

Electronic Supplementary Information for

Modification of electro-optical properties of an orthoconic chiral biphenyl smectogen with its isostructural carborane analog

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1. Synthetic Details

¹H NMR spectra were recorded at 400 or 300 MHz in CDCl₃ and referenced to the solvent. S(+)-2-Octanol (ChiraSelect, *S*:*R* ≥99.5:0.5) was purchased from Fluka.

Preparation of esters 1 and 2. General Procedure. Carboxylic acid **3H** or **3F**¹ (0.22 mmol), phenol **4** or **5** (0.20 mmol), DCC (52 mg, 0.25 mmol), and DMAP (3 mg) were stirred in CH₂Cl₂ (10 mL) for 18 h. The reaction mixture was condensed and loaded directly onto a silica gel column. The column was eluted with 3:1 hexane / ethyl acetate to give 80-90 % yield of ester **1** or **2**. The product was recrystallized to obtain colorless solid.

4'-[(1*S*)-1-Methylheptyloxycarbonyl]biphenyl-4-yl 4-(3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctyloxy)benzoate (1F).² Crude product was recrystallized from heptane followed by MeCN to give **1F** as colorless platelets: ¹H NMR (300 MHz) δ 0.86 (t, *J* = 7.4 Hz, 3H), 0.88 (t, *J* = 7.4 Hz, 3H), 1.36 (d, *J* = 6.2 Hz, 3H), 1.07-1.42 (m, 9H), 1.56-1.66 (m, 1H), 1.70-1.82 (m, 1H), 2.70 (tt, *J*₁ = 18.2 Hz, *J*₂ = 6.8 Hz, 2H), 4.38 (t, *J* = 6.7 Hz, 2H), 5.18 (sext, *J* = 6.3 Hz, 1H), 7.01 (d, *J* = 8.7 Hz, 2H), 7.31 (d, *J* = 8.6 Hz, 2H), 7.66 (d, *J* = 8.1 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 8.12 (d, *J* = 8.2 Hz, 2H), 8.20 (d, *J* = 8.7 Hz, 2H). Anal. Calcd for C₃₆H₃₃F₁₃O₅: C, 54.55; H, 4.20. Found: C, 54.50; H, 4.16. [α]_D²⁶ = +20.1° (0.0250 g mL⁻¹; CHCl₃).

4'-[(1*S*)-1-Methylheptyloxycarbonyl]biphenyl-4-yl 4-Octyloxybenzoate (1H).^{2,3} Crude product was recrystallized from heptane followed by MeCN to give **1H** as colorless platelets: ¹H NMR (300 MHz) δ 0.88 (t, *J* = 6.9 Hz, 3H), 0.90 (t, *J* = 6.2 Hz, 3H), 1.36 (d, *J* = 6.2 Hz, 3H), 1.25-1.50 (m, 19H), 1.55-1.66 (m, 1H), 1.71-1.80 (m, 1H), 1.83 (quin, *J* = 6.6, 2H), 4.05 (t, *J* = 6.6 Hz, 2H), 5.18 (sext, *J* = 6.3 Hz, 1H), 6.98 (d, *J* = 8.8 Hz, 2H), 7.31 (d, *J*

= 8.5 Hz, 2H), 7.66 (d, $J = 8.2$ Hz, 2H), 7.67 (d, $J = 8.5$ Hz, 2H), 8.11 (d, $H = 8.2$ Hz, 2H), 8.16 (d, $J = 8.7$ Hz, 2H); IR (film) 1721 cm^{-1} (C=O). Anal. Calcd for $\text{C}_{36}\text{H}_{46}\text{O}_5$: C, 77.38; H, 8.30. Found: C, 77.00; H, 8.05. $[\alpha]_{\text{D}}^{26} = +26.4^\circ$ (0.0300 g mL^{-1} ; CHCl_3).

