Electronic Supplementary Information for

Anion-Driven Mesogenicity: A Comparative Study of Ionic Liquid Crystals Based on the [*closo*-1-CB_9H_{10}]$^-$ and [*closo*-1-$CB_{11}H_{12}$]$^-$ Clusters.

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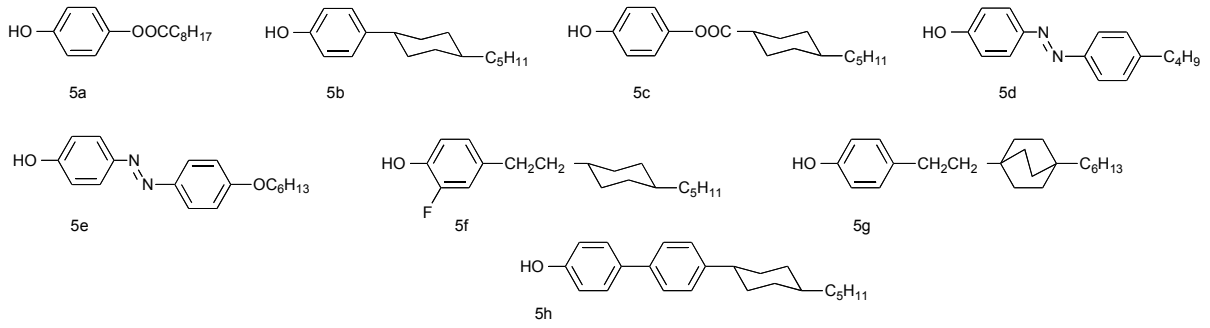
1. Synthetic and analytical details

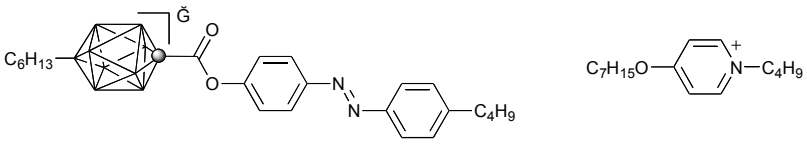
^{1}H NMR spectra were obtained at 400 MHz for all compounds in acetone-d_6 (δ 2.04 ppm) or $CDCl_3$ (δ 7.26 ppm). ^{11}B NMR spectra were recorded at 128 MHz. Chemical shifts were referenced to the solvent (^{1}H) or to an external sample of $B(OH)_3$ in MeOH (^{11}B, δ = 18.1 ppm). The preparation and characterization details of *N*-butyl-4-heptyloxypyridinium bromide (**[Pyr]Br**),[1] phenols **5a**,[2] **5b**,[3] **5c**,[4] **5d**,[5] **5e**,[6] and **5h**,[7] and also ion pairs **1a[Pyr]–1c[Pyr]**[1] were reported previously.



General Procedure for Preparation of Esters 1 and 2

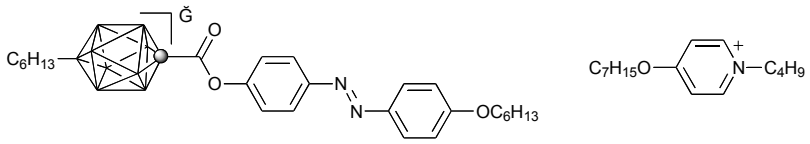
Phenol **5** (1.5 equivalents) was added to a colorless solution of acid [*closo*-1-CB_9H_8-1-COOH-10-C_6H_{13}]$^-$ $[NMe_4]^+$ (**3[NMe$_4$]**) or [*closo*-1-$CB_{11}H_{10}$-1-COOH-12-C_6H_{13}]$^-$ $[NEt_4]^+$ (**4[NEt$_4$]**), DCC (1.0 equivalent), and DMAP (0.1 equivalents) in anhydrous CH_2Cl_2. The reaction mixture was stirred overnight at rt, and the reaction progress was monitored by TLC (R_f = 0.5, CH_3CN/CH_2Cl_2, 1:9). The solvent was removed *in vacuo*, and the crude product was isolated by column chromatography (SiO_2, CH_3CN/CH_2Cl_2, 1:9). The resulting ester was washed with hot hexane and used in the subsequent step for cation exchange without further purification. Typical yields for this procedure are above 80 %.

N-Butyl-4-heptyloxypyridinium bromide (**[Pyr]Br**, 1.0 equivalent) or cetyltrimethylammonium bromide ([**Cetyl**]Br, 1.0 equivalent) were added to a solution of ester **1[NMe$_4$]** or **2[NEt$_4$]** in CH_2Cl_2. Water was added, and the biphasic system was stirred vigorously until all the precipitate had dissolved. The CH_2Cl_2 layer was separated, and the aqueous layer was extracted with additional CH_2Cl_2. The CH_2Cl_2 layers were combined, washed with H_2O, dried (Na_2SO_4), and evaporated giving **1[Pyr]**, **2[Pyr]** or **1[Cetyl]**, **2[Cetyl]** as crystalline solids, which were further purified by recrystallization from aqueous alcohol. Some pyridinium salts were purified further by column chromatography (CH_3CN/CH_2Cl_2, 1:9) and then by repeated recrystallization from aqueous alcohol. The resulting crystals were dried in vacuum at ambient temperature, and typical yields range from 20%-40% based on the starting hexyl acid **3[NMe$_4$]** or **4[NEt$_4$]**.



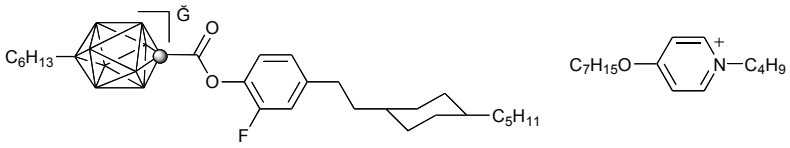
1d[Pyr]:

Recrystallized from EtOH/H_2O mixtures (1x) and MeOH/H_2O mixtures (7x) providing the pure salt as orange microcrystals: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 8H), 0.87 (t, J = 6.9 Hz, 3H), 0.92 (t, J = 7.1 Hz, 3H); 0.94 (t, J = 7.4 Hz, 3H), 0.95 (t, J = 7.4 Hz, 3H), 1.23-1.44 (m, 16H), 1.45-1.52 (m, 2H), 1.53-1.61 (m, 2H), 1.66 (quint, J = 7.6 Hz, 2H), 1.85-1.92 (m, 4H), 1.95-2.04 (m, 2H), 2.73 (t, J = 7.7 Hz, 2H), 4.46 (t, J = 6.5 Hz, 2H), 4.64 (t, J = 7.5 Hz, 2H), 7.42 (d, J = 8.4 Hz, 2H), 7.51 (d, J = 8.8 Hz, 2H), 7.67 (d, J = 7.6 Hz, 2H), 7.88 (d, J = 8.4 Hz, 2H), 8.03 (d, J = 8.8 Hz, 2H), 8.92 (d, J = 7.6 Hz, 2H); ^{11}B {^{1}H} NMR (128 MHz, acetone-d_6) δ -23.8 (4B), -15.8 (4B), 49.4 (1B). Anal. Calcd. for $C_{40}H_{66}B_9N_3O_3$: C, 65.43; H, 9.06; N, 5.72. Found: C, 65.96; H, 9.02; N, 6.00.



1e[Pyr]:

Recrystallized from EtOH/H_2O mixtures (4x) providing the pure salt as orange microcrystals: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 8H), 0.88 (t, J = 7.0 Hz, 3H), 0.92 (t, J = 7.0 Hz, 3H), 0.93 (t, J = 6.5 Hz, 3H), 0.96 (t, J = 7.4 Hz, 3H), 1.27-1.32 (m, 4H), 1.33-1.45 (m, 12H), 1.46-1.62 (m, 6H), 1.80-2.09 (m, 10H), 4.14 (t, J = 6.5 Hz, 2H), 4.47 (t, J = 6.5 Hz, 2H), 4.64 (t, J = 7.4 Hz, 2H), 7.12 (d, J = 9.0 Hz, 2H), 7.50 (d, J = 8.8 Hz, 2H), 7.68 (d, J = 7.4 Hz, 2H), 7.95 (d, J = 8.9 Hz, 2H), 8.01 (d, J = 8.8 Hz, 2H), 8.92 (d, J = 7.4 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -23.9 (d, J = 143 Hz, 4B), -15.9 (d, J = 139 Hz, 4B), 49.0 (1B). Anal. Calcd. for $C_{42}H_{70}B_9N_3O_4$: C, 64.81; H, 9.07; N, 5.40. Found: C, 64.70; H, 9.11; N, 5.35.

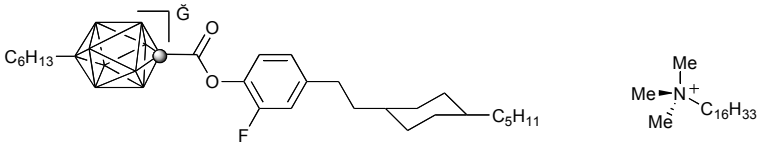


1f[Pyr]:

Recrystallized from MeOH/H_2O mixtures (4x) providing the pure salt as white crystals: ^{1}H NMR (500 MHz, acetone-d_6) δ 0.40-2.50 (m, 8H), 0.87 (t, J = 7.0 Hz, 6H), 0.91 (t, J = 7.1 Hz, 3H), 0.95 (t, J = 7.4 Hz, 3H), 0.96-1.03 (m, 2H), 1.15-1.20 (m, 2H), 1.21-1.33 (m, 12H), 1.34-1.44 (m, 8H), 1.45-1.51 (m, 2H), 1.52-1.59 (m, 4H), 1.77 (br d, J = 12.3 Hz, 2H), 1.82-1.98 (m, 8H), 1.99-2.04 (m, 4H), 2.68 (t, J = 8.1 Hz, 2H), 4.47 (t, J = 6.5 Hz, 2H), 4.64 (t, J = 7.5 Hz, 2H), 7.08 (d, J = 8.2 Hz, 1H), 7.13 (dd, J_1 = 11.5 Hz, J_2 = 1.8 Hz, 1H), 7.24 (t, J = 8.2 Hz, 1H), 7.68 (d, J = 7.5 Hz, 2H), 8.92 (d, J = 7.5 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -23.9 (d, J

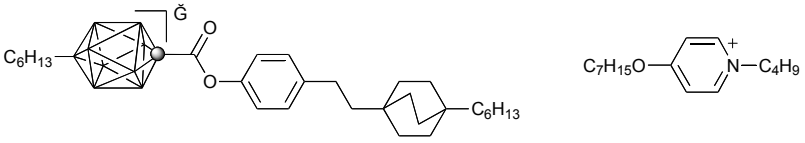
= 140 Hz, 4B), -15.9 (d, J = 150 Hz, 4B), 49.0 (s, 1B). Anal. Calcd. for $C_{43}H_{77}B_9FNO_3$: C, 66.87; H, 10.05; N, 1.81. Found: C, 67.06; H, 10.07; N, 1.89.

