956617193\C,2.2241
494765,-4.2427828784,-1.8408159885\C,2.35711746,-4.528352735,-0.346269
725\C,0.9610752028,-4.6484310634,-4.02194137\C,2.0647826862,-5.3801399
749,-4.7983018981\C,1.9361825687,-5.1994929114,-6.3143074957\H,0.83935
78487,-1.2034054585,-1.7167259216\H,-1.5589816756,-1.5205147214,0.7459
174167\H,0.9113149454,-1.740345441,3.1247099064\H,3.3096550758,-1.4213
422879,0.6846363432\H,-0.5386863345,-5.6529352792,-0.1743506436\H,-1.3
598304421,-4.0951198908,0.0413999804\H,-0.3588176556,-3.2109048892,-2.
0392552675\H,-1.1863781727,-4.7276226044,-2.3710382915\H,0.9914814468,
-5.9490816416,-2.3073927958\H,3.1309550069,-4.639742612,-2.3109345284\
H,2.2277324253,-3.1608811274,-2.0094761478\H,2.4513261662,-5.599837323
5,-0.1428053148\H,3.2140936122,-4.0164579433,0.0970812696\H,-0.0127551
952,-4.9804155438,-4.4071467422\H,1.0167493289,-3.5709779401,-4.232286
7984\H,3.0527462671,-5.0247424889,-4.4808252306\H,2.0305843031,-6.4504
873204,-4.5526172091\H,0.9763557498,-5.5815158908,-6.6794063285\H,1.99
87866717,-4.1420668967,-6.5937510582\H,2.7305646224,-5.7314364817,-6.8
468082688\C,0.9148031755,8.4432809426,4.4247346284\N,0.9300872134,9.51
82570591,4.869978973\\Version=EM64L-G09RevC.01\State=1-A\HF=-1491.9077
317\RMSD=7.990e-09\RMSF=4.603e-06\Dipole=0.1432582,-5.6045635,-1.83995
81\Quadrupole=7.4248311,-8.5642166,1.1393855,1.4960538,-3.2258969,-6.6
999158\PG=C01 [X(C17H28B9N1O2S1)]\\@

**4[5]a-trans**

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C23H43B9O2S1\PIOTR\01-May-2010
\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck freq(nor
aman)\\C5-C5S-CB9-COO-PhC5 start at the HF/6-31G* geom\\0,1\B,-0.11096
61673,0.0065589271,0.6406172951\B,-0.4054918217,-0.1196476622,2.484218
8462\B,1.4161431303,-0.1750336982,2.7715773652\B,1.7110293492,-0.04917
11152,0.9285783835\C,0.6697797444,0.8397529434,1.7714268997\C,0.712124
5528,2.331218494,1.8252193342\O,0.5569656609,2.7628129814,3.110901641\
C,0.574024728,4.1245940388,3.4232751495\C,1.5299121911,5.0087850931,2.
9250994644\C,1.5113749115,6.3325272544,3.3623982533\C,0.5656847172,6.7
910697835,4.2892791534\C,0.592066389,8.2204862334,4.7853016\C,1.514742
2655,8.4229362014,6.0038504231\C,1.5514876077,9.8725315818,6.500557218
5\C,2.4730989562,10.0816586166,7.7087479306\C,2.5093149557,11.53264624
14,8.1975858721\H,1.5126524734,11.874465839,8.4992368975\H,3.175015401
3,11.6491699187,9.0589937113\H,2.863836019,12.2072125651,7.40988418\H,
2.148598764,9.4265596666,8.5285491409\H,3.4895048007,9.7575355461,7.44

