Electronic Supplementary Information for

High Δε nematic liquid crystals: fluxional zwitterions of the [*closo*-1-CB_9H_{10}]$^-$ cluster

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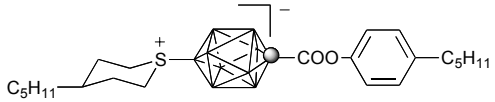
1. Synthetic Details

Reagents and solvents were obtained commercially. NEt_3 was distilled over CaH_2, and DMF was stored over freshly activated 4 Å molecular sieves. *N*,*N*-Dimethylthioformamide was distilled (80 °C, 0.25 mm Hg) prior to use. All other reagents were used as supplied. Reactions were carried out under Ar, and subsequent manipulations were conducted in air. NMR spectra were obtained in $CDCl_3$ or CD_3OD. ^1H NMR spectra were referenced to the solvent, and ^{11}B NMR chemical shifts were referenced to an external boric acid sample in CH_3OH that was set to 18.1 ppm.

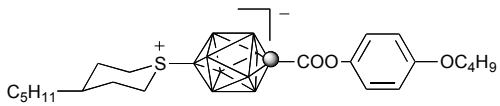
General Procedure for Preparation of Esters. A suspension of acid **6** (0.25 mmol) in anhydrous CH_2Cl_2 (1 mL) was treated with a 0.5 M solution of $(COCl)_2$ in CH_2Cl_2 (0.75 mL, 0.375 mmol) and 0.1 M solution of anhydrous DMF in CH_2Cl_2 (0.25 mL, 0.025 mmol) at rt. The mixture began to bubble, and the reaction became homogeneous. After 30 mins, the light yellow solution was evaporated to dryness, redissolved in anhydrous CH_2Cl_2 (1 mL), and phenol (1.5 equivalents) and a 0.5 M solution of freshly distilled NEt_3 in CH_2Cl_2 (0.25 mL, 0.75 mmol) were added. The reaction was stirred overnight at rt and evaporated to dryness. The product was isolated by column chromatography (SiO_2, CH_2Cl_2 or CH_2Cl_2/hexane, 1:1), the eluent was filtered through a cotton plug, and the solvent was evaporated. The resulting ester was washed with hot hexane, and repeatedly recrystallized until constant temperature and narrow transition peaks.

Preparation of ester of [*closo*-1-CB_9H_8-1-COOH-10-(1-(1-(4-C_5H_{11})-C_5H_9S)] and 4-pentylphenol (4a).



Following the General Method, ester **4a** was obtained in 93% yield as an off-white solid after chromatography. The product was recrystallized twice from cold *iso*-octane/toluene (-20 ^oC) and three times from cold CH_3CN (-40 ^oC) giving pure **4a** as a white powder: R_f = 0.74 (CH_2Cl_2/hexane, 1:1); mp 96.9 ^oC (DSC); ^1H NMR (400.1 MHz, $CDCl_3$, δ): (equatorial epimer, 78%) 0.6-2.5 (br m, 8H), 0.88-0.94 (m, 6H), 1.25-1.40 (m, 12H), 1.64-1.80 (m, 4H), 2.25-2.39 (m, 1H), 2.39 (br d, *J* = 14.7 Hz, 2H), 2.63 (t, *J* = 7.7 Hz, 2H), 3.43 (t, *J* = 12.3 Hz, 2H), 3.72 (br d, *J* = 12.2 Hz, 2H), 7.24 (s, 4H); (axial epimer, 22%, characteristic signals) δ 2.07-2.15 (m, 2H), 3.54-3.61 (m, 2H); ^{11}B NMR (128.4 MHz, $CDCl_3$, δ): -19.7 (d, *J* = 133 Hz, 4B), -14.1 (d, *J* = 151 Hz, 4B), 31.6 (s, 1B); HRMS (ESI, *m/z*): $[M+H]^+$ calcd. for $C_{23}H_{44}B_9O_2S$, 483.3899; found, 483.3907.

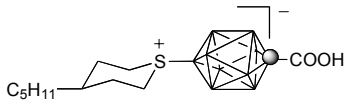
Preparation of ester of [*closo*-1-CB_9H_8-1-COOH-10-(1-(1-(4-C_5H_{11})-C_5H_9S)] and 4-butoxyphenol (4b).