4-[12-[(*IS*)-1-Methylheptyloxycarbonyl]-*p*-carboran-1-yl]phenyl 4-(3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctyloxy)benzoate (2F). Crude product was recrystallized from heptane followed by MeCN to obtain colorless micro-needles: ^1H NMR (400 MHz) δ 0.89 (t, $J = 6.9$ Hz, 3H), 1.15 (d, $J = 6.2$ Hz, 3H), 1.20-1.32 (m, 8H), 1.45-1.52 (m, 2H), 1.6-3.5 (brm, 10H), 2.68 (tt, $J_1 = 18.3$ Hz, $J_2 = 6.7$ Hz, 2H), 4.36 (t, $J = 6.7$ Hz, 2H), 4.75 (sext, $J = 6.3$ Hz, 1H), 6.98 (d, $J = 9.0$ Hz, 2H), 7.02 (d, $J = 8.9$, 2H), 7.23 (d, $J = 9.0$ Hz, 2H), 8.12 (d, $J = 9.0$ Hz, 2H); IR (film) 1732 (C=O), 2619 (B-H) cm^{-1} . Anal. Calcd for $\text{C}_{32}\text{H}_{39}\text{B}_{10}\text{F}_{13}\text{O}_5$: C, 44.76; H, 4.58. Found: C, 44.68; H, 4.55.

4-[12-[(*IS*)-1-Methylheptyloxycarbonyl]-*p*-carboran-1-yl]phenyl 4-Octyloxybenzoate (2H). Crude product was recrystallized from EtOH to obtain colorless micro-needles: ^1H NMR (400 MHz) δ 0.89 (t, $J = 6.8$ Hz, 6H), 1.14 (d, $J = 6.2$ Hz, 3H), 1.25-1.35 (m, 20H), 1.40-1.52 (m, 2H), 1.81 (quint, $J = 7.1$ Hz, 2H), 1.6-3.5 (brm, 10H), 4.03 (t, $J = 6.6$ Hz, 2H), 4.75 (sext, $J = 6.3$ Hz, 1H), 6.95 (d, $J = 9.0$ Hz, 2H), 7.02 (d, $J = 8.9$ Hz, 2H), 7.22 (d, $J = 8.9$ Hz, 2H), 8.08 (d, $J = 9.0$ Hz, 2H); IR (film) 1731 (C=O), 2632 (B-H) cm^{-1} . Anal. Calcd for $\text{C}_{32}\text{H}_{52}\text{B}_{10}\text{O}_5$: C, 61.51; H, 8.39. Found: C, 61.70; H, 8.45.

(*IS*)-1-Methylheptyl 4'-Hydroxy-4-biphenylcarboxylate (4).^{3,4} Mp. 83-85 °C, lit.⁴ mp. 87-89 °C; ^1H NMR (300 MHz) δ 0.88 (t, $J = 6.8$ Hz, 3H), 1.29-1.46 (m, 8H), 1.35 (d, $J = 6.2$ Hz, 3H), 1.58-1.68 (m, 1H), 1.70-1.79 (m, 1H), 4.94 (brs, 1H), 5.17 (sext, $J = 6.3$ Hz, 1H), 6.93 (d, $J = 8.6$ Hz, 2H), 7.53 (d, $J = 8.6$ Hz, 2H), 7.60 (d, $J = 8.4$ Hz, 2H), 8.08 (d, $J =$

8.4 Hz, 2H). $[\alpha]_{\text{D}}^{26} = +40.9^{\circ}$ (0.0300 g mL⁻¹; CHCl₃), lit.⁴ $[\alpha]_{\text{D}}^{\text{rt}} = +38.8^{\circ}$ (0.0232 g mL⁻¹; CHCl₃).