1f[Cetyl]:



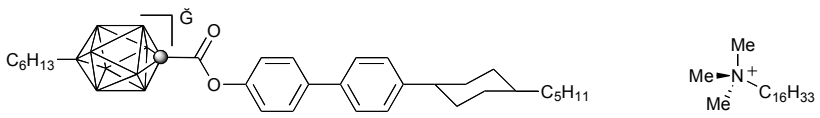
Recrystallized from MeOH/H_2O mixtures (4x) providing the pure salt as white crystals: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 8H), 0.87 (t, J = 7.0 Hz, 3H), 0.88 (t, J = 6.8 Hz, 3H), 0.92 (t, J = 7.0 Hz, 3H), 0.96-1.03 (m, 2H), 1.15-1.43 (m, 42H), 1.52-1.61 (m, 4H), 1.78 (br d, J = 12.6 Hz, 2H), 1.83-2.00 (m, 8H), 2.69 (t, J = 8.1 Hz, 2H), 3.37 (s, 9H), 3.54-3.60 (m, 2H), 7.09 (d, J = 8.3 Hz, 1H), 7.14 (dd, J_1 = 11.5 Hz, J_2 = 1.9 Hz, 1H), 7.25 (t, J = 8.1 Hz, 1H); ^{11}B NMR (128 MHz, acetone-d_6) δ -23.9 (d, J = 135 Hz, 4B), -15.9 (d, J = 150 Hz, 4B), 49.3 (s, 1B). Anal. Calcd. for $C_{46}H_{91}B_9FNO_2$: C, 68.50; H, 11.37; N, 1.74. Found: C, 68.92; H, 11.24; N, 1.86.

1g[Pyr]:

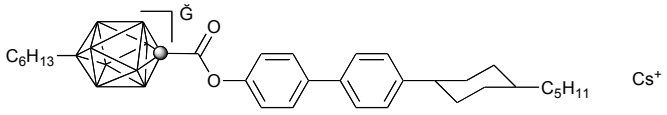


Recrystallized from MeOH/H_2O mixtures (4x) providing the pure salt as white crystals: ^{1}H NMR (500 MHz, acetone-d_6) δ 0.40-2.50 (m, 8H), 0.87 (t, J = 7.0 Hz, 6H), 0.91 (t, J = 7.1 Hz, 3H), 0.95 (t, J = 7.4 Hz, 3H), 1.06-1.10 (m, 2H), 1.18-1.51 (m, 36H), 1.56 (quint, J = 7.2 Hz, 2H), 1.84-1.96 (m, 6H), 1.98-2.04 (m, 2H), 2.52-2.57 (m, 2H), 4.46 (t, J = 6.5 Hz, 2H), 4.63 (t, J = 7.5 Hz, 2H), 7.15 (d, J = 8.5 Hz, 2H), 7.24 (d, J = 8.5 Hz, 2H), 7.67 (d, J = 7.5 Hz, 2H), 8.91 (d, J = 7.5 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -23.9 (d, J = 139 Hz, 4B), -16.0 (d,

J = 152 Hz, 4B), 49.0 (s, 1B). Anal. Calcd. for $C_{46}H_{82}B_9NO_3$: C, 69.54; H, 10.40; N, 1.76. Found: C, 69.68; H, 10.21; N, 1.87.

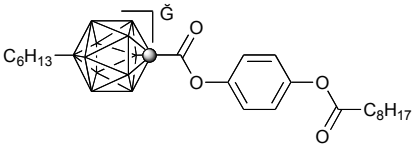
1h[Cetyl]: 

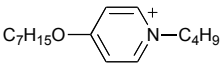
Due to low solubility of **1h[NMe$_4$]** salt it was converted directly to **1h[Cetyl]** and purified chromatographically. Product was recrystallized from EtOH (3x) providing the pure salt **1h[Cetyl]** as a white wax: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 8H), 0.88 (t, J = 7.0 Hz, 3H), 0.91 (t, J = 7.0 Hz, 3H), 0.93 (t, J = 7.1 Hz, 3H), 1.00-1.17 (m, 3H), 1.22-1.45 (m, 46H), 1.50-1.62 (m, 2H), 1.87-2.00 (m, 4H), 2.52 (tt, J_1 = 12.2 Hz, J_2 = 3.0 Hz, 1H), 3.35 (s, 9H), 3.53-3.60 (m, 2H), 7.34 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 8.7 Hz, 2H), 7.62 (d, J = 8.2 Hz, 2H), 7.73 (d, J = 8.6 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -23.9 (d, J = 137 Hz, 4B), -16.0 (d, J = 151 Hz, 5B), 49.0 (s, 1B). Anal. Calcd. for $C_{50}H_{92}B_9NO_2$: C, 71.79; H, 11.08; N, 1.67. Found: C, 72.00; H, 11.15; N, 1.92.



Preparation of 1h[Cs]. Purified salt **1h[NMe$_4$]** (75 mg, 0.12 mmol) was suspended in 10% HCl (20 mL), Et_2O (50 mL) was added and the mixture was stirred until precipitation had dissolved (0.5 h). The Et_2O layer was separated, washed with water and a solution of CsCl (2 mL, ~5.7 M) was added followed by H_2O (2 mL) and CH_2Cl_2 (10 mL). The mixture was stirred for 15 min, Et_2O was evaporated, and CH_2Cl_2 added. After short stirring, the organic layer was separated the aqueous layer extracted (CH_2Cl_2), extracts dried ($NaSO_4$), and the solvent

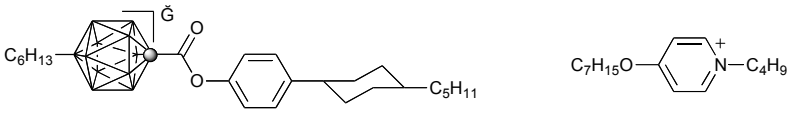
evaporated leaving 70 mg (86% yield) of cesium salt **1h[Cs]** as a white solid. Analytically pure sample was obtained by recrystallization from toluene containing small amounts of MeCN: mp >290 ^{o}C dec; ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 8H), 0.88 (t, J = 7.0 Hz, 3H), 0.90 (t, J = 7.2 Hz, 3H), 1.00-1.14 (m, 3H), 1.20-1.43 (m, 12H), 1.44-1.58 (m, 4H), 1.82-1.97 (m, 8H), 2.09 (s, 3H, MeCN), 2.53 (tt, J_1 = 12.2 Hz, J_2 = 2.9 Hz, 1H), 7.33 (d, J = 8.2 Hz, 2H), 7.35 (d, J = 8.6 Hz, 2H), 7.60 (d, J = 8.2 Hz, 2H), 7.70 (d, J = 8.8 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -23.7 (d, J = 135 Hz, 4B), -16.1 (d, J = 143 Hz, 4B), 49.0 (s, 1B). Anal. Calcd. For $C_{31}H_{50}B_9CsO_2$: C, 54.36; H, 7.36; calcd for $C_{31}H_{50}B_9CsO_2$•MeCN: C, 54.60; H, 7.36; N, 1.93. Found: C, 54.81; H, 7.26; N, 1.83.





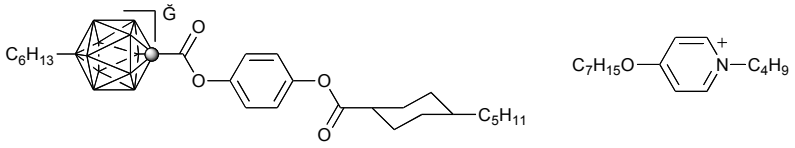
2a[Pyr]:

Recrystallized from MeOH/H_2O mixtures (3x) providing the pure salt as white flakes: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.50-2.50 (m, 10H), 0.53-0.59 (m, 2H), 0.85 (t, J = 7.1 Hz, 3H), 0.87 (t, J = 6.9 Hz, 6H), 0.95 (t, J = 7.4 Hz, 3H), 1.26-1.44 (m, 26H), 1.45-1.53 (m, 2H), 1.70 (quint, J = 7.4 Hz, 2H), 1.89 (quint, J = 7.0 Hz, 2H), 1.98-2.06 (m, 2H), 2.55 (t, J = 7.4 Hz, 2H), 4.47 (t, J = 6.5 Hz, 2H), 4.64 (t, J = 7.5 Hz, 2H), 7.01 (d, J = 9.0 Hz, 2H), 7.10 (d, J = 9.0 Hz, 2H), 7.68 (d, J = 7.6 Hz, 2H), 8.92 (d, J = 7.6 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -14.1 (d, J = 157 Hz, 5B), -12.0 (d, J = 137 Hz, 5B), 5.1 (s, 1B). Anal. Calcd. for $C_{39}H_{72}B_{11}NO_5$: C, 62.13; H, 9.63; N, 1.86. Found: C, 62.40; H, 9.63; N, 1.81.

2b[Pyr]: 

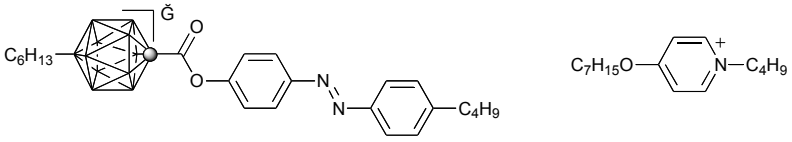
Recrystallized from EtOH/H_2O mixtures (3x) providing the pure salt as white crystals: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 10H), 0.53-0.59 (m, 2H), 0.86 (t, J = 7.1 Hz, 3H), 0.88 (t, J = 6.9 Hz, 3H), 0.89 (t, J = 6.8 Hz, 3H), 0.96 (t, J = 7.4 Hz, 3H), 0.96-1.06 (m, 3H), 1.20-1.54 (m, 28H), 1.80-1.94 (m, 8H), 2.40 (tt, J_1 = 12.3 Hz, J_2 = 3.2 Hz, 1H), 4.48 (t, J = 6.5 Hz, 2H), 4.65 (t, J = 7.5 Hz, 2H), 6.88 (d, J = 8.5 Hz, 2H), 7.21 (d, J = 8.5 Hz, 2H), 7.69 (d, J = 7.3 Hz, 2H), 8.93 (d, J = 7.3 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -14.0 (d, J = 157 Hz, 5B), -12.0 (d, J = 137 Hz, 5B), 5.0 (s, 1B).