Following the General Method, ester **4b** was obtained in 86% yield as an off-white solid after chromatography. The product was recrystallized twice from cold *iso*-octane/toluene (-20 ^oC) and twice from cold CH_3CN (-40 ^oC) giving pure ester **4b** as white leaflets: R_f = 0.7 (CH_2Cl_2/hexane, 1:1); mp 101.2 ^oC (DSC); ^1H NMR (400.1 MHz, $CDCl_3$, δ): (equatorial

epimer, 80%) 0.6-2.5 (br m, 8H), 0.91 (t, J = 6.9 Hz, 3H), 0.99 (t, J = 7.4 Hz, 3H), 1.26-1.42 (m, 8H) 1.51 (sext, J = 7.4 Hz, 2H), 1.65-1.83 (m, 4H), 2.26-2.39 (m, 1H), 2.39 (br d, J = 13.6 Hz, 2H), 3.43 (t, J = 12.1 Hz, 2H), 3.72 (d, J = 12.6 Hz, 2H), 3.98 (t, J = 6.5 Hz, 2H), 6.94 (d, J = 9.0 Hz, 2H), 7.24 (d, J = 9.0 Hz, 2H); (axial epimer, 20%, characteristic signals) δ 2.07-2.16 (m, 2H), 3.53-3.63 (m, 2H); ^{11}B NMR (128.4 MHz, $CDCl_3$, δ): -19.6 (d, J = 138 Hz, 4B), -14.0 (d, J = 163 Hz, 4B), 31.7 (s, 1B); HRMS (ESI, *m/z*) $[M+H]^+$ calcd. for $C_{22}H_{42}B_9O_3S$, 485.3692; found, 485.3707.

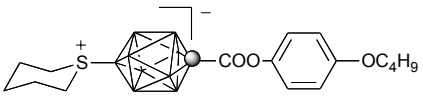
Preparation of acid [*closo*-1-CB_9H_8-1-COOH-10-(1-(4-C_5H_{11})-C_5H_9S)] (5).



A solution of crude protected mercaptan[1] [*closo*-1-CB_9H_8-1-COOH-10-$SCHN(CH_3)_2$] (**6**, 0.062 g, 0.25 mmol) in anhydrous CH_3CN (4 mL) was treated with a solution of $NMe_4^+OH^-$ •$5H_2O$ (0.180 g, 0.99 mmol) in anhydrous CH_3CN (6 mL) resulting in the formation of a white precipitate after mild heating with a heat gun. The suspension was cooled to rt, and dibromide[2] **7** (0.077 g, 0.257 mmol) was added, and the reaction mixture was stirred for 24 hrs at rt. The reaction mixture was evaporated to dryness and stirred in a methanolic solution (4 mL) of NaOH (0.01 g, 0.250 mmol) at 50 °C for 4 hrs. Solvent was removed to dryness, and 10% HCl (10 mL) was added. The suspension was stirred vigorously with Et_2O (5 mL) until the aqueous layer became homogeneous. The Et_2O layer was separated, and the aqueous layer was further extracted with Et_2O (2 x 5 mL). The Et_2O layers were combined, washed with H_2O, dried (Na_2SO_4), and evaporated leaving crude product as an orange crystalline film. The crude material was passed through a short silica gel plug (CH_3OH/CH_2Cl_2, 1:19, R_f = 0.4) and

washed with hot hexane giving 0.036 g (44% yield) of acid [*closo*-1-CB_9H_8-1-COOH-10-(1-$C_5H_{11}C_5H_{10}S$)] (**5**) as an off-white solid. An analytical sample of **5** was prepared by passing the acid through a cotton plug and recrystallizing twice from cold CH_3CN (-20 ^oC), once from cold *iso*-octane/toluene (-20 ^oC), and dried *in vacuo* at 110 ^oC for 2 hr: mp 215-216 ^oC; ^1H NMR (400.1 MHz, CD_3OD, δ): (equatorial epimer, 75%) 0.6-2.5 (br m, 8H), 0.92 (t, J = 6.7 Hz, 3H), 1.28-1.42 (m, 6H) 1.63-1.80 (m, 4H), 2.17-2.29 (m, 1H), 2.37 (br d, J = 9.4 Hz, 2H), 3.41 (t, J = 12.5 Hz, 2H), 3.75 (br d, J = 12.7 Hz, 2H), (COOH not observed); (axial epimer, 25%, characteristic signals) 2.05-2.12 (m, 2H), 3.50 (d, J = 14.0 Hz, 2H), 3.61 (br t, J = 11.2 Hz, 2H); ^{11}B NMR (128.4 MHz, CD_3OD, δ): (equatorial epimer) -20.1 (d, J = 143 Hz, 4B), -14.6 (d, J = 166 Hz, 4B), 31.9 (s, 1B); (axial epimer, characteristic signal) 29.8 (s, 1B). Anal. Calcd for $C_{12}H_{29}B_9O_2S$: C, 43.06; H, 8.73; found: C, 43.13; H, 8.72.