(1*S*)-1-Methylheptyl 12-(4-Hydroxyphenyl)-*p*-carborane-1-carboxylate (5). A mixture of Pd/C (10%, 57 mg) and ester **8** (265 mg, 0.54 mmol) in EtOAc (10 mL) was stirred under hydrogen atmosphere (1 atm) overnight (18 hrs.). The reaction was filtered through Celite® and condensed. The crude product was recrystallized from hexane giving 0.210 g (95% yield) of phenol **5** as colorless needles: mp 118-119 °C; ¹H NMR (400 MHz) δ 0.89 (t, *J* = 6.9 Hz, 3H), 1.14 (d, *J* = 6.2 Hz, 3H), 1.19-1.32 (m, 8H), 1.39-1.47 (m, 1H), 1.50-1.57 (m, 1H), 1.90-3.13 (brm, 10H), 4.74 (sext, *J* = 6.3 Hz, 1H), 5.0 (brs, 1H), 6.61 (d, *J* = 8.9 Hz, 2H), 7.05 (d, *J* = 8.9 Hz, 2H). Anal. Calcd for C₁₇H₃₂B₁₀O₃: C, 52.02; H, 8.02. Found: C, 52.14; H, 8.21. $[\alpha]_{\text{D}}^{26} = +23.7^{\circ}$ (0.0150 g mL⁻¹; CHCl₃).

1-(4-Benzyloxyphenyl)-*p*-carborane (6). Following a general literature procedure,⁵ *n*-BuLi (2.5 M, 2.9 mL, 7.25 mmol) was added dropwise to a solution of *p*-carborane (1.00 g, 6.93 mmol) in dry DME (30 mL) under argon at -10 °C. The reaction was allowed to warm to room temperature for 30 min.; then dry CuCl (0.913 g, 9.22 mmol) was added at once. After stirring 45 min., pyridine (4.4 mL) and 4-benzyloxyiodobenzene⁶ (2.50 g, 8.07 mmol) were added. The reaction was stirred 2 days at 110 °C. The reaction was cooled to room temperature, diluted with Et₂O (50 mL), and filtered through Celite®. The filtrate was washed with 10% HCl, water, and brine and dried (MgSO₄). After removing solvent, the brown product was purified by flash chromatography (hexane), giving 1.47 g (65% yield) of the monoarylated carborane **6** as off-white crystals: mp 96.5 – 97 °C (not recrystallized); ¹H NMR (400 MHz) δ 1.6-3.3 (brm, 10H), 2.75 (brs, 1H), 4.99 (s, 2H), 6.75 (d, *J* = 9.0 Hz, 2H),

7.11 (d, $J = 9.0$ Hz, 2H), 7.30-7.35 (m, 1H), 7.37-7.40 (m, 4H). Anal. Calcd for $C_{15}H_{21}B_{10}O$: C, 55.19; H, 6.79. Found: C, 55.31; H, 6.81.

12-(4-Benzyloxyphenyl)-*p*-carborane-1-carboxylic acid (7). Following a similar literature procedure,⁷ 1.8 M *n*-BuLi in hexanes (0.78 mL, 1.4 mmol) was added to a solution of carborane derivative **6** (0.42 g, 1.28 mmol) in dry THF (30 mL) at -78 °C. The orange solution turned dull green as it warmed to room temperature over 30 min. Dry CO_2 was bubbled through the solution until all solvent was removed. Aqueous HCl (1 M, 12 mL) was added, and the product was extracted with Et_2O . The organic layer was dried (Na_2SO_4) and condensed. The resulting crude product was recrystallized successively from toluene followed by EtOH giving 0.43 g (90% yield) of acid **7** as off-white crystals: mp 228 – 232 °C; 1H NMR (400 MHz) δ 1.8-3.3 (brm, 10H), 4.99 (s, 2H), 6.76 (d, $J = 9.0$ Hz, 2H), 7.08 (d, $J = 9.0$ Hz, 2H), 7.31-7.35 (m, 1H), 7.37-7.40 (m, 4H). Anal. Calcd for $C_{16}H_{22}B_{10}O_3$: C, 51.88; H, 5.99. Found: C, 52.03; H, 6.01.