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.40-2.50 (m, 10H), 0.53-0.61 (m, 2H), 0.82 (t, J = 7.0 Hz, 3H), 0.87 (t, J = 7.2 Hz, 3H), 0.88 (t, J = 7.0 Hz, 3H), 0.92 (t, J = 7.3 Hz, 3H), 0.96-1.06 (m, 3H), 1.16-1.46 (m, 28H), 1.78-1.92 (m, 8H), 2.40 (br t, J = 12.2 Hz, 1H), 4.23 (t, J = 6.5 Hz, 2H), 4.30 (t, J = 7.5 Hz, 2H), 6.89 (d, J = 8.5 Hz, 2H), 7.11 (d, J = 8.6 Hz, 2H), 7.30 (d, J = 7.1 Hz, 2H), 8.37 (d, J = 7.1 Hz, 2H). Anal. Calcd. for $C_{41}H_{76}B_{11}NO_3$: C, 65.66; H, 10.21; N, 1.87. Found: C, 65.46; H, 10.40; N, 1.81.

2c[Pyr]: 

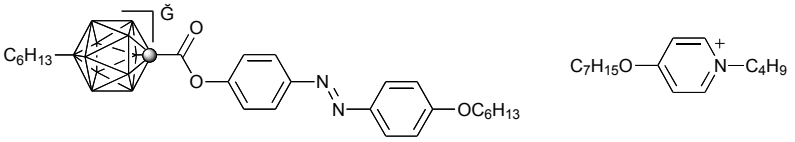
Recrystallized from EtOH/H_2O mixtures (3x) providing the pure salt as white crystals: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 10H), 0.52-0.59 (m, 2H), 0.85 (t, J = 7.1 Hz, 3H), 0.87 (t, J = 7.0 Hz, 3H), 0.88 (t, J = 6.8 Hz, 3H), 0.95 (t, J = 7.4 Hz, 3H), 0.98-1.07 (m, 1H), 1.17-1.56 (m, 32H), 1.82-1.93 (m, 4H), 1.98-2.13 (m, 2H), 2.48 (tt, J_1 = 12.2 Hz, J_2 = 3.6 Hz, 1H),

4.47 (t, *J* = 6.5 Hz, 2H), 4.64 (t, *J* = 7.5 Hz, 2H), 7.00 (d, *J* = 9.0 Hz, 2H), 7.09 (d, *J* = 9.0 Hz, 2H), 7.68 (d, *J* = 7.6 Hz, 2H), 8.92 (d, *J* = 7.5 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -14.1 (d, *J* = 152 Hz, 5B), -12.0 (d, *J* = 140 Hz, 5B), 5.9 (s, 1B). Anal. Calcd. for $C_{42}H_{76}B_{11}NO_5$: C, 63.53; H, 9.65; N, 1.76. Found: C, 63.79; H, 9.69; N, 1.70.



2d[Pyr]:

Recrystallized from an EtOH/H_2O mixture (1x) and MeOH/H_2O mixtures (3x) providing the pure salt as orange crystals: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 10H), 0.53-0.60 (m, 2H), 0.85 (t, *J* = 7.1 Hz, 3H), 0.87 (t, *J* = 7.0 Hz, 3H), 0.93 (t, *J* = 7.3 Hz, 3H), 0.95 (t, *J* = 7.3 Hz, 3H), 1.18-1.52 (m, 18H), 1.59-1.68 (m, 4H), 1.89 (quint, *J* = 7.0 Hz, 2H), 1.97-2.07 (m, 2H), 2.71 (t, *J* = 7.7 Hz, 2H), 4.46 (t, *J* = 6.5 Hz, 2H), 4.64 (t, *J* = 7.5 Hz, 2H), 7.20 (d, *J* = 8.9 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 7.5 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.93 (d, *J* = 8.9 Hz, 2H), 8.92 (d, *J* = 7.6 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -14.0 (d, *J* = 158 Hz, 5B), -11.9 (d, *J* = 139 Hz, 5B), 5.7 (s, 1B). Anal. Calcd. for $C_{40}H_{68}B_{11}N_3O_3$: C, 63.39; H, 9.04; N, 5.54. Found: C, 63.73; H, 9.14; N, 5.87.



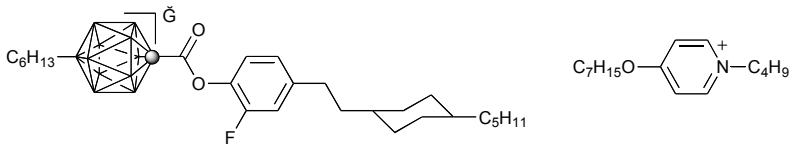
2e[Pyr]:

Recrystallized from an EtOH providing the pure salt as orange crystals: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 10H), 0.52-0.61 (m, 2H), 0.86 (t, *J* = 7.3 Hz, 3H), 0.88 (t, *J* = 7.2 Hz, 3H), 0.91 (t, *J* = 7.0 Hz, 3H), 0.96 (t, *J* = 7.4 Hz, 3H), 1.19-1.27 (m, 6H), 1.28-1.34 (m,

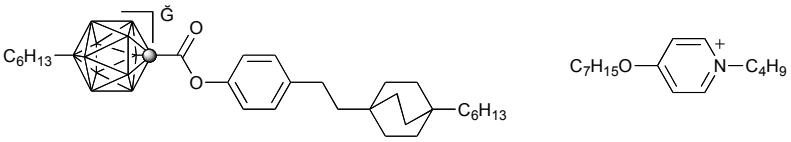
4H), 1.35-1.45 (m, 6H), 1.46-1.55 (m, 4H), 1.82 (quint, J = 7.1 Hz, 4H), 1.90 (quint, J = 7.0 Hz, 4H), 1.99-2.09 (m, 2H), 4.12 (t, J = 6.5 Hz, 2H), 4.47 (t, J = 6.5 Hz, 2H), 4.65 (t, J = 7.4 Hz, 2H), 7.10 (d, J = 9.0 Hz, 2H), 7.19 (d, J = 8.8 Hz, 2H), 7.69 (d, J = 7.5 Hz, 2H), 7.90 (d, J = 8.8 Hz, 2H), 7.91 (d, J = 9.0 Hz, 2H), 8.93 (d, J = 7.5 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -14.0 (d, J = 154 Hz, 5B), -11.9 (d, J = 138 Hz, 5B), 5.0 (s, 1B). Anal. Calcd. for $C_{42}H_{72}B_{11}N_3O_4$: C, 62.90; H, 9.05; N, 5.24. Found: C, 63.13; H, 9.03; N, 5.18.

After a solution of **2e[Pyr]** in acetone-d_6 was exposed to intense fluorescent tube light for 1 hr, ^{1}H NMR spectrum showed new distinct signals ascribed to the *cis* isomer: 6.96 (d, J = 8.8 Hz, 2H), 6.84-6.88 (m, 6H), 3.96 (t, J = 6.5 Hz, 2H), 1.73 (quint, J = 7.1 Hz, 4H).

2f[Pyr]:

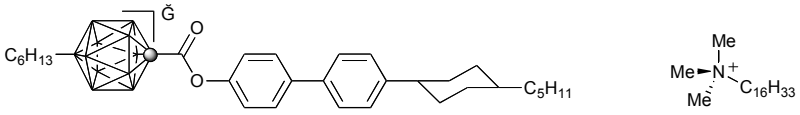


Recrystallized from MeOH/H_2O mixtures (4x) providing the pure salt as white crystals: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 10H), 0.52-0.58 (m, 2H), 0.85 (t, J = 7.2 Hz, 3H), 0.86 (t, J = 6.9 Hz, 3H), 0.87 (t, J = 7.0 Hz, 3H), 0.98-0.99 (m, 4H), 0.95 (t, J = 7.4 Hz, 3H), 1.12-1.52 (m, 30H), 1.74 (br d, J = 11.1 Hz, 2H), 1.80 (br d, J = 11.8 Hz, 2H), 1.89 (quint, J = 7.1 Hz, 2H), 1.98-2.08 (m, 2H), 2.61 (t, J = 8.1 Hz, 2H), 4.47 (t, J = 6.5 Hz, 2H), 4.65 (t, J = 7.4 Hz, 2H), 6.94 (t, J = 7.8 Hz, 1H), 6.98 (dd, J_1 = 10.4 Hz, J_2 = 1.8 Hz, 1H), 7.02 (dd, J_1 = 11.4 Hz, J_2 = 1.6 Hz, 1H), 7.68 (d, J = 7.5 Hz, 2H), 8.93 (d, J = 7.5 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -14.0 (d, J = 157 Hz, 5B), -11.9 (d, J = 141 Hz, 5B), 5.4 (s, 1B). Anal. Calcd. for $C_{43}H_{79}B_{11}FNO_3$: C, 64.88; H, 10.00; N, 1.76. Found: C, 65.06; H, 10.05; N, 1.82.



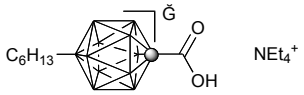
2g[Pyr]:

Recrystallized from EtOH/H_2O mixtures (2x) and MeOH/H_2O mixtures (2x) providing the pure salt as white flakes: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 10H), 0.52-0.58 (m, 2H), 0.85 (t, J = 7.2 Hz, 3H), 0.87 (t, J = 7.1 Hz, 3H), 0.88 (t, J = 6.9 Hz, 3H), 0.95 (t, J = 7.4 Hz, 3H), 1.04-1.08 (m, 2H), 1.16-1.46 (m, 38H), 1.49 (quint, J = 7.3 Hz, 2H), 1.89 (quint, J = 7.1 Hz, 2H), 1.99-2.06 (m, 2H), 2.45-2.50 (m, 2H), 4.47 (t, J = 6.5 Hz, 2H), 4.64 (t, J = 7.5 Hz, 2H), 6.85 (d, J = 8.5 Hz, 2H), 7.14 (d, J = 8.5 Hz, 2H), 7.68 (d, J = 7.4 Hz, 2H), 8.92 (d, J = 7.4 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -14.1 (d, J = 154 Hz, 5B), -12.0 (d, J = 137 Hz, 5B), 5.1 (s, 1B). Anal. Calcd. for $C_{46}H_{84}B_{11}NO_3$: C, 67.53; H, 10.35; N, 1.71. Found: C, 67.76; H, 10.44; N, 1.88.



2h[Cetyl]:

Recrystallized from MeOH (1x) and EtOH (2x) providing the pure salt as a white powder: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.40-2.50 (m, 10H), 0.50-0.60 (m, 2H), 0.83-0.91 (m, 9H), 1.03-1.14 (m, 3H), 1.15-1.45 (m, 44H), 1.46-1.57 (m, 2H), 1.85-2.01 (m, 4H), 2.52 (br t, J = 12.2 Hz, 1H), 3.34-3.37 (m, 9H), 3.53-3.60 (m, 2H), 7.05 (d, J = 8.6 Hz, 2H), 7.30 (d, J = 8.2 Hz, 2H), 7.54 (d, J = 8.2 Hz, 2H), 7.61 (d, J = 8.5 Hz, 2H); ^{11}B NMR (128 MHz, acetone-d_6) δ -14.0 (d, J = 158 Hz, 5B), -11.9 (d, J = 138 Hz, 5B), 5.0 (s, 1B). Anal. Calcd. for $C_{50}H_{94}B_{11}NO_2$: C, 69.81; H, 11.01; N, 1.63. Found: C, 70.00; H, 10.82; N, 1.73.