Preparation of ester of [*closo*-1-CB_9H_8-1-COOH-10-$C_5H_{10}S$] and 4-butoxyphenol (8).

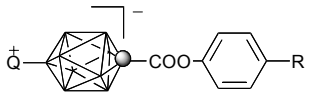


Following the General Method, ester **8** was obtained in 88% yield from acid [*closo*-1-CB_9H_8-1-COOH-10-$C_5H_{10}S$][1] as an off-white solid after chromatography. The product was recrystallized twice from cold *iso*-octane/toluene (-20 ^oC) and twice from cold CH_3CN (-20 ^oC) giving pure ester **8** as white blades: R_f = 0.55 (CH_2Cl_2); mp 138.5 ^oC (DSC); ^1H NMR (400.1 MHz, $CDCl_3$, δ): 0.6-2.5 (br m, 8H), 0.99 (t, J = 7.4 Hz, 3H), 1.51 (sext, J = 7.5 Hz, 2H) 1.63-1.76 (m, 1H), 1.78 (quint, J = 7.0 Hz, 2H), 2.00-2.13 (m, 3H), 2.38-2.48 (m, 2H), 3.42 (td, J_1 = 12.4 Hz, J_2 = 2.6 Hz, 2H), 3.64 (br d, J = 11.4 Hz, 2H), 3.98 (t, J = 6.5 Hz, 2H), 6.94 (d, J = 9.1 Hz, 2H), 7.24 (d, J = 9.0 Hz, 2H); ^{11}B NMR (128.4 MHz, $CDCl_3$, δ): -19.6 (d, J = 143 Hz, 4B), -14.1 (d,

J = 161 Hz, 4B), 31.2 (s, 1B). Anal. Calcd. for $C_{17}H_{31}B_9O_3S$: C, 49.46; H, 7.57; found: C, 49.48; H, 7.66.

2. DSC data

Table S1. Transition temperatures (°C) and enthalpies (kJ) for compounds **3** and **4**.[a]



R		Q: $C_7H_{15}O$–(N)– **3** [b]	Q: C_5H_{11}–(S)– **4**
a	C_5H_{11}	Cr 120 (N 114) I *22.8 0.7*	Cr 97 I *29.5*
b	OC_4H_9	Cr_1 100 Cr_2 122 N 156 I *2.9 12.7 0.7*	Cr 101 (N 97) I *28.6 0.6*
c	CN	Cr 128 (N 129) I *35.7 0.2*	[c]

[a] Cr-crystal, N-nemtic, I-isotropic. Monotropic transitions in parentheses. Transition enthalpies are given below in italics. [b] Ref [3] [c] Not prepared.

Ester **8**: Cr 138 I, enthalpy of melting: 33.2 kJ/mol

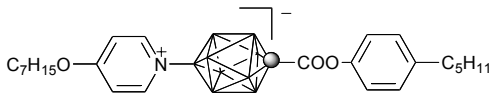
3. Binary mixtures

Binary mixtures preparation. Solutions of esters in an appropriate host (10 mg of ClEster, [4] 6-CHBT[5] or ZLI-1132) were prepared in an open vial with agitation using a closed-end capillary tube with moderate heating supplied by a heat gun. The mixtures were then allowed to condition for 3 hr at room temperature, and subsequently analyzed by polarized optical microscopy (POM) to verify their homogeneity.

Thermal analysis. The clearing temperature of each homogeneous mixture was determined by DSC typically on a second heating cycle as the peak of the transition. The results are shown in Tables S2 – S7. The virtual N-I transition temperature, [T_{NI}], was determined by linear

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.