(1*S*)-1-Methylheptyl 12-(4-Benzyloxyphenyl)-*p*-carborane-1-carboxylate (8). Dicyclohexylcarbodiimide (DCC, 0.308 g, 1.49 mmol) was added to a mixture of acid **7** (0.504 g, 1.36 mmol), (*S*)-2-octanol (0.26 mL, 1.63 mmol), and 4-dimethylaminopyridine (DMAP, 40 mg, 0.33 mmol) in dry CH_2Cl_2 (10 mL) at 0 °C under argon. The reaction was allowed to stir overnight (18 h) at room temperature. The reaction mixture was condensed and applied directly to a silica gel column (4:1 hexane/EtOAc). The isolated product (0.350 g, 53% yield) solidified upon standing, and it was used directly in the following step. An analytical sample of **8** was obtained by recrystallization from pentane at -78 °C: mp 34-35 °C; 1H NMR (300 MHz) δ 0.89 (t, $J = 6.7$ Hz, 3H), 1.14 (d, $J = 6.2$ Hz, 3H), 1.20-1.30 (m, 8H), 1.44-1.55 (m, 2H), 4.75 (sext, $J = 6.3$ Hz, 1H), 4.99 (s, 2H), 6.75 (d, $J = 8.9$ Hz, 2H),

7.09 (d, $J = 8.9$ Hz, 2H), 7.30-7.38 (m, 5H). Anal. Calcd for $C_{24}H_{38}B_{10}O_3$ C, 59.72; H, 7.94.
Found: C, 59.62; H, 7.88.

2. Thermal Analysis of 1F

A virgin sample obtained by crystallization of **1F** from solution shows two melting transitions (Figure S1). The first melting is observed at 94 °C, which is followed by partial crystallization and subsequent second melting at 98 °C. The relative proportion of the two endotherms is a function of the rate of heating: at a higher rate (5 K min⁻¹) practically only the first melting is visible, but at a slower rate the exotherm of crystallization and the second melting are clearly visible. The second DSC run showed practically only the high temperature melting peak what is consistent with thermal behavior of **1F** reported in the literature.²

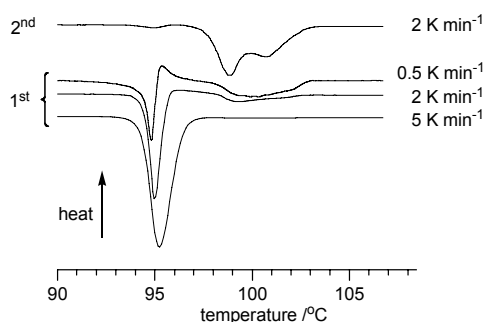


Figure S1. First heating DSC traces for **1F** obtained at different scanning rates. The top curve is the second heating DSC trace

3. Thermo-optical measurements

Thermo-optical measurements were done using a 1.6 μm cell with planar orienting layers obtained by spin-coating of polyimide PI-2610 (DuPont). Subsequently, after drying and baking the antiparallel rubbing was applied on both surfaces of the cell for uniform orientation. Cells were assembled using glass microspheres and sealed using UV curable

adhesives. The cell with uniformly oriented material was placed in the computer-controlled hot stage (Instec) placed in a microscope (Biolar PI, PZO) birefractive setup. The uniform SmA* structure was obtained upon slow cooling from the isotropic state. The optical axis of the cell was oriented at the maximum transmission increment (22.5 °). The light intensity transmitted through the birefractive setup was recorded by using the linear silicone photodetector (FLC PIN 20, FLC Electronics, Sweden) on cooling (5 K min⁻¹) from the isotropic state. The recorded intensity vrs temperature for the host and each binary mixture is shown in Figure S2.