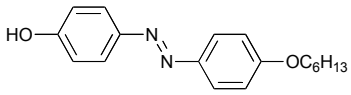


Preparation of [*closo*-1-$CB_{11}H_{10}$-1-COOH-12-C_6H_{13}]$^-$ [NEt_4]$^+$ (4[NEt_4]).

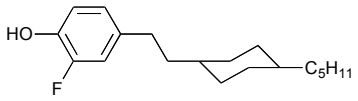
A solution of anhydrous $ZnCl_2$ (5.84 g, 42.8 mmol) in anhydrous THF (30 mL) under Ar was treated with $C_6H_{13}MgBr$ (21.5 mL, 40.8 mmol, 1.9 M in Et_2O) at 0 ^oC forming a white, thick slurry which was stirred for 15 min. Anhydrous NMP (15 mL), $Pd_2(dba)_3$ (0.062 g, 2 mol %), and $[HPCy_3]^+$ $[BF_4]^-$ (0.100 g, 8 mol %) were added and the reaction mixture turned dark green but slowly faded to red/orange. After 5 mins, [*closo*-1-$CB_{11}H_{10}$-1-COOH-12-I]$^-$ $[NEt_4]^+$ (**6[NEt_4]**, 1.50 g, 3.40 mmol) was added, and the reaction mixture was refluxed at 90 °C for 24 hr. ^{11}B NMR of a small aliquot (quenched in sat. $[NH_4]^+Cl^-$ and extracted into ether) showed complete conversion to product. Sat. $[NH_4]^+$ Cl^- (50 mL) was added, excess THF was removed, and the remaining aqueous layer was extracted with Et_2O (3 x 20 mL). The organic layers were combined, dried (Na_2SO_4), and removed giving a black sludge. Excess NMP and 1-hexanol were removed under vacuum (60 °C, 0.5 mm Hg) and the residue was separated by column chromatography (SiO_2, CH_3CN/CH_2Cl_2, 1:9).

The crude acid extract was re-dissolved in 10 % HCl (50 mL) and extracted with Et_2O (3 x 20 mL). The organic layers were combined, and water (10 mL) was added. The Et_2O was removed *in vacuo*, and the aqueous layer was filtered. $[NEt_4]^+$ Br^- (0.790 g, 3.73 mmol) was added to the filtrate, and the resulting precipitate formed was filtered, washed (H_2O), and dried *in vacuo* giving 0.830 g (61% yield) of **4[NEt_4]** as a light yellow crystalline solid. Further purification was achieved by recrystallization from aqueous CH_3OH: mp 122-124 ^oC; ^1H NMR (400 MHz, CD_3CN) δ 0.40-2.50 (m, 10H), 0.46 (br t, J = 8.9 Hz, 2H), 0.85 (t, J = 7.0 Hz, 3H), 1.20 (tt, J_1 = 7.3 Hz, J_2 = 1.9 Hz, 12H), 1.07-1.29 (m, 8H), 3.15 (q, J = 7.3 Hz, 8H), 8.81 (br s, 1H); ^{11}B NMR (128 MHz, CD_3CN) δ -14.3 (d, J = 155 Hz, 5H), -12.2 (d, J = 137 Hz, 5B), 4.6

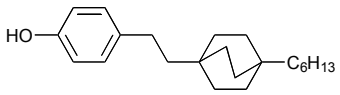
(s, 1H). Anal. Calcd. for $C_{16}H_{44}B_{11}NO_2$: C, 47.87; H, 11.05; N, 3.49. Found: C, 48.38; H, 11.25; N, 3.55.



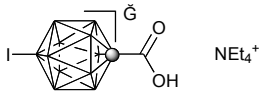
4-(4-Hexyloxyphenylazo)phenol (5e).[6] Mp 105-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.92 (t, J = 7.0 Hz, 3H), 1.32-1.39 (m, 4H), 1.45-1.54 (m, 2H), 1.82 (quint, J = 7.0 Hz, 2H), 4.04 (t, J = 6.6 Hz, 2H), 5.1 (s, 1H), 6.93 (d, J = 8.8, Hz, 2H), 6.99 (d, J = 8.9 Hz, 2H), 7.83 (d, J = 8.8 Hz, 2H), 7.85 (d, J = 9.0 Hz, 2H).



2-Fluoro-4-(2-(4-pentylcycloxexyl)ethyl)phenol (5f). Mp 72-73 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, J = 7.2 Hz, 3H), 0.82-0.99 (m, 4H), 1.12-1.35 (m, 10H), 1.42-1.49 (m, 2H), 1.75 (br t, J = 11.5 Hz, 4H), 2.54 (t, J = 8.1 Hz, 2H), 4.88 (d, J = 3.8 Hz, 1H), 6.82 (dd, J_1 = 8.3 Hz, J_2 = 1.8 Hz, 1H), 6.86 (t, J = 11.4 Hz, 1H), 6.89 (dd, J_1 = 11.9 Hz, J_2 = 1.9 Hz, 1H). Anal. Calcd. for $C_{19}H_{29}FO$: C, 78.04; H, 10.00. Found: C, 78.33; H, 9.89.



4-(2-(4-Hexylbicyco[2.2.2]-1-octyl)ethyl)phenol (5g). Mp 103-104 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, J = 6.8 Hz, 3H), 1.04-1.08 (m, 2H), 1.15-1.45 (m, 22H), 2.40-2.46 (m, 2H), 4.49 (s, 1H), 6.72 (d, J = 8.3 Hz, 2H), 7.02 (d, J = 8.3 Hz, 2H). Anal. Calcd. for $C_{22}H_{34}O$: C, 84.02; H, 10.90. Found: C, 83.48; H, 9.96.



Preparation of [*closo*-1-$CB_{11}H_{10}$-1-COOH-12-I]$^-$ [NEt_4]$^+$ (6[NEt_4]).

A solution of dried [*closo*-1-$CB_{11}H_{11}$-12-I]$^-$ Cs^+ (**7[Cs]**, 1.67 g, 4.15 mmol) in anhydrous THF (20 mL) in a three-necked flask at –78 °C under Ar was treated with freshly distilled TMEDA (0.80 mL, 5.90 mmol) followed by dropwise addition of *n*-BuLi (2.90 mL, 5.80 mmol) over 30 min. The reaction mixture was slowly warmed to 0 °C (addition of THF may be necessary) and stirred for 1.5 hr. Dry CO_2 gas was bubbled through the solution for 40 mins, and the mixture became significantly more homogeneous. Water (30 mL) was added, and the volatiles evaporated. Insoluble material was removed by filtration, the filtrate washed with Et_2O (3 x 20 mL); the Et_2O layers were evaporated leaving a yellowish oil. The aqueous layer was acidified with 10 % HCl, extracted with Et_2O (3 x 20 mL), and the organics layers combined. Water (25 mL) was added, and the Et_2O removed. The aqueous layer was filtered, and [NEt_4]$^+$ Br^- (1.10 g, 5.23 mmol) was added producing a white precipitate. The solid was collected by filtration, washed with water, and dried giving typically 1.20–138 g (65-75% yield) of **6[NEt_4]** as a white crystalline solid. An analytical sample of **6[NEt_4]** was prepared by recrystallization from water containing with a few drops of EtOH: ^{1}H NMR (400 MHz, acetone-d_6) δ 0.50-2.50 (m, 10H), 1.40 (tt, J_1 = 7.3 Hz, J_2 =1.9 Hz, 12H), 3.50 (q, J = 7.3 Hz, 8H), COOH was not observed; ^{11}B NMR (128 MHz, acetone-d_6) δ -16.2 (s, 1B), -13.5 (d, J = 155 Hz, 5B), -11.3 (d, J = 146 Hz, 5B). Anal. Calcd. for $C_{10}H_{31}B_{11}INO_2$: C, 27.10; H, 7.05; N, 3.16. Found: C, 27.02; H, 7.18; N, 3.18.

A similar result was obtained using [*closo*-1-$CB_{11}H_{11}$-12-I]$^-$ [$NHMe_3$]$^+$ (**7[$NHMe_3$]**) and doubled amounts of BuLi. Thus, *n*-BuLi (3.35 mL, 7.50 mmol) was added slowly to a stirred

solution of [*closo*-1-$CB_{11}H_{11}$-12-I]$^-$[$NHMe_3$]$^+$ (0.824 g, 2.51 mmol, dried over P_2O_5) in THF (5 mL) and TMEDA (0.57 mL) at –78 ºC under N_2. The reaction mixture was stirred for 40 min, the temperature was slowly raised to 0 ºC, and CO_2 (g) was bubbled through for 30 min before quenching the reaction with methanol (10 mL). Volatiles were removed *in vacuo*. The resulting yellowish oil was dissolved in H_2O (25 ml), and the solution was washed with Et_2O (3 x 15 mL). The aqueous was checked to ensure basicity, then half the required [NEt_4]$^+$Br$^-$ (0.29 g, 1.38 mmol) was added and the solution filtered. The other half of [NEt_4]$^+$Br$^-$ (0.29 g, 1.38 mmol) was added and the solution was acidified with 20% HCl (10 mL). The precipitate was filtered to provide a white crystalline solid, 0.746 g (90 %), which was recrystallized from hot H_2O (20 ml) with a few drops of EtOH, to yield 0.623 g (75%) of carboxylic acid **6[NEt_4]**.