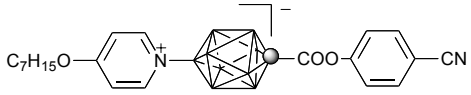
Table S2. T_{NI} for solutions of **3a** in **ClEster**.



	Mole fraction, *x*			
T_{NI} /°C	0.00(host)	0.0549	0.0929	0.1588
Onset		50.0	52.0	55.4
Peak	47.0	50.3	52.4	55.9

[T_{NI}] = 103±1 °C, r^2 = 0.999. (First run)

Table S3. T_{NI} for solutions of **3c** in ClEster.



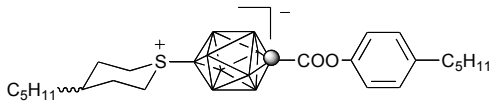
	Mole fraction, *x*				
T_{NI} /°C	0.00(host)	0.0152	0.0311	0.0564	0.0979
onset		45.0	46.8	48.5	50.7 [a]
peak	46.2	45.5	47.2	49.0	51.2 [a]

[T_{NI}] = 96.5±0.5 °C, r^2 = 0.999.

Non-linear behavior. T_{NI} extrapolated using 5.64 mol% and 9.79 mol% concentrations.

[a] inhomogenous at rt.

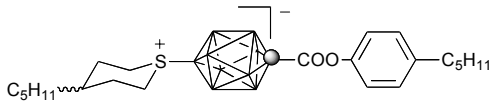
Table S4. T_{NI} for solutions of **4a** in ClEster.



	Mole fraction, *x*			
T_{NI} /°C	0.00(host)	0.0283	0.0628	0.1156
onset		46.1	47.6	49.4
peak	46.4	47.2	49.1	50.6

$[T_{NI}]$ = 89±2 °C, r^2 = 0.987.

Table S5. T_{NI} for solutions of **4a** in 6-CHBT.

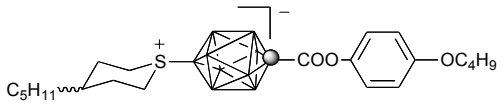


	Mole fraction, *x*				
T_{NI} /°C	0.00(host)	0.021	0.0519	0.0767	0.1098
onset	39.5	38.9	42.6	45.0	43.7
peak	40.4	41.6	44.3	46.0	45.6

$[T_{NI}]$ = 112±2 °C, r^2 = 0.993; excluding the 10.98 mol% concentration.

For 2.80 % w/w of **4a** (sulfonim C5C5) in ZLI-1132 the peak of T_{NI} changed from 68.1 °C to 67.2 °C.

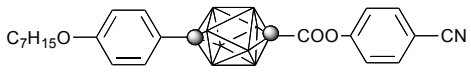
Table S6. T_{NI} for solutions of **4b** in 6-CHBT.



	Mole fraction, *x*			
T_{NI} /°C	0.00(host)	0.027	0.0551	0.1126
onset	39.5	41.5	43.2	48.6
peak	40.4	43.5	45.7	51.1

$[T_{NI}]$ = 133±2 °C, r^2 = 0.996; from first run data.

Table S7. T_{NI} for solutions of **11** in ClEster.



	Mole fraction, x			
T_{NI} /°C	0.00(host)	0.0628	0.1125	0.16.41
onset	45.2	49.1	51.7	54.0
peak	46.2	49.5	52.1	54.7

$[T_{NI}] = 98\pm1$ °C, $r^2 = 0.998$

Dielectric measurements. Dielectric properties of solutions of esters **3**, **4** and **11** in appropriate host (ClEster,[4] 6-CHBT[5-7] or ZLI-1132) were measured by a Liquid Crystal Analytical System (LCAS - Series II, LC Analytical Inc.) using GLCAS software version 0.951, which implements literature procedures for measuring of dielectric constants.[8] The homogeneous binary mixtures were loaded into ITO electro-optical cells by capillary forces with moderate heating supplied by a heat gun. The cells (about 4 μm thick, electrode area of 0.581 cm^2 and anti-parallel rubbed polyimide layer 2°–3° pretilt) were obtained from LCA Inc., and their precise thickness (±0.05 □m) was measured by LCAS using the capacitance method before the cells were filled. The filled cells were heated to an isotropic phase and were cooled to room temperature before measuring the dielectric properties. Default parameters were used for measurements: triangular shaped voltage bias ranging from 0.1–15 V for **3** and **4** and 0.1–30 V for **11** at 1 kHz frequency. The threshold voltage V_{th} was measured at a 5% change. For each mixture, the measurement was repeated seven times for two cells. The first two measurements for each cell were discarded as conditioning measurements, and the remaining ten results were averaged to calculate the mixture's parameters. Results are in shown in Tables S8–S14. Dielectric parameters of pure hosts 6-