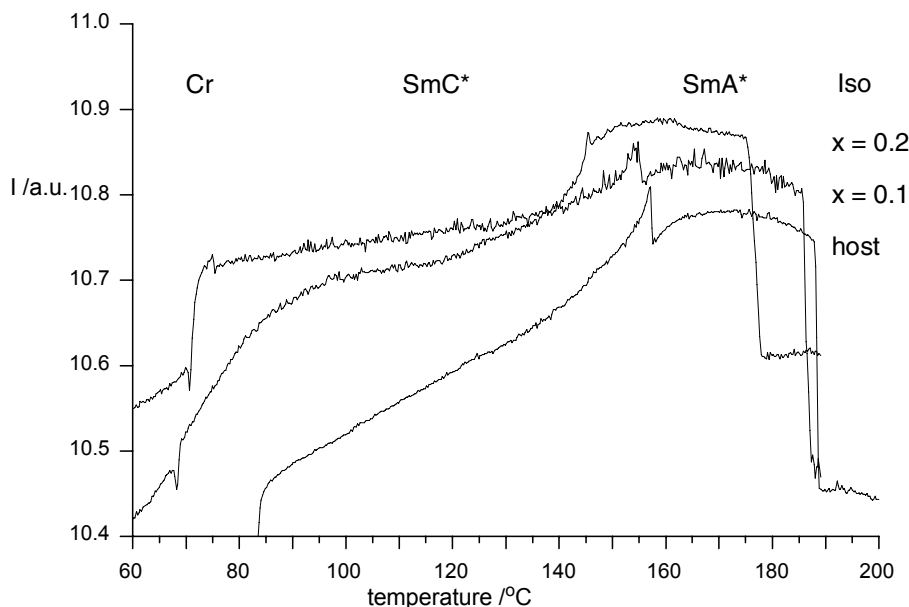


Figure S2. A plot intensity of transmitted light vs temperature for host **1F** and its solutions with 10 mol% and 20 mol% of **2F**.

Table S1. Transition temperatures for **1F** and its mixtures with **2F** obtained on cooling.^a

	SmC–SmA / °C	SmA-I / °C
1F	157	188.5
10 mol% of 2F	155	186.5

20 mol% of 2F	146	176.5
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^a Temperatures were obtained in 1.6 μm electro-optical cells by thermo-optical methods and taken as the middle of the light transmission change region (see Figure S2).

4. Dielectric Data

According to the Cole-Cole model, a plot of the real part of permittivity ϵ' (x axis) vs the imaginary component ϵ'' (y axis) gives a semicircle shown in Figure S3.⁸⁻¹⁰ On the basis of the original Cole-Cole equation,⁸ the plot was numerically analyzed using the least square method (an algorithm implemented in MS Excel) to find coordinates of the semicircle points and its radius. This permitted the calculation of maximum ϵ'' and the corresponding relaxation frequency f_r .

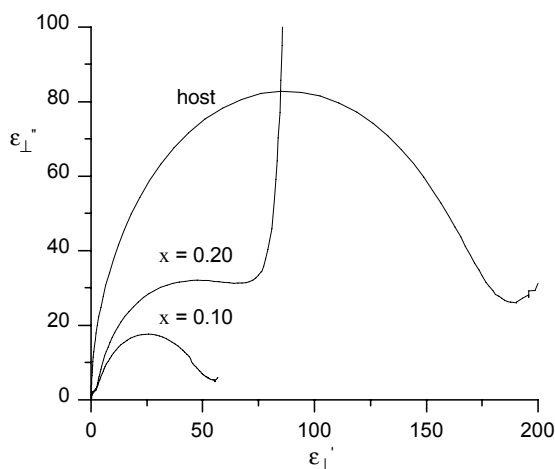


Figure S3. The Cole-Cole diagram for **1F** (host) and its solutions with 10 mol% and 20 mol% of **2F** at 120 °C in a planar 23 μm cell.

5. Procedure for Goldstone mode elastic constant calculations.

The Goldstone mode elastic constant K_ϕ was calculated using equation 2:¹¹

$$K_\phi = \frac{p^2}{2\pi\epsilon_0\Delta\epsilon_G} \cdot \left(\frac{P_s}{\theta}\right)^2 \quad \text{Eq 2.}$$

In which:

- p stands for the value of the length of the helical pitch obtained from the wavelength of selective reflection λ assuming that refractive index n for the binary mixtures is the same as for the pure host ($n = 1.46$) according to ref¹².
- P_s is the spontaneous polarization measured by using of the reversal current method,¹³
- θ is the molecular tilt obtained from electrooptical methods,
- $\Delta\epsilon_G$ stands for the dielectric strength obtained for the Goldstone mode relaxation.

Example of calculations of elastic constant K_ϕ of the host at $T-T_c = 25$ K.