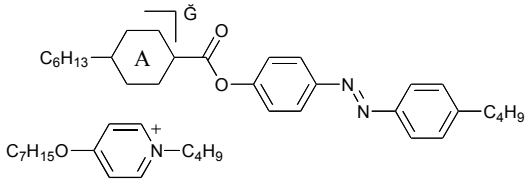
Preparation of [*closo*-1-$CB_{11}H_{11}$-12-I]$^-$ [$NHMe_3$]$^+$ (7[$NHMe_3$])

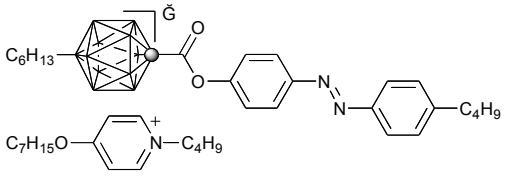
Following the literature procedure,[8] [*closo*-1-$CB_{11}H_{12}$]$^-$$Cs^+$ (2.85, 10.3 mmol), prepared from [*closo*-1-$CB_{11}H_{11}$-1-NMe_3],[9] was extracted to Et_2O (3 x 20 mL) from 10 % HCl (100 mL). The ether was evaporated, and the free acid residue was dissolved in glacial acetic acid (35 mL) and treated with molecular I_2 (5.1 g, 20 mmol). The reaction was stirred at rt 45-50 ^{o}C for 3-4 days, and the reaction progress was monitored by ^{11}B NMR. Most of the acetic acid was removed *in vacuo*, solid Na_2SO_3 (1.0 g, 7.9 mmol) was added, followed by 10 % HCl (50 mL). The product was extracted to Et_2O (3 x 20 mL), organic layers were combined, and solvent evaporated in the presence of H_2O (30 mL). The aqueous layer was filtered, and the filtrate treated with [$NHMe_3$]$^+$Cl$^-$ (2.5 g, 11.9 mmol) to precipitate a white solid that was filtered and dried. Recrystallization from hot aqueous EtOH gave 3.10 g (75% yield) of pure **7[$NHMe_3$]**. ^{11}B NMR data was consistent with the literature.[8]

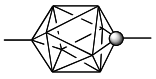
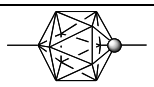
2. Transition temperatures for binary mixtures

Table S1. Transition temperatures for binary mixtures of **d[Pyr]** in **2e[Pyr]**.

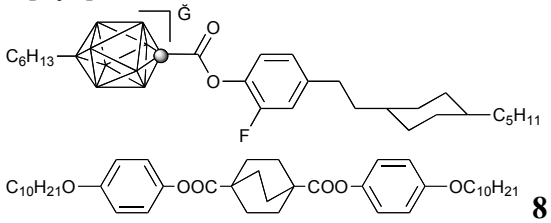
additive: **d[Pyr]** host: **2e[Pyr]**



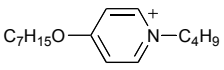


A	Mol fraction x in **2e[Pyr]**	T_{NI} peak /°C	T_{SN} peak /°C	Extrapolation to pure y = a+ x •T_{NI}
 **1d[Pyr]**	0.000 0.0927 0.1998 0.2980	144.3 141.4 138.1 134.1	132.9 129.7 126.2 122.2	y = 144.5-33.8•T_{NI} R^2 = 0.997 y = 133.0-35.5•T_{SN} R^2 = 0.997
 **2d[Pyr]**	0.0000 0.0994 0.2000 0.2972	144.3 142.6 139.8 137.9	132.85 129.7 125.0 122.30	y = 144.5-22.2•T_{NI} R^2 = 0.992 y = 132.9-36.6•T_{SN} R^2 = 0.992

1f[Pyr] in diester **8**: 9.7 mol%



8



1f[Pyr]

Pure components: SmA-I (peak):

Host (**8**):	175.3 °C
Additive (**1f[pyr]**):	150.4 °C
Mixture:	175.1 °C

3. Powder XRD raw data

Table S2. X-ray Diffraction Data.

1e[Pyr]		**1f[Pyr]**		**2f[Pyr]**		**1g[Pyr]**		**2g[Pyr]**	
T /°C	d_{001}/Å	T /°C	d_{001}/Å	T /°C	d_{001}/Å	T /°C	d_{001}/Å	T /°C	d_{001}/Å
129.0	27.659	141.0	24.457	140.0	24.340	162.0	26.337	177.0	26.412
128.0	27.692	140.0	24.459	139.0	24.343	160.0	26.335	176.0	26.420
127.0	27.728	139.0	24.461	138.0	24.345	158.0	26.332	175.0	26.433
126.0	27.762	138.0	24.464	137.0	24.344	156.0	26.331	174.0	26.444
125.0	27.799	137.0	24.467	136.0	24.347	154.0	26.328	173.0	26.453
124.0	27.833	136.0	24.470	135.0	24.350	152.0	26.323	172.0	26.465
123.0	27.866	135.0	24.472	134.0	24.352	150.0	26.320	171.0	26.481
122.0	27.898	134.0	24.475	133.0	24.352	148.0	26.319	170.0	26.499
121.0	27.929	133.0	24.478	132.0	24.355	146.0	26.314	169.0	26.507
120.0	27.961	132.0	24.480	131.0	24.358	144.0	26.310	168.0	26.517
119.0	27.991	131.0	24.482	130.0	24.358	142.0	26.306	167.0	26.527
118.0	28.029	130.0	24.484	129.0	24.359	140.0	26.301	166.0	26.530
117.0	28.064	129.0	24.486	128.0	24.362	138.0	26.300	165.0	26.541
116.0	28.099	128.0	24.489	127.0	24.365	136.0	26.296	164.0	26.543
115.0	28.140	127.0	24.491	126.0	24.364			163.0	26.547
		126.0	24.493	125.0	24.365			162.0	26.559
				124.0	24.369				
				123.0	24.370				
				122.0	24.369				
				121.0	24.372				
				120.0	24.375				
$\kappa = -3.38 \pm 0.02$ pm K^{-1}		$\kappa = -0.25 \pm 0.004$ pm K^{-1}		$\kappa = -0.17 \pm 0.005$ pm K^{-1}		$\kappa = +0.16 \pm 0.005$ pm K^{-1}		$\kappa = -1.02 \pm 0.04$ pm K^{-1}	

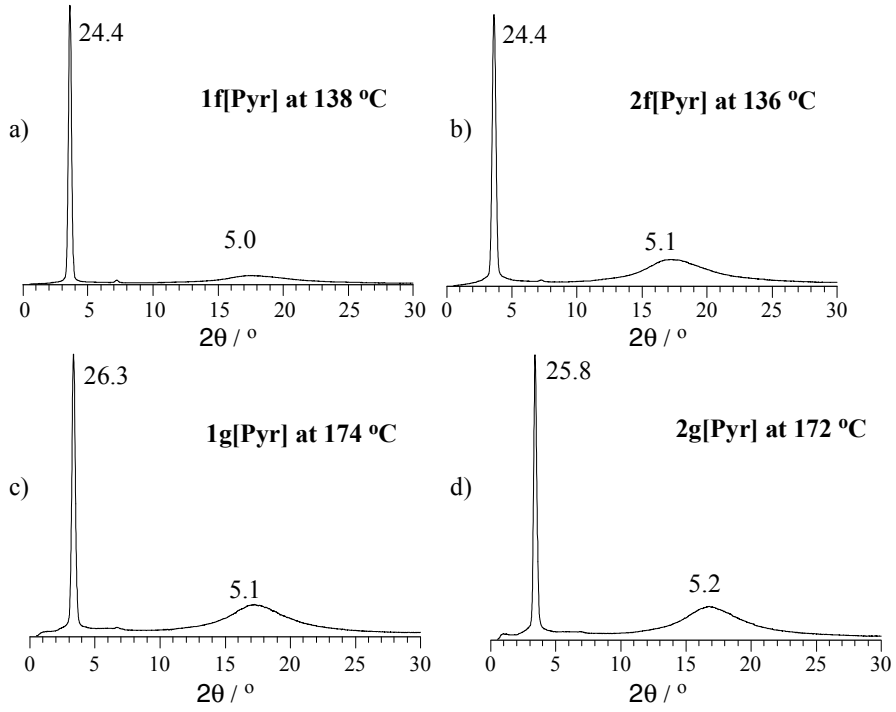
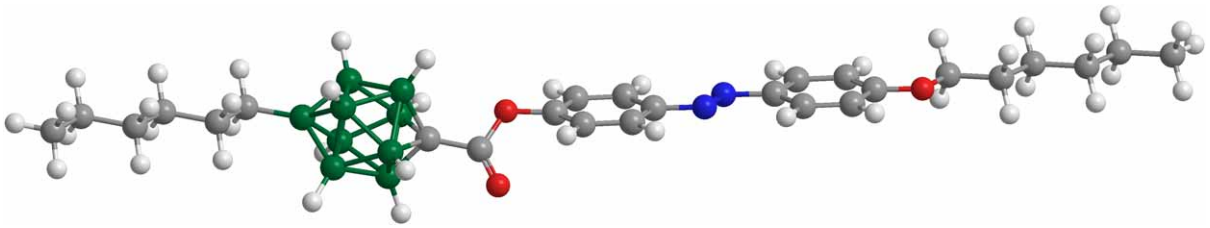


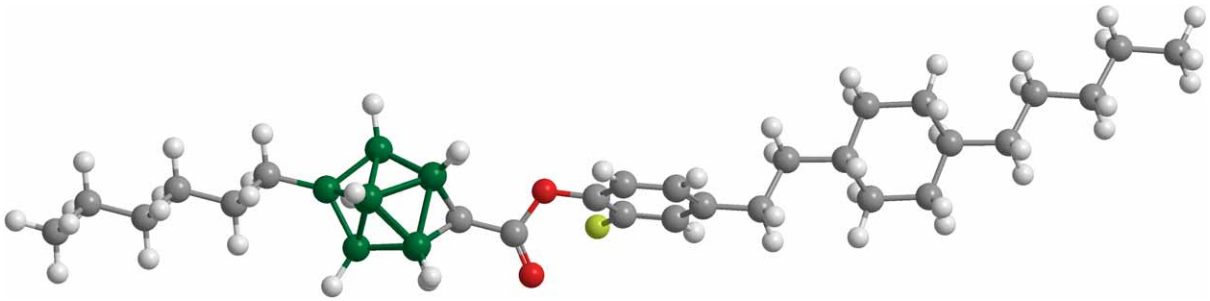
Figure S1. X-ray diffraction patterns for a) **1f[Pyr]** (138 °C, SmA, *c* = 24.4 Å); b) **2f[Pyr]** (136 °C, SmA, *c* = 24.4 Å); c) **1g[Pyr]** (174 °C, SmA, *c* = 26.3 Å); and d) **2g[Pyr]** (172 °C, SmA, *c* = 25.8 Å).

4. Computational details and molecular modeling

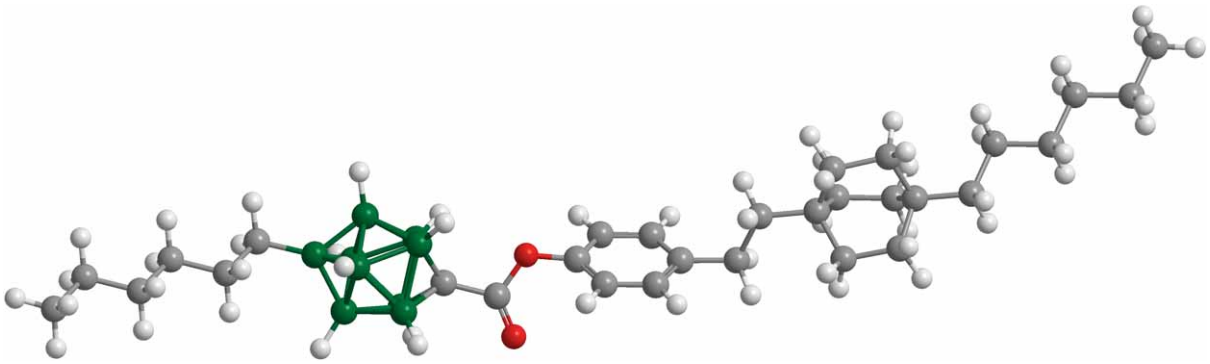
Geometry optimization for **1e**–**1h**, and **2e**–**2h** was undertaken without symmetry constraints and default convergence limits with the HF/6-31G(d) method using the Gaussian 09 computational package.[10] The optimized geometries of the models were perturbed several times to assure conformational minimum and the fully optimized structures are shown in Figure S2.