CHBT and ZLI-1132 were obtained using the same protocol. For consistency, dielectric parameters ClEster were obtained by averaging values obtained by extrapolation from a series of measurements for each additive. The averaged extrapolated values are higher than those measured in a set of homeotropic cells by about 0.2 for $\varepsilon_{||}$ and $\varepsilon_{\perp}$ and lower by 0.03 for $\Delta\varepsilon$. The value for elastic constant K_{11} of 10±0.3 pN was assumed from the measurement in homeotropic cells. The viscosity γ from these measurements was not used for comparison purposes.

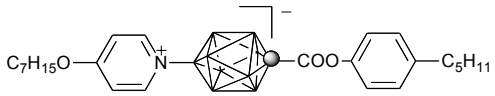
E-4-(4-Hexylcyclohexyl)phenyl isothiocyanate[5-7] (6-CHBT) and ClEster[4] were vacuum distilled prior to measurements. ZLI-1132 was used as supplied (E. Merck, Ind). Pure hosts at 23 ^{o}C:

6-CHBT: $\varepsilon_{||}$ = 11.65±0.05 $\varepsilon_{\perp}$ = 4.02±0.05; $\Delta\varepsilon$ = 7.63±0.05, K_{11} = 13.7±0.7 pN, γ = 111±1 mP·s

ZLI-1132: $\varepsilon_{||}$ = 16.12±0.06 $\varepsilon_{\perp}$ = 4.64±0.01; $\Delta\varepsilon$ = 11.48±0.05, γ = 225±1.5 mP·s.

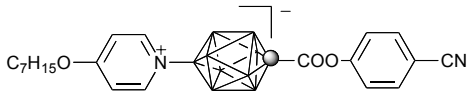
Standard deviation of the resulting values typically is ≤ ±0.03. All measurements were run at 25 ^{o}C. Error on concentration is estimated at about 1.5%. The dielectric values obtained for each concentration were fitted to a linear funtion in which the intercept was set at the value extrapolated for the pure host. The resulting extrapolated values for pure additives are shown in Table 3 in the main text.

Table S8. Dielectric parameters for solutions of **3a** in ClEster at 25 °C.



Parameter	mole fraction, *x*			
	0.00(host)	0.0549	0.0929	0.158
$\varepsilon_{\|\|}$	2.86±0.01	5.63±0.04	7.72±0.01	11.11±0.02
$\varepsilon_{\perp}$	3.42±0.01	3.95±0.01	4.28±0.01	4.91±0.02
$\Delta\varepsilon$	-0.56±0.01	1.69±0.04	3.45±0.02	6.20±0.02
γ /P•s		0.15±0.004	0.28±0.01	0.65±0.006
K_{11} p□	10.0±0.3	17.5±0.1	19±2	20.5±0.2

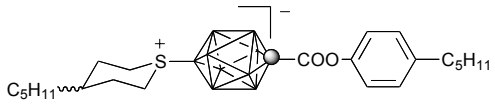
Table S9. Dielectric parameters for solutions of **3c** in ClEster at 25 °C.



Parameter	mole fraction, *x*			
	0.00(host)	0.0152	0.0311	0.0564 [a]
$\varepsilon_{\|\|}$	2.86±0.01	4.90±0.015	7.00±0.015	10.01±0.03
$\varepsilon_{\perp}$	3.42±0.01	3.70±0.01	4.035±0.01	4.49±0.01
$\Delta\varepsilon$	-0.56±0.01	1.20±0.017	2.97±0.01	5.52±0.02
γ /P•s		0.08±0.002	0.32±0.005	0.54±0.01
K_{11} p□	10.0±0.3	14±1	15.7±0.2	16.6±0.1

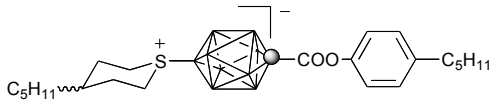
[a] Not used for extrapolation.