73542685\H,1.8749561631,10.5299880583,5.6806114451\H,0.5331376553,10.1
94935264,6.7615069866\H,1.1851089989,7.7611881759,6.816012152\H,2.5299
366605,8.0964974089,5.7414545038\H,0.9208559629,8.8843634177,3.9756219
482\H,-0.424567713,8.5367821323,5.0508828513\C,-0.3779715473,5.8749977
599,4.7716994058\C,-0.3797637781,4.5483027236,4.3451627915\H,-1.108614
3564,3.8354290156,4.7159668282\H,-1.1260936746,6.2033092531,5.48895621
48\H,2.2511770086,7.0252805656,2.9688420988\H,2.2607753556,4.674463111
6,2.2007436963\O,0.863365165,3.051591638,0.8690542783\H,-0.7345846641,
0.5880908319,-0.1801456061\H,-1.2671689399,0.3596656048,3.1397900388\H
,2.0617583134,0.2576612568,3.6644734095\H,2.5900649708,0.4882245732,0.
3456546139\B,0.833020172,-1.4856381646,0.2995433887\B,-0.6776742096,-1
.536732486,1.3968785609\B,0.4159102083,-1.6664906025,2.905143238\B,1.9
249093765,-1.61589133,1.8074486287\B,0.6037271404,-2.6096932336,1.5265
653511\S,0.5604682284,-4.4889116731,1.4020537355\C,2.1215807915,-4.928
8287055,0.5266721128\C,2.048935066,-6.3540615003,-0.0226035658\C,0.938
5084225,-6.5780822274,-1.0696257943\C,-0.4542717689,-6.2649335348,-0.4
861234214\C,-0.6116086123,-4.8301858606,0.0204124512\C,1.0235336038,-8
.0101807206,-1.6323147786\C,0.1197054853,-8.2993408806,-2.8388852963\C
,0.336014556,-9.7007470772,-3.4245748918\C,-0.5662152383,-10.0081234,-
4.6261011779\C,-0.3396019965,-11.406668279,-5.2074250485\H,1.001667591
3,-1.8360688032,-0.8287508031\H,-1.78830213,-1.914269606,1.1888777514\
H,0.2327254902,-2.1705108099,3.9669877927\H,3.0205084392,-2.0619186918
,1.9485666106\H,2.2662682296,-4.1816690142,-0.2581214219\H,2.912752487
8,-4.8076860584,1.2693272907\H,1.9237045001,-7.0636846793,0.8059928837
\H,3.0231168504,-6.5758108042,-0.4749557628\H,1.1179428021,-5.87703783
21,-1.8997161918\H,-1.2214645499,-6.414864732,-1.2531268708\H,-0.68111
39679,-6.9715293465,0.3235337382\H,-0.4111368343,-4.0869933921,-0.7557
0492\H,-1.604642992,-4.6400691407,0.4326425702\H,2.065178366,-8.201131
3036,-1.9238595802\H,0.8005202291,-8.72602381,-0.8277714173\H,-0.93618
18279,-8.1939159343,-2.5573644451\H,0.3047518535,-7.5476114718,-3.6193
33922\H,1.3879674525,-9.8106179392,-3.7241141858\H,0.1645812442,-10.45
27786579,-2.6411891285\H,-1.6174425594,-9.9022342962,-4.3255886982\H,-
0.3970897184,-9.2545243664,-5.4070860896\H,-0.9963125574,-11.595087243
8,-6.0625534572\H,0.6942644808,-11.5314649201,-5.5486515106\H,-0.53608
13147,-12.1835047118,-4.4598654097\\Version=EM64L-G09RevA.02\State=1-A
\HF=-1674.8865527\RMSD=5.656e-09\RMSF=3.075e-06\Dipole=0.0800887,-3.79
04274,-0.8804738\Quadrupole=-15.8960307,30.5974084,-14.7013776,1.05823
45,-1.2109348,24.9424581\PG=C01 [X(C23H43B9O2S1)]\\@