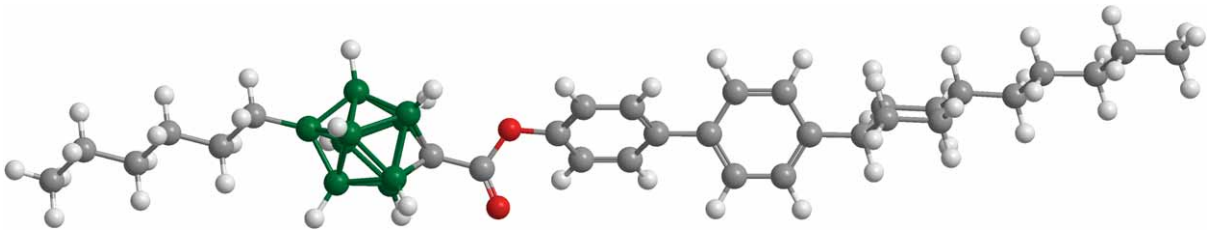
1e



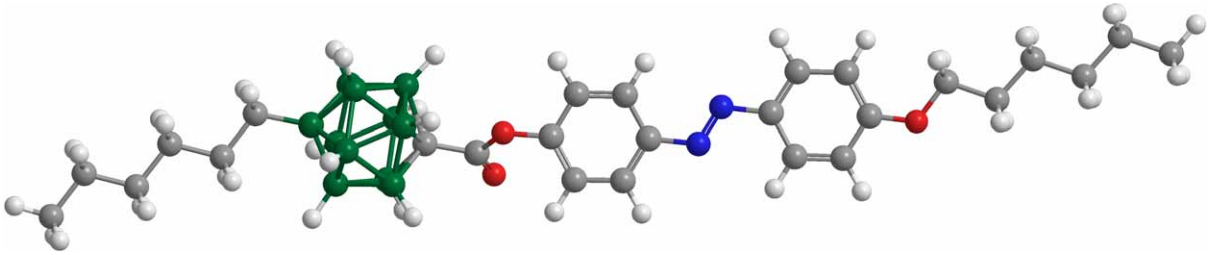
1f



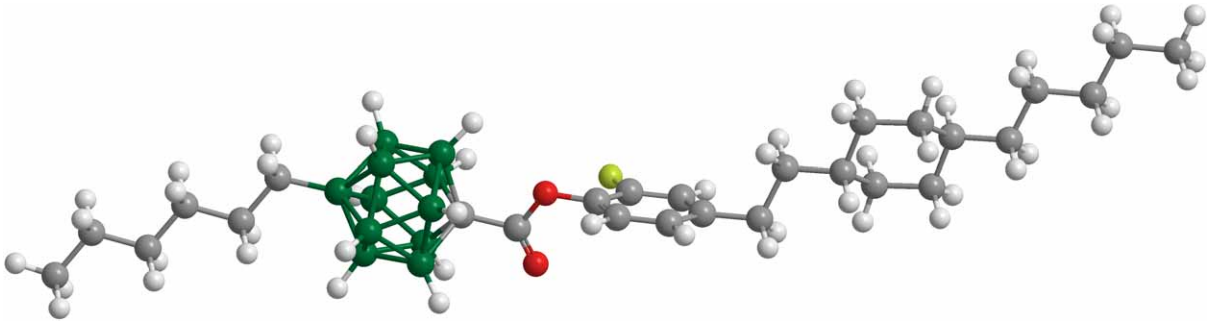
1g



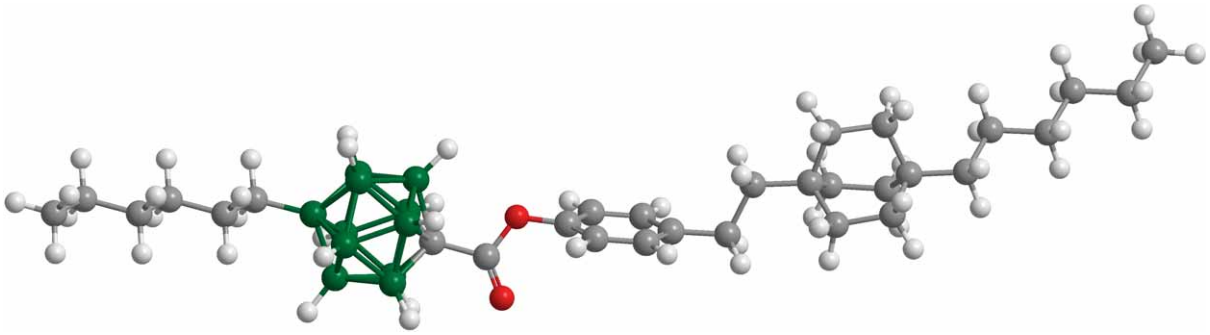
1h



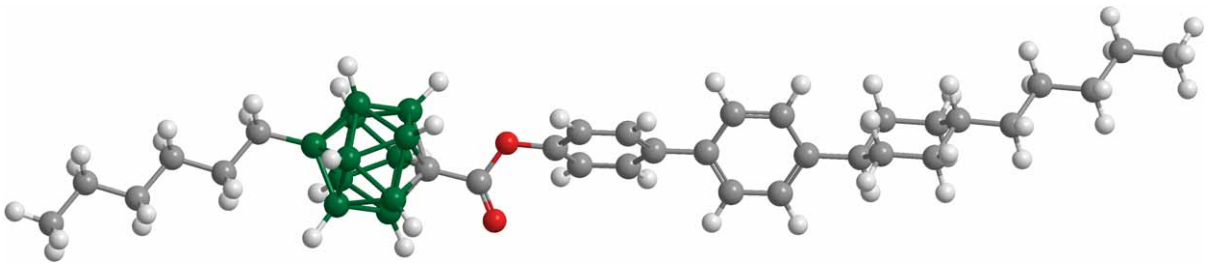
2e



2f



2g



2h

Figure S2. Molecular structures of selected anions obtained by full geometry optimization at the HF/6-31G(d) level of theory.

Table S3. Molecular dimensions for selected anions.

anion	length L [a] /Å	Interchain angle [b] /°
1e	34.0	11
1f	31.8	28
1g	32.7	26
1h	33.8	25
2e	33.8	9
2f	31.8	4
2g	32.4	31
2h	33.8	24
Pyr	18.9	88
Cetyl	23.4	–

[a] H···H distance measured for most extended molecular conformation optimized at the HF/6-31G(d) level of theory. [b] Angle between planes of terminal alkyl chains in all-trans conformation. First three carbon atoms from the core of each chain were used for the measurement.

5. Archive for HF/6-31G(d) computational results

1e

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1f

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1g

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\H,1.3722945479,-1.8026010456,-1.7659769642\H,1.8552023565,7.886128191
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,8.6838827835,3.2843675994\H,-0.706845248,8.3777534048,3.8647084351\C,
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,2.1820328384,-4.9221523879,-0.4529070462\C,2.1580479751,-6.4483922726
,-0.5778189003\C,3.297515683,-7.0117939449,-1.4299219624\C,3.273612784
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718,-1.9873483882\H,4.3720949986,-10.1733410204,-2.4782184954\H,3.3192
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4\H,0.37030633,12.9674569064,9.8871969567\H,1.6606067943,13.7448007289
,7.9177952488\H,0.1879374907,14.1055625945,7.0668849346\O,1.0392804141
,3.0159465078,0.1630075481\H,-1.448680328,17.9225163931,13.1030156316\
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1h

1\1\GINC-OCTOPUS\FOpt\RHF\6-31G(d)\C31H50B9O2(1-)\PIOTR\07-Apr-2011\0\
\#P HF/6-31G* FOpt geom(noangle,nodistance) fcheck\\C6-CB9-COO-PhPhChx
-C5, restart\\-1,1\B,-6.311957769,-1.7696262197,0.3567984607\B,-5.7819
960718,-1.0477557654,-1.2811769791\B,-5.7664476889,0.6396458264,-0.531
0667611\B,-6.2933548088,-0.0825620529,1.1054395482\B,-7.8675622559,-0.
8868278193,0.6780474585\B,-7.50119878,-1.578513029,-1.0070132117\B,-7.
1238897434,0.1280781463,-1.6267153849\B,-7.4776564171,0.8162708415,0.0
580611455\B,-8.5465102252,-0.2469497877,-0.7545482381\C,-5.148648132,-
0.67935577,0.1480526261\C,-3.7428486958,-0.8759467834,0.5580953246\O,-
2.8853385598,-0.4654538199,-0.4030345711\C,-1.5323484644,-0.5343315036
,-0.2144072814\C,-0.8097021445,0.6334899908,-0.3628174841\C,0.57073440
92,0.6063295458,-0.2636716557\C,1.2494314244,-0.581669677,-0.013626646
9\C,2.7347721017,-0.6102117827,0.0973027893\C,3.3697753812,-1.32080843
23,1.1096290823\C,4.751715942,-1.345380684,1.208228466\C,5.5561626243,
-0.661663464,0.3063733033\C,0.4968667588,-1.7457513497,0.1298514532\C,
-0.8814285984,-1.7313435279,0.0289312386\H,-6.0327660124,-2.8167386648
,0.8377733811\H,-5.0847651181,-1.5167988989,-2.118318968\H,-5.05478334
39,1.5635755533,-0.7497946935\C,9.8898386433,-0.0302127128,-0.34983289
51\H,-6.0014641173,0.2577660855,2.202684322\H,9.4445738051,0.058221055
,1.754007132\H,9.5813288412,1.6298556591,1.0119670949\H,7.4334521249,1
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.7508594838,-1.3525432201,-0.7805611921\H,7.3013648382,-1.3180650768,1
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H,7.3536504834,-2.3526528827,-0.9283121291\H,7.5096598863,-0.788923944
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\C,13.683612339,1.0142753836,-0.0839638292\H,-7.8548596728,1.892044324