Table S10. Dielectric parameters for solutions of **4a** in ClEster at 25 °C.



Parameter	mole fraction, *x*			
	0.00(host)	0.0283	0.0628	0.1156
$\varepsilon_{\parallel}$	2.86±0.01	3.79±0.02	4.91±0.04	6.54±0.01
$\varepsilon_{\perp}$	3.42±0.01	3.58±0.00	3.84±0.04	4.12±0.01
$\Delta\varepsilon$	-0.56±0.01	0.21±0.02	1.08±0.01	2.42±0.01
γ /P•s		0.003±0.001	0.06±0.003	0.24±0.004
K_{11} pN	10.0±0.3	14.3±1.5	15.7±0.6	19.3±0.1

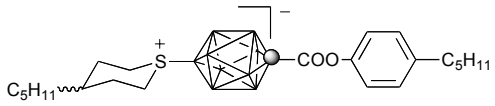
Table S11. Dielectric parameters for solutions of **4a** in 6-CHBT at 25 °C.



Parameter	mole fraction, *x*				
	0.00(host)	0.021	0.0519	0.0767[a]	0.1098[b]
$\varepsilon_{\parallel}$	11.65±0.05	12.25±0.04	13.18±0.09	13.94±0.19	14.51±0.09
$\varepsilon_{\perp}$	4.02±0.05	4.21±0.03	4.41±0.02	4.62±0.02	4.79±0.02
$\Delta\varepsilon$	7.63±0.05	8.04±0.03	8.77±0.08	9.31±0.16	9.71±0.08
γ /P•s	0.11±0.01	0.13±0.01	0.13±0.01	0.14±0.04	0.17±0.003
K_{11} pN	13.7±0.6	13.3±0.1	13.6±0.2	13.8±0.3	13.7±0.2

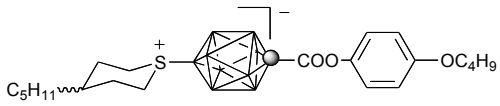
[a] Average of 3 cells. [b] Not used in correlation.

Table S12. Dielectric parameters for solutions of **4a** in ZLI-1132 at 25 °C.



Parameter	**weight fraction**	
	0.00(host)	0.028
$\varepsilon_{\parallel}$	16.11±0.05	16.97±0.14
$\varepsilon_{\perp}$	4.64±0.01	4.88±0.01
$\Delta\varepsilon$	11.47±0.05	12.09±0.13
γ /P•s	0.23±0.002	0.24±0.01

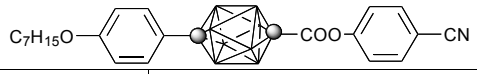
Table S13. Dielectric parameters for solutions of **4b** in 6-CHBT at 25 °C.



Parameter	**mole fraction, *x***			
	0.00(host)	0.027 [a]	0.055 [a]	0.1126
$\varepsilon_{\parallel}$	11.65±0.05	12.63±0.11	13.63±0.13	[b]
$\varepsilon_{\perp}$	4.02±0.02	4.24±0.02	4.47±0.02	[b]
$\Delta\varepsilon$	7.63±0.05	8.39±0.011	9.16±0.012	[b]
γ	0.11±0.01	0.13±0.01	0.14±0.02	[b]
K_{11} /p□	13.7±0.6	13.8±0.9	14.0±0.3	[b]

[a] Average of 3 cells. [b] Inhomogenous mixture at 25 C.

Table S14. Dielectric parameters for solutions of **11** in ClEster at 25 °C.



Parameter	mole fraction, *x*			
	0.00(host)	0.0628	0.1125	0.1641 [a]
$\varepsilon_{\parallel}$	2.86±0.01	4.00±0.03	4.90±0.03	5.68±0.03
$\varepsilon_{\perp}$	3.42±0.01	3.58±0.02	3.68±0.03	3.84±0.02
$\Delta\varepsilon$	-0.56±0.01	0.42±0.01	1.22±0.01	1.84±0.02
γ /P•s		0.01±0.001	0.07±0.004	0.14±0.004
K_{11} ~ p□	10.0±0.3	17.0±0.6	16.6±0.1	16.3±0.8

[a] Not used for extrapolation.