Taking

$$P_s = 174 \text{ nC/cm}^2$$

$$\theta = 43.8^\circ$$

$$\epsilon_r = 157.13 \text{ (from Cole-Cole analysis)}$$

$$p = \lambda/n = (426 \cdot 10^{-9} \text{ m})/1.46 = 293.8 \cdot 10^{-9} \text{ m}$$

$$\Delta\epsilon_G = \epsilon_r \times \epsilon_0 = 157.13 \times 8.85 \cdot 10^{-12} \text{ F/m} = 1.39 \cdot 10^{-9} \text{ F/m}$$

The resulting value of K_ϕ is 50.8 pN, which a typical value for SmC* materials.¹⁴

6. Archive for computational results

1F

```
1\1\GINC-MONSTER\FOpt\RHF\6-31G(d)\C36H33F13O5\PIOTR\04-Mar-2007\0\#P
HF/6-31G* FOPT GEOM(NOANGLE,NODISTANCE) FCHECK\C6F13CH2CH2O-Ph-COO-P
hPh-COO-Oc* (S), C1\0,1\C,0.6885112668,-1.9778598057,1.9562653594\C,0
.5072695053,-1.7357330902,0.6150625235\C,0.1298127816,-0.4679848592,0.
1699250428\C,-0.0588545135,0.5419059379,1.0998134485\C,0.1209771807,0.
3119824611,2.4536400258\C,0.4961515871,-0.9539465501,2.8827551519\O,0.
6983375712,-1.2893147096,4.1699756725\C,0.5276278221,-0.3361358344,5.1
854415627\C,0.8315915257,-1.0628556668,6.4891183916\C,0.7321480715,-0.
1343241262,7.6799665245\C,0.9310565859,-0.8511805518,9.0266347634\C,1.
1081181953,0.0762250883,10.2503711902\C,0.8857354663,-0.6397603774,11.
6029521735\C,1.4683444116,0.1238309213,12.8107104358\C,0.9447549702,-0.
3463285668,14.1773559961\F,-0.4709278678,0.4537710209,7.7076717478\F,
1.6501329542,0.8397674966,7.5926927033\F,2.0169479178,-1.6164641718,8.
9408437768\F,-0.1239449737,-1.6396034471,9.2271975373\F,0.246407827,1.
0809715882,10.1756243354\F,2.3417831366,0.5659083552,10.2232254588\F,1.
4549715795,-1.838361946,11.5655923293\F,-0.4207431342,-0.7927160539,1
1.7826327115\F,1.1828399446,1.4155333639,12.6989774282\F,2.7843151864,
-0.031858825,12.8122115491\F,1.6569067569,0.2244919813,15.1187880871\F
,1.0568719513,-1.649203331,14.2900157301\F,-0.3105568164,-0.0079071928
,14.3369280837\C,-0.0810645176,-0.148295874,-1.2623435829\O,0.14524979
35,-1.2071948947,-2.0538965794\C,0.0158367008,-1.08606061,-3.422746410
3\C,1.1530432921,-1.1903360205,-4.195227638\C,1.0441327554,-1.14708936
```