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1897,-0.0242463,-1.1723081183\C,-11.0120523786,-1.21789885,-0.91283332
02\C,-12.4660932854,-0.9644650802,-1.3215729083\C,-13.3920181544,-2.15
51316749,-1.0630318267\C,-14.844881783,-1.902055483,-1.4711321417\C,-1
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65469\H,11.8963377274,1.7969566414,-0.9877183477\H,11.8540103,1.755816
4214,0.7525744574\H,11.6333388479,-0.7213358423,0.7090747851\H,11.8052
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38104,-0.7062742132\C,3.5406263231,0.0752051801,-0.8100319205\H,3.0829
328184,0.6180197657,-1.6176527723\H,5.5007693117,0.5903236155,-1.43328
66232\H,5.2073469846,-1.9017990332,2.0095720487\H,2.7796226559,-1.8441
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2e

1\1\GINC-OCTOPUS\FOpt\RHF\6-31G(d)\C26H44B11N2O3(1-)\PIOTR\10-Mar-2011
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8,0.1608686126\C,-1.2000127433,0.5207373255,0.1955429198\C,-0.63137582
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,1.7099444656\C,1.5509293414,0.7590592611,0.0997253375\C,0.9653207252,
-0.502899092,0.144639711\B,-5.3158049537,-0.0677022652,-0.6635836024\C
,-0.4079672363,-0.6181495731,0.1929989091\B,-5.758655213,1.5652125611,
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64385728,2.6273265252,-0.1253282777\H,7.8610522341,-1.6181846738,-0.07
49394777\H,5.4182632774,-1.8266328804,0.0112979525\H,1.5846672173,-1.3
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2f

1\1\GINC-OCTOPUS\FOpt\RHF\6-31G(d)\C27H51B11F1O2(1-)\PIOTR\09-Mar-2011
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3.8840885288\C,-0.7570038188,1.0669621253,-8.5266266445\C,0.2264536363

,0.7167630275,-9.6502711492\C,-0.3393292938,0.9622704559,-11.052112596
9\C,0.6385339588,0.6140617632,-12.1765361527\C,0.0738649356,0.85926241
75,-13.5773941499\C,1.0579064073,0.508491438,-14.693751667\H,1.9668851
236,1.098752084,-14.6137290387\H,1.3430059232,-0.5392661818,-14.649009
1559\H,0.6291167028,0.6929494522,-15.6753432919\H,-0.8371210883,0.2775
939475,-13.7054949149\H,-0.2177388756,1.9037295235,-13.6704914593\H,1.
5512772748,1.1952443745,-12.0526346919\H,0.9319395688,-0.4310648955,-1
2.0876636537\H,-1.2520416856,0.3805964772,-11.1789641638\H,-0.63238210
74,2.0077877649,-11.1439888957\H,1.1394533843,1.2961162256,-9.53012353
78\H,0.521633683,-0.3269798442,-9.5651179328\H,-1.6699189318,0.4894075
609,-8.6763752633\H,-1.0526242565,2.110437607,-8.6413514651\C,-1.71013
38436,0.1918897687,15.3751386636\H,-0.2729298868,-2.0445429879,-0.3831
630121\H,0.1358157671,-2.4945454895,2.0098757564\C,1.2018999346,-0.814
3907522,3.8812565773\C,0.014861469,-0.3574243891,4.7439027625\H,1.7631
378592,1.438769986,2.4141528678\F,1.3922477462,2.057618398,-0.02486856
72\H,-1.5289479044,-0.8585065775,15.5857770815\H,-0.8444811635,0.75067
32972,15.7199880537\H,-2.5637385532,0.505491066,15.9685995016\H,-2.167
69423,1.4739357719,13.7113003606\H,-2.8475026375,-0.12283134,13.578405
6892\H,-0.5669180503,-1.0628152989,13.1836700094\H,0.1154548806,0.5333
823931,13.3205321846\H,-1.2110605546,1.2775000277,11.3419008183\H,-1.9
140197006,-0.310685991,11.2174197348\H,0.3295060924,-1.2915708938,10.7
79310423\H,1.069897519,0.2634323596,11.0278333202\O,2.34667181,0.00253
01176,-2.1923694398\H,-0.158416624,1.1593934684,9.0512006183\\Version=
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06\Dipole=-0.6418843,-1.1540866,11.0485861\Quadrupole=39.6489264,48.60
71458,-88.2560722,2.0686832,3.0913731,8.6210044\PG=C01 [X(C27H51B11F1O
2)]\\@

2g

1\1\GINC-OCTOPUS\FOpt\RHF\6-31G(d)\C30H56B11O2(1-)\PIOTR\09-Mar-2011\0
\\#P HF/6-31G* FOpt geom(noangle,nodistance) fcheck\\C6-CB11-COO-Ph-CH
2CH2-BCO-C6\\-1,1\B,5.6992790125,-0.701314944,-1.3162084486\B,6.155063
9671,-2.1816317596,-0.4088793472\B,5.2780209803,0.5738936178,-0.131696
1966\B,5.9991837787,-1.8266759433,1.3340990583\B,5.4503827149,-0.12402
40791,1.5052578845\B,8.0699547966,-0.1065588174,0.2516590588\C,4.95196
10172,-1.0958933032,0.179135484\C,3.5380939906,-1.6056634652,0.1558429
468\B,7.1604907956,-0.5492280856,1.7484041389\O,2.6409675509,-0.606081
1524,0.111911898\C,1.2982279344,-0.8920388648,0.1116898423\B,7.6002164
441,-1.8192316539,0.5587001878\C,0.6880588676,-1.4562401843,-0.9927262
815\C,-0.6799007307,-1.6596300125,-0.9804620247\B,6.7179144415,0.93209
2569,0.8391496337\C,-1.4570933132,-1.3028794242,0.1168828453\C,-0.8171
219533,-0.735920765,1.2109473591\B,7.4114689883,-1.1278513955,-1.08641
40506\C,0.5530471584,-0.5293198805,1.2145940655\B,6.8723361215,0.57581
50952,-0.9120800225\H,7.1548708146,1.4170299734,-1.7065561982\C,-7.889
3349708,-0.3314092093,-0.6130410353\H,8.066937781,-1.4947107047,-2.008
4959546\H,-7.7533043159,1.2524224457,-2.087877245\H,-7.5679853228,1.80
00434253,-0.4456906175\H,-5.2962803409,1.791732668,-0.8807394484\H,6.8
981109415,2.0236305917,1.2793862582\H,-5.4822811548,0.8114254486,-2.30
54752111\H,8.3985024432,-2.6682148003,0.8038061229\C,-5.7648945607,-1.
5917865985,-1.2252068478\C,-5.8580596983,-0.3157455447,0.9089391938\C,
-7.3892666556,-0.5345030297,0.8300300995\H,7.6528885711,-0.5018268457,
2.8315268968\H,-7.8938612745,0.1429301091,1.5107556176\H,4.6519186418,
0.1428264138,2.340329192\H,-7.6449923502,-1.54117895,1.1531051157\H,-5
.4101629173,-1.0751574443,1.5403960766\H,5.5498633237,-2.6484280942,2.
0568999368\H,-5.6361996187,0.6411787538,1.3753679957\C,-7.2863560399,-
1.4615865037,-1.4718149006\H,4.3817070101,1.3063834409,-0.3639224125\H
,-7.786009979,-2.4005837592,-1.2486786265\H,-7.4848459014,-1.251085515
2,-2.5200916573\H,-5.2386607441,-1.727922215,-2.1663467427\H,5.8121147
062,-3.2340490487,-0.8213990826\H,-5.5599442424,-2.4745555526,-0.62740
91581\C,-5.2357420272,-0.3404079533,-0.5002908344\H,5.0584893817,-0.80
62808847,-2.3092031014\H,-3.339090446,-0.1116671697,-1.4804095964\H,-3
.401114352,0.6006272407,0.1014900501\H,-3.1958351661,-2.3815113707,-0.
4817315734\H,-3.2973792005,-1.7022758952,1.1163304247\C,-5.7699836922,
0.8908548591,-1.2601619588\C,-7.3076089963,0.9975476584,-1.1294322803\

C,-9.4238962595,-0.3873746843,-0.7172982569\C,-10.216484993,0.7535622235,-0.0698849443\C,-11.7292050323,0.5556063042,-0.1996075422\C,-12.5435549535,1.6893781271,0.4260879613\C,9.6027467443,0.4094075559,0.3350558281\C,10.5303251312,-0.0299282994,-0.8047152493\C,11.9628607212,0.4915729351,-0.6583913072\C,12.8917963994,0.0560904623,-1.793833063\C,14.3232823864,0.5766504988,-1.6481063834\C,15.2435142478,0.136457586,-2.7869788431\H,15.3073557206,-0.9470472113,-2.841771941\H,14.8762941398,0.4916531903,-3.7461817133\H,16.2516634794,0.5209511597,-2.655851054\H,14.3079330585,1.6638089727,-1.598296095\H,14.7358870172,0.2355423386,-0.7004747308\H,12.9109349231,-1.0316309994,-1.8461396418\H,12.4829557161,0.3967239836,-2.7441528007\H,11.9463239788,1.5799513723,-0.6073059585\H,12.37468113,0.1509073979,0.2912172823\H,10.5525171601,-1.1163126707,-0.8592869426\H,10.1255088731,0.308887093,-1.756091298\H,9.608182589,1.4989400197,0.3819845026\H,10.0363647354,0.0764720598,1.2787286172\C,-14.0553363966,1.4925872844,0.2987480217\H,1.2817291648,-1.7393254266,-1.841227069\H,-1.14849238,-2.1076858128,-1.840252083\C,-2.9594515199,-1.4997967857,0.1050875202\C,-3.6984802964,-0.2779516259,-0.4669175353\H,-1.391296685,-0.4534878715,2.0771198992\H,1.0492228306,-0.0906434395,2.0604156543\H,-14.3190766348,1.4011704102,-0.7529104263\H,-14.3363385174,0.5509288093,0.7658583044\C,-14.8619524626,2.6292742543,0.9259386534\H,-12.282168635,1.7823627119,1.4790628874\H,-12.2649063966,2.6331628573,-0.0400799356\H,-11.9916792884,0.4642061587,-1.2524494314\H,-12.0104323532,-0.3875200371,0.266164973\H,-9.9632181048,0.8400481186,0.9834650115\H,-9.945799271,1.7006722437,-0.5290752283\H,-9.6899690207,-0.4289752454,-1.7728882924\H,-9.7588053571,-1.3307934941,-0.2879900284\O,3.2167970351,-2.7443963385,0.1767479726\H,-15.929516493,2.4611249586,0.8196962943\H,-14.6460998052,2.7242253723,1.9865069619\H,-14.628731536,3.5808639919,0.4563529216\\Version=EM64L-G09RevA.02\State=1-A\HF=-1590.1270602\RMSD=5.408e-09\RMSF=2.157e-06\Dipole=-12.226751,0.9638562,-0.7214916\Quadrupole=-111.7649077,50.9062721,60.8586357,8.0642436,-5.8930489,2.3524264\PG=C01 [X(C30H56B11O2)]\\@