4. Background for calculations in the nematic phase

The Equations derived from the Maier-Meier theory used in this work were adopted from literature[9,10] and had the following form:

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

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

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

All quantities were in SI units.

• Dielectric permittivity of vacuum:

$\varepsilon = 1.114\times10^{-10}/4\pi = 8.865\times10^{-12}$ F•m^{-1}.

• The matrix of electronic polarizabilities α in a.u. units listed in the output file for each molecule was diagonalized. The resulting principal values were converted to F•m^2 units by multiplying with

$1.482 \times 4\pi\varepsilon \times 10^{-31} = 1.651 \times 10^{-41}$.

• Computed dipole moments μ 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 and h in equations 1–3 were obtained according to equation 4 and 5 assuming ε_s to be experimental average permittivity calculated from $\varepsilon_{||}$ and $\varepsilon_{\perp}$.

$$F = \frac{1}{1 - \bar{\alpha} \bullet f} \quad \text{where} \quad f = \frac{2(\bar{\varepsilon}_s - 1)}{2\bar{\varepsilon}_s + 1} \bullet \frac{N}{3\varepsilon_0} \qquad h = \frac{3\varepsilon_s}{(2\varepsilon_s + 1)}$$

equation 4 equation 5

5. 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 $\varepsilon_{||}$ (equations 1 and 2). The unknown g from the expression for $\Delta\varepsilon$ (equation 1) was substituted into the expression for $\varepsilon_{||}$ (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 $\varepsilon_{||}$ and $\varepsilon_{\perp}$. The obtained value S was substituted to the expression for parameter g (equation 7).

$$S = \frac{\Delta\varepsilon\varepsilon_0}{\Delta\alpha NFh + (1 - 3\cos^2\beta)\left[\Delta\varepsilon\varepsilon_0 - \frac{3}{2}\left(\varepsilon_{||}\varepsilon_0 - \varepsilon_0 - \bar{\alpha}NFh\right)\right]}$$

equation 6

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

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

6. Assumptions and models for Maier-Meier calculations

Number density *N* used in all calculations was obtained for each ester **3**, **4** and **11** assuming density of the liquid to be 1000 kg•m^{-3}. For the hosts, the density at 25 ^{o}C was taken as 1.009 g/cm^3 for 6-CHBT[5] and 1.02 g/cm^3 for ClEster[11] as reported in the literature.

For the pure hosts ε_s was assumed 6.56 for 6-CHBT and 3.07 for ClEster. In Method A polarizability α of the host was calculated at the B3LYP/6-31G(d,p) level. In Method B, the polarizability was obtained from optical measurements (α = 53.8 Å^3 for ClEster[4]and α = 39.04±0.03 Å^3 for 6-CHBT[5]). These parameters were used to calculate the order parameter *S* and Kirkwood factor *g* using computed dipole moment vectors (*vide infra*) and according to equations 6 and 7. Results are shown in Tables S15 and S16.

Table S15. Calculated parameters *S* and *g* for host ClEster.

Method	ε_s	α	μ	β	S_{calcd}	g_{calcd}
A	Exptl	Calcd	Calcd	Calcd	1.23	1.73
B	Exptl	Exptl [a]	Calcd	Calcd	0.83	1.375
B	Exptl	Exptl [a]	Calcd [b]	Calcd [b]	0.81	0.545

[a] From ref [4] [b] Calculated using the HF/6-31G* method.

Table S16. Calculated parameters *S* and *g* for 6-CHBT.

Method	ε_s	α	μ	β	S_{calcd}	g_{calcd}
A	Exptl	Calcd	Calcd	Calcd	0.61	0.31
B	Exptl	Exptl [a]	Calcd	Calcd	0.68	0.29

[a] From ref [5].

Results show that the calculated polarizability α is lower than that calculated from optical data by 10% for ClEster and 6% for 6-CHBT. The $\Delta\alpha$ is higher than that from optical data by a factor of about 2.8 for ClEster and 2.2 for 6-CHBT. No corrections were used in Maier-Meier analysis.