**4[5]a-cis**

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C23H43B9O2S1\PIOTR\02-May-2010
\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck freq(nor
aman)\\C5-C5S-CB9-COO-PhC5, cis, CB9 axial, at HF/6-31G* geom\\0,1\B,-
0.4724630517,0.4732894816,0.9271714499\B,-0.6533286663,-0.1836305709,2
.6392003576\B,-1.283931448,-1.8050148968,1.9514622759\B,-1.1049296039,
-1.1455649217,0.2375248343\C,-0.0106417213,-0.9892668358,1.4058549675\
C,1.3684013987,-1.558207763,1.338004037\O,2.2769451588,-0.6386311487,1
.7740105384\C,3.6420799902,-0.9284720078,1.839182071\C,4.3080956401,-0
.4231535666,2.9537671557\C,5.6851117695,-0.5983477605,3.0673263364\C,6
.4144617242,-1.2743870713,2.0800892356\C,7.9161672129,-1.4268868332,2.
1891033616\C,8.6926376514,-0.242659167,1.5795674935\C,10.2136918951,-0
.3905849378,1.6986336923\C,10.9914783214,0.7856986966,1.0955447403\C,1
2.5104180354,0.6341324258,1.2205931328\C,5.7152137878,-1.7686289191,0.
9714766205\C,4.3368581533,-1.6020757123,0.8356019013\O,1.6375016241,-2
.6710082358,0.9563685367\H,0.3263883689,1.2197285642,0.4734587825\H,-0
.0032386449,0.0153416901,3.6084463162\H,-1.1324107047,-2.9043034864,2.
3630377924\H,-0.8047572729,-1.7021460219,-0.7632507173\H,3.7389399527,
0.0990008874,3.7155727892\H,6.1999046363,-0.2060447121,3.9408305166\H,

8.1990495718,-1.532634184,3.2442375252\H,8.2287739037,-2.3532968341,1.
6910010462\H,8.4124253004,-0.1373900816,0.5229561133\H,8.3723109689,0.
6857963215,2.0710266184\H,10.4872419563,-0.500050972,2.7580728139\H,10
.528883936,-1.3228347108,1.2080223113\H,10.7197755875,0.8935812264,0.0
367624816\H,10.6750358223,1.7167513086,1.5850468394\H,12.8620121948,-0
.2703088445,0.7111354541\H,13.0360260983,1.4881875638,0.7812023613\H,1
2.8161652329,0.5601748592,2.2704667824\H,6.2573471846,-2.3008148174,0.
1936908168\H,3.8123131153,-2.0017189766,-0.0216363887\B,-2.1551455237,
0.3258207971,0.2690857795\B,-1.8335537015,0.9955401222,1.9768961773\B,
-2.4127118769,-0.615902003,2.713811561\B,-2.7248305176,-1.2945835245,1
.002908996\B,-3.2599736304,0.2135511258,1.5267092159\S,-4.9371475328,1
.0618393934,1.6788802677\C,-5.7981462166,0.8982380756,0.0545082694\C,-
6.2049543892,-0.527997255,-0.3100279527\C,-7.1092204561,-1.2199544685,
0.7287970938\C,-6.3842830243,-1.3552544585,2.0820138024\C,-6.001562908
6,-0.0234228484,2.7247007327\C,-7.5871340015,-2.5836582286,0.191876258
6\C,-8.65987542,-3.2806840108,1.0396397535\C,-9.1898243283,-4.57037731
41,0.3988438088\C,-10.2491048543,-5.2816820459,1.2491509863\C,-10.7793
300193,-6.5656659202,0.6042368293\H,-2.4298649245,0.869664391,-0.75515
2989\H,-1.8749708344,2.1066491574,2.3999419081\H,-2.9056854068,-0.8719
348952,3.7685025944\H,-3.4734559523,-2.1292739032,0.6029620403\H,-6.66
44699191,1.5630730382,0.1320598722\H,-5.0989551349,1.3251924957,-0.668
0608974\H,-5.3064739376,-1.1302313792,-0.478015239\H,-6.7317569133,-0.
4689656705,-1.2709798732\H,-7.9998133305,-0.5873555226,0.8799449262\H,
-7.0289401217,-1.8690287443,2.8038547948\H,-5.4892143687,-1.9741388191
,1.9593303823\H,-6.8812073002,0.586352241,2.9546595475\H,-5.4261013156
,-0.1602851616,3.6428659572\H,-7.985447703,-2.4317301178,-0.8205859343
\H,-6.7190376531,-3.24801532,0.0783568991\H,-8.2614814835,-3.521771400
6,2.0336292189\H,-9.4982089143,-2.5885481979,1.2057347591\H,-9.6122505
69,-4.338963539,-0.5893111694\H,-8.3509898179,-5.2567578465,0.21610882
39\H,-9.8236007943,-5.5159009472,2.2343799622\H,-11.0848059272,-4.5934
938199,1.436123335\H,-11.5325644443,-7.0483219088,1.2350347338\H,-11.2
4214075,-6.3594890597,-0.3674877531\H,-9.972490163,-7.288323543,0.4382
125279\\Version=EM64L-G09RevA.02\State=1-A\HF=-1674.8849855\RMSD=6.377
e-09\RMSF=2.668e-06\Dipole=-3.4721305,0.7239292,-0.026613\Quadrupole=3
8.7791475,-22.6087429,-16.1704046,-4.6800127,2.6951157,-0.2597175\PG=C
01 [X(C23H43B9O2S1)]\\@