2h

1\1\GINC-OCTOPUS\FOpt\RHF\6-31G(d)\C31H52B11O2(1-)\PIOTR\10-Mar-2011\0\\#P HF/6-31G* FOpt geom(noangle,nodistance) fcheck\\C6-CB11-COO-PhPhChx-C5\\-1,1\B,-5.7254705242,-1.3499621539,-1.1216009811\B,-5.844081421,0.2374519857,-0.3085330747\B,-6.042899135,-2.6184505803,0.1039405534\B,-6.2505501373,-0.0479218858,1.4187433992\B,-6.3771774148,-1.8127930178,1.6705828934\B,-7.8442874976,-0.8295152575,1.4930513282\B,-8.4544478702,-1.0270045991,-0.1940319036\C,-5.2663750946,-1.1466273652,0.5316969724\C,-3.8155581091,-1.1977507531,0.9195827803\O,-3.0046203547,-1.0314790995,-0.1405522349\C,-1.6439585954,-1.0181996693,0.0222629979\B,-7.5146193911,0.4436539749,0.2701174917\C,-0.9641561822,0.1240254139,-0.3498457675\C,0.4182232217,0.1527232032,-0.2786127275\B,-7.7179061162,-2.4238315608,0.6800474948\C,1.1376633992,-0.9521214734,0.1643821839\C,2.6250317559,-0.9190071318,0.2440196209\C,3.2995756738,-1.4148142843,1.3539287206\C,4.683138731,-1.382879579,1.4231691532\B,-7.1916050156,-0.366039279,-1.2986518742\C,5.4494772667,-0.8539405984,0.3931559684\B,-7.3130415188,-2.1366380248,-1.0447932826\C,0.4256203342,-2.0925184801,0.5315355866\H,-7.6663779066,-2.8763447096,-1.9082887958\C,-0.9539399407,-2.1336758049,0.4610923376\H,-7.4606701568,0.1447110292,-2.3399286036\C,9.7492825229,-0.2457925679,-0.4734016343\H,-8.3519417694,-3.3683998149,1.032333073\H,9.3371221536,0.2160348575,1.5886122819\H,9.4308950692,1.6228405368,0.5631262191\H,7.2566077306,1.0934826329,-0.4541323282\H,-8.0050473129,1.5272348109,0.3324378335\H,7.0918990764,1.1799553178,1.2776546966\C,7.6434277508,-1.6752598017,-0.598704862\H,7.2317270377,-1.2672926532,1.4496655106\H,-8.5598904347,-0.6458922839,2.4246985224\C,9.1694295627,-1.6676917581,-0.464828161\H,9.598549021,-2.2585374225,-1.2681677881\H,-5.9516134392,-2.2893553193,2.6636220196\H,9.4522869485,-2.1591914138,0.4662396824\H,7.2722926226,-2.6949315236,-0.5501868153\H,7.3684817878,-1.2939672275,-1.5797847698\H,-5.7338912698,0.6213945642,2.2469961604\C,6.9656419217,-0.827374863,0.4899521657\C,7.5365273708,0.5999898177,0.47407826\H,-5.395199964,-3.6123201457,0.0909381431\C,9.0614849079,0.6010169268,0.6069438267\C,11.2741875525,-0.215831672

2,-0.296002038\H,-5.0722694789,1.093935436,-0.5834455473\C,12.07912156
41,-0.8547355633,-1.431395611\H,-4.8890848673,-1.5297581355,-1.9358347
439\C,13.5898049058,-0.6840707596,-1.256123162\C,14.4068943616,-1.3254
45468,-2.3791887049\C,-10.0193635762,-0.9761522846,-0.6073959362\C,-11
.0181162601,-0.7498946726,0.5344141329\C,-12.4766115087,-0.7147944151,
0.0685167501\C,-13.4767921632,-0.4890179884,1.204491552\C,-14.93420416
16,-0.4539505879,0.7396416076\C,-15.9256515784,-0.2279344068,1.8813783
809\H,-15.8521250043,-1.0167981911,2.6252487712\H,-15.7338262273,0.715
7945347,2.3850069741\H,-16.9507870356,-0.2079491097,1.5207132097\H,-15
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.2351500118\H,-13.3584343983,-1.2744089391,1.9497367401\H,-13.24098674
7,0.4457741359,1.7112582436\H,-12.5978124012,0.0713555854,-0.676282218
\H,-12.7153974646,-1.6497457048,-0.4377240792\H,-10.9032093503,-1.5332
009589,1.2806861572\H,-10.786047556,0.1835212803,1.0429559013\H,-10.16
35032642,-0.1913571428,-1.3508037873\H,-10.2809775518,-1.9059707652,-1
.1137652452\C,15.9142561415,-1.1483361144,-2.1988009144\H,-1.522321115
4,0.9773556038,-0.6873515497\H,0.9380261126,1.0536050358,-0.5515060969
\H,0.9572189863,-2.9684599619,0.8575104543\H,-1.4927108016,-3.01757255
57,0.7430943981\H,16.1853209324,-0.0964495119,-2.1751729779\H,16.25302
67012,-1.5963936253,-1.2687594624\H,16.4660932333,-1.6136426742,-3.010
0263805\H,14.1728809195,-2.3865465901,-2.434025825\H,14.1054000358,-0.
8977095012,-3.3330903698\H,13.8292020024,0.3766917056,-1.2000595104\H,
13.8926777801,-1.1141970004,-0.3025989658\H,11.8515240015,-1.914936714
2,-1.5020268777\H,11.7765537038,-0.4128392562,-2.3796293207\H,11.58641
8525,0.8223594005,-0.1958358205\H,11.5329776128,-0.700092693,0.6449890
178\O,-3.3995831496,-1.3576018563,2.0156581264\H,9.5167302804,0.202323
0069,-1.4409154051\C,4.772499764,-0.3563129178,-0.7173947943\C,3.39236
8917,-0.3891494028,-0.7916610482\H,2.9035064981,-0.015777437,-1.673703
4291\H,5.324034662,0.0567022886,-1.5438405466\H,5.1702049895,-1.770424
7057,2.3017240802\H,2.7391805087,-1.8116641929,2.1813818816\\Version=E
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799167,56.3546889,-4.0618801,6.426883,-3.643496\PG=C01 [X(C31H52B11O2)
]\\@

Pyr

1\1\GINC-MONSTER\FOpt\RHF\6-31G(d)\C16H28N1O1(1+)\PIOTR\10-Apr-2009\0\
\#P HF/6-31G* FOPT GEOM(NOANGLE,NODISTANCE) FCHECK\\N-Butyl-4-heptylox
ypyridinium cation, C1\\1,1\O,-0.4779317225,0.6473135911,-0.6046062704
\C,-0.5829497383,0.6219629894,0.6869122492\C,0.3891925078,0.1297234366
,1.5710664884\C,0.1379665964,0.1708898476,2.9128926094\N,-0.996797342,
0.6646018415,3.4190152364\C,-1.2420655221,0.6441022159,4.8844143598\C,
-1.9592777963,-0.6269818176,5.3312875634\C,-2.2081563108,-0.6323158001
,6.842618898\C,-2.9252230211,-1.8990134168,7.3076456886\H,-2.34322938,
-2.7865543369,7.080376677\H,-3.0874087366,-1.8749461796,8.3787604753\H
,-3.8934736279,-2.00154498,6.8280315937\H,-1.2596637935,-0.5397600738,
7.3657417668\H,-2.7982126984,0.2391287317,7.114994767\H,-2.9046057814,
-0.7125917022,4.8018389404\H,-1.3637523946,-1.4922356673,5.0519109577\
H,-0.2806138454,0.7461549164,5.3673069632\H,-1.8175980702,1.5280497172
,5.1202487773\C,-1.9413912538,1.1381139687,2.5811934049\C,-1.774766368
9,1.1357685884,1.2357786917\H,-2.5346150037,1.521854196,0.5859652598\H
,-2.8316173837,1.5210455807,3.0391454148\H,0.8545126063,-0.1942259258,
3.6219816942\H,1.3199518538,-0.2730317892,1.2293362856\C,0.6861081661,
0.1573197111,-1.2950316311\C,0.449798274,0.3491524281,-2.779795684\C,1
.6382869452,-0.1438176892,-3.6101161811\C,1.4197163272,0.0411089286,-5
.1135112354\C,2.6009153603,-0.447975251,-5.9533130356\C,2.3857542868,-
0.2645595954,-7.4568509997\C,3.5686600053,-0.7547541218,-8.2906855099\
H,4.4777746472,-0.2175667331,-8.0364139298\H,3.7527591144,-1.812637073
7,-8.1272468315\H,3.385886573,-0.6113279185,-9.3504006384\H,1.48595508
96,-0.7958768691,-7.7588488098\H,2.205435932,0.7869781017,-7.668708398
5\H,3.5019298621,0.0834874628,-5.6520415917\H,2.7819756387,-1.50045816
25,-5.7422346553\H,0.5187196335,-0.4904806205,-5.412432008\H,1.2386744
68,1.0934268774,-5.3222509758\H,2.5383943715,0.3891291211,-3.309894554
7\H,1.8176821959,-1.1964852838,-3.4001443538\H,-0.4521615877,-0.185478

0153,-3.0600354333\H,0.269613374,1.402409822,-2.9696885288\H,1.5469317
582,0.7187681484,-0.9536255922\H,0.8163796123,-0.8882994985,-1.0449638
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.339e-06\Dipole=-1.0113661,0.6234517,4.2700995\PG=C01 [X(C16H28N1O1)]\
\@

Cetyl

1\1\GINC-OCTOPUS\FOpt\RHF\6-31G(d)\C19H42N1(1+)\PIOTR\08-Apr-2011\0\\#
P HF/6-31G* FOpt geom(noangle,nodistance) fcheck\\C16H33NMe3 cation\\1
,1\N,8.701261562,0.1057818378,0.0000000864\C,7.335663524,0.7723679844,
0.0000001055\C,6.1245034178,-0.1554176111,0.0000000664\C,4.8321483499,
0.6744493028,0.0000000649\C,3.5774683441,-0.2023230949,0.0000000491\C,
2.2835363448,0.6144521523,0.00000005\C,1.0263776858,-0.2576298881,0.00
00000366\C,-0.2689061763,0.5565620112,0.0000000366\C,-1.5269557937,-0.
3139823855,0.0000000366\C,-2.822798809,0.499210533,0.0000000182\C,-4.0
812574589,-0.3707028298,0.0000000131\C,-5.3773802746,0.4420240361,0.00
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