93, -5.5748088538\C, -0.193519657, -0.9962873372, -6.1914457356\C, -1.3245170262, -0.8943907823, -5.3839773112\C, -1.2275928883, -0.9423798035, -4.006055942\C, -0.3076890421, -0.945665004, -7.6760193734\C, -1.1114651258, 0.0083535805, -8.2957626964\C, -1.219563871, 0.0582937408, -9.6733281592\C, -0.5222707393, -0.8477196113, -10.4621535265\C, 0.2822328704, -1.802386368, -9.8525127002\C, 0.3875043937, -1.8507442271, -8.4762141017\C, -0.6018542546, -0.8379401229, -11.9509629493\O, -0.0075089587, -1.6045373946, -12.644796778\O, -1.3966263508, 0.1103461315, -12.4165150824\O, -0.4119144154, 0.9141362343, -1.6742323301\C, -1.565164412, 0.2475860157, -13.8363344646\C, -2.6329182039, -0.7290142922, -14.3057047332\C, -1.9065727217, 1.716653038, -14.0610360224\C, -1.9932364383, 2.1198531258, -15.5352407584\C, -2.1980551852, 3.6253305642, -15.7188735045\C, -2.3003117423, 4.0445260017, -17.1862972045\C, -2.5014895321, 5.5495286673, -17.3727174458\C, -2.6031675085, 5.9612193842, -18.8409784373\H, 0.9782122147, -2.9477702952, 2.3140069092\H, 0.6567590729, -2.5278107753, -0.092403688\H, -0.3490125579, 1.5168835123, 0.757450194\H, -0.0321458437, 1.1146714153, 3.1476994392\H, -0.4872735158, 0.0412262689, 5.1824489584\H, 1.2086125754, 0.4944250545, 5.0422451579\H, 1.8300834089, -1.4748464546, 6.4483809579\H, 0.1335962759, -1.8797417841, 6.620833527\H, 2.109527572, -1.3003069242, -3.7188916496\H, 1.9345363942, -1.2106694605, -6.1731159813\H, -2.2943639233, -0.7974533372, -5.8365201782\H, -2.1041491762, -0.8689563561, -3.3907722394\H, -1.6378501153, 0.7299023379, -7.698052786\H, -1.8372196663, 0.8036020834, -10.1351758965\H, 0.8136312422, -2.5048790095, -10.4655702582\H, 0.99609683, -2.6087505693, -8.0179300873\H, -0.6210888677, 0.0101998233, -14.3048964722\H, -2.7579651292, -0.6727919015, -15.3809873859\H, -3.5857380289, -0.5058254281, -13.8358763941\H, -2.3500905118, -1.7438905424, -14.0568969485\H, -1.1403678195, 2.3107840817, -13.5710560919\H, -2.8439877698, 1.9416890969, -13.5581536438\H, -2.8091537416, 1.5911472907, -16.0206810773\H, -1.0819957499, 1.8172258018, -16.0485702994\H, -1.3752460097, 4.1599813141, -15.248060805\H, -3.1008299296, 3.9315630855, -15.193210803\H, -3.1250916529, 3.5117746531, -17.6568831272\H, -1.3988710799, 3.7354344171, -17.7129222161\H, -1.6771591189, 6.0834367031, -16.9047433997\H, -3.4025343347, 5.8599078718, -16.8478778625\H, -2.7452116242, 7.0329045641, -18.9403151484\H, -3.4404005443, 5.4700728396, -19.3289131461\H, -1.701902173, 5.6952000843, -19.3861063161\\Version=x86-Linux-G98R evA.9\HF=-3049.5624479\RMSE=6.476e-09\RMSF=1.102e-06\Dipole=-0.3408888, -0.0538273, 0.2590407\PG=C01 [X(C36H33F13O5)]\\

Dipole moment (Debye):

X= 0.5753 Y= 0.1309 Z= 0.9246 Tot= 1.0968

Results for B3LYP/3-21G//HF/6-31G(d):

Dipole moment (Debye):

X= 0.1828 Y= 0.3195 Z= 0.8096 Tot= 0.8893

Exact polarizability: 619.256 -4.321 298.628 -2.545 30.562 232.301

2F

1\1\GINC-MONSTER\FOpt\RHF\6-31G(d)\C32H39B10F13O5\PIOTR\23-Mar-2007\0\
\#P HF/6-31G* FOPT GEOM(NOANGLE,NODISTANCE) FCHECK\C6F13CH2CH2O-Ph-CO
O-PhC2B10-COO-OC* (S), C1\0,1\B, -1.341249634, -1.6385189918, -7.7499420
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Dipole moment (Debye):

X= -0.0110 Y= 0.5895 Z= -0.1580 Tot= 0.6104

Results for B3LYP/3-21G//HF/6-31G(d):

Dipole moment (Debye):

X= -0.4201 Y= 0.8023 Z= 0.0407 Tot= 0.9066

Exact polarizability: 655.699 -7.727 340.344 -3.895 15.473 319.189

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