**4[7]j-trans** COOPhCOOPhOCF3

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C28H40B9F3O5S1\PIOTR\03-Feb-20
14\0\\#P B3LYP/6-31G(d,p) Fopt SCF=tight Geom(NoAngle, noDistance) Pol
ar\\C7_C5S_CB9COOPhCOOPhOCF3, trans\\0,1\B,-0.0887833043,-1.1078033435
,-3.7071928949\B,1.5173743817,-0.2326046138,-3.3041516953\B,0.60853967
3,1.3672846496,-3.158520226\B,-0.9960222547,0.4925415309,-3.5627727238
\C,0.1212741561,-0.0309991322,-2.5315946685\C,-0.1494327687,-0.3198936
756,-1.0955700994\O,0.8549453693,0.1902376027,-0.3122666814\C,0.862418
338,0.0504974115,1.0682927373\C,-0.2835698027,0.1206078244,1.865473701
8\C,-0.1457770685,0.02895533,3.247569361\C,1.1181653301,-0.1233551535,
3.8348087843\C,2.2565126934,-0.1783571949,3.0166663354\C,2.1309771704,
-0.0919726834,1.6373111306\H,2.9964700327,-0.1323333937,0.9852869137\H
,3.2295701991,-0.2926228418,3.4811198362\H,-1.0260949049,0.0771320299,
3.8769998104\H,-1.2593739368,0.228417954,1.4142719248\O,-1.1057009466,
-0.9221589176,-0.6758781254\H,-0.4330147519,-2.2053636664,-3.428926040
6\H,2.4582398196,-0.633317165,-2.7075072395\H,0.7984803052,2.290776322
9,-2.4425572295\H,-2.0890564859,0.7137456888,-3.1657616224\B,-0.648511
7581,-0.2287853556,-5.1714961952\B,1.1342943942,-0.7536472288,-4.99222
04695\B,1.6205055205,1.0074316179,-4.6041354278\B,-0.1623213922,1.5320
950712,-4.7851822519\B,0.6407731044,0.5680525686,-5.8976762934\S,0.933
6695523,0.8974829876,-7.7296583323\C,-0.6470852044,1.6412096656,-8.319

8331953\C,-0.7415855821,1.5730842941,-9.8444832898\C,-0.7455159847,0.1
411508253,-10.4171876714\C,0.5400613338,-0.6184157357,-10.0322698728\C
,0.7570493535,-0.7572294683,-8.5245111952\C,-0.9633980329,0.1776910088
,-11.9423761406\C,-1.2159002739,-1.1854913718,-12.6013209576\C,-1.5489
455805,-1.0767340954,-14.0951524921\H,-1.5404790215,-0.6752348873,-5.8
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,-1.3247792083,-1.8165052897,-16.779899227\C,-2.7418045813,-3.57356652
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**4[7]j-cis** COOPhCOOPhOCF3