Results of Maier-Meier calculations for 6-CHBT appear to be much less sensitive to the values of molecular parameters than those for ClEster. In both calculations, however, the use of experimental polarizabilities appears to improve the values of order parameter *S*. For 6-CHBT the order parameter is lower than experimental by 0.06,[9] when both polarizatibity and dipole are DFT-derived, which is a reasonable good agreement the experiment. The use of DFT-derived dipole moment components gives unrealistic values of *S* and *g* for ClEster (Table S15). In contrast, higher dipole moment values obtained at the HF/6-31G* level and increase of the β from 85^o to 89^o gave reasonable values of *S* and *g*.

Models for analysis of the additives.

The computations for the additives were performed using 2 models and set of assumptions:

1) It was assumed that the additive does not change properties of the host (density, density number, polarizability, dielectric strength) and that dipole moment of the additive does not change in response to dielectric medium (gas phase value). Therefore, Maier-Meier calculations used *F* and *h* values derived for the appropriate pure host, extrapolated

dielectric parameters $\varepsilon_{||}$ and $\varepsilon_{\perp}$ and density number *N* for the pure additive assuming density 1.0 g/cm^3.

2) Dielectric parameters $\varepsilon_{||}$ and $\varepsilon_{\perp}$ extrapolated for the pure additive were used to calculate average dielectric permittivity ε_s, which together with DFT-calculated polarizability α (uncorrected) and density number *N* for the additive (assuming density of 1.0 g/cm^3) gave the values of field parameters *F* and *h* for the pure additive (equation 4 and 5). These parameters and DFT-derived gas phase molecular dipoles were used to calculate the *S* and *g* values. The resulting values are shown in Table 3 of the main text.

Results show that the differences between the two methods are small due to partial compensation of the decrease density number *N* and increase ε.

7. Quantum-mechanical computations

Quantum-mechanical calculations were carried out using Gaussian 09 suite of programs.[12] Geometry optimizations for unconstrained conformers of **3**, **4** and **11** with the most extended molecular shapes were undertaken at the B3LYP/6-31G(d,p) level of theory using default convergence limits. The alkoxy groups were set in all-*trans* conformation co-planar with the aromatic ring in the input structure. The aromatic ring and the carboxyl group were set staggered with the carborane cage as found experimentally and computationally in a related structure.[1] The orientation of the alkyl and carbonyloxy substituents on the alicyclic ring in the input structure was set according to conformational analysis of 1-ethyl and 1-acetoxy derivatives of bicyclo[2.2.2]octane and cyclohexane.

Dipole moment components and polarizability tensors for selectd molecules

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)

3a

```
Dipole moment (field-independent basis, Debye):
     X= 13.9883    Y= 3.2199    Z= 0.7821  Tot= 14.3754
Exact polarizability:
     644.996   6.722 303.100  -0.386   4.911  288.097
diagonal components: 645.1, 304.4, 286.6
```

3c

```
Dipole moment (field-independent basis, Debye):
    X= 20.2283    Y= -1.7478    Z=  0.3709  Tot=  20.3070
Exact polarizability:
     605.944   3.154 269.206   6.539   4.294  238.337
diagonal components: 606.1, 269.7, 237.7
```

4a-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
diagonal components: 574.7  305.3  279.1
```

4a-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
diagonal components: 544.3  318.1   286.1
```

4b-trans

```
Dipole moment (field-independent basis, Debye):
    X=  -8.8937    Y=  -2.5141    Z=  0.7418  Tot= 9.2719
Exact polarizability: 572.364   0.297 305.983  -0.494   5.867 262.106
diagonal components:  572.4  306.8  261.3
```

4b-cis

```
Dipole moment (field-independent basis, Debye):
    X= 7.6865    Y=  -3.4510    Z= 0.0419  Tot= 8.4257
Exact polarizability: 541.509  -7.981 320.164   3.452  12.931 269.033
diagonal components: 541.8 323.0  265.9
```

11

```
Dipole moment (field-independent basis, Debye):
     X= 8.0974    Y= -0.4732    Z= -0.1920  Tot= 8.1135
Exact polarizability:
596.018   1.464 267.694   5.478   4.491 236.374
diagonal components: 596.1, 268.3, 235.7
```

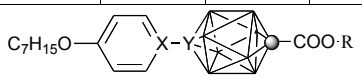
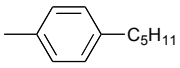
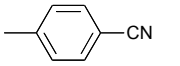