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C28H40B9F3O5S1\PIOTR\03-Feb-20
14\0\\#P B3LYP/6-31G(d,p) Fopt SCF=tight Geom(NoAngle, noDistance) Pol
ar\\C7_C5S_CB9COOPhCOOPhOCF3, cis in vacuum\\0,1\B,0.2254725589,0.4992
667028,-0.2643076808\B,0.0477975691,0.3995667637,1.5955599579\B,1.8829
594388,0.3493148569,1.7684873156\B,2.0626202575,0.4456231179,-0.090619
7543\C,1.0762329202,1.3487112793,0.8028646853\C,1.1136089808,2.8379447
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,4.6388463693,2.4393965011\C,1.7457442948,5.6049318736,1.7979680656\C,
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461046991\C,0.1205123725,6.2823470189,3.9815349905\C,0.15773931,4.9705
420624,3.5310270044\H,-0.4255885749,4.190388282,4.0073973818\H,-0.4993
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,-0.6491015951\B,-0.2905760254,-1.0346908674,0.5433462683\B,0.89407758

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19709206,-2.006306037\H,-1.2055632331,-4.7280204782,-2.2926546031\H,0.
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,-8.0768599479,-8.9889046444\H,4.4165597121,-7.513446023,-11.343801804
5\H,2.6700904187,-7.3296051719,-11.1356014075\H,3.7105476948,-5.901566
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44098\PG=C01 [X(C28H40B9F3O5S1)]\

**20-I**

1\1\GINC-OCTOPUS\SP\RB3LYP\6-31G(d,p)\C6H19B9S1\PIOTR\01-Dec-2013\0\\#
P B3LYP/6-31G(d,p) SCF=tight fcheck Polar SCRF(Solvent=Generic,Read)\\
1-ThiaCB9 Cs, ecliped at the DFT geometry in ClEster\\0,1\B,0,2.899618
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273166\B,0,2.7209377809,1.8353280907,-0.9247842653\B,0,2.7209377809,1.
8353280907,0.9247842653\B,0,1.3264461656,0.7755902321,1.3178053106\B,0
,1.3264461656,0.7755902321,-1.3178053106\B,0,1.4552471419,-0.543908737
7,0.\B,0,1.2002679808,2.0836455447,0.\C,0,0.4048642581,0.6746418483,0.
\S,0,-1.3639330903,0.5588825119,0.\C,0,-1.7592293399,-0.581641414,1.39
38168448\C,0,-1.7592293399,-0.581641414,-1.3938168448\C,0,-3.206098899
3,-1.0708428477,1.2804031909\C,0,-3.2060988993,-1.0708428477,-1.280403
1909\C,0,-3.4780261775,-1.8751008994,0.\B,0,3.894931399,1.0155771133,0
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42,0.\H,0,-3.4043845492,-1.6911065622,-2.1615412437\H,0,-3.4043845492,
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-2.7801016585,0.\\Version=EM64L-G09RevC.01\State=1-A'\HF=-862.0577849\
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78108,189.2633158,0.,0.,193.3506342\HyperPolar=-810.0020848,-140.41897
05,-27.5564183,28.6682171,0.,0.,0.,-21.6034239,11.325927,0.\Quadrupole
=-6.4923487,1.0886541,5.4036946,-0.0719238,0.,0.\PG=CS [SG(C2H5B3S1),X
(C4H14B6)]\\

**20-II**

1\1\GINC-OCTOPUS\SP\RB3LYP\6-31G(d,p)\C6H19B9S1\PIOTR\01-Dec-2013\0\\#
P B3LYP/6-31G(d,p) SCF=tight fcheck Polar SCRF(Solvent=Generic,Read)\\
10-ThiaCB9 Cs at the DFT geometry in ClEster\\0,1\B,0,2.9717199004,0.0
078142209,0.9253369131\B,0,2.9717199004,0.0078142209,-0.9253369131\B,0
,2.8101823357,1.858826162,-0.9249436027\B,0,2.8101823357,1.858826162,0
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74885447,0.\\Version=EM64L-G09RevC.01\State=1-A'\HF=-862.1112211\RMSD=
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528112,34.0554166,0.,0.,0.,-1.4809404,12.4903952,0.\Quadrupole=5.75258
7,-4.6114691,-1.1411179,3.2885901,0.,0.\PG=CS [SG(C2H5B3S1),X(C4H14B6)
]\\@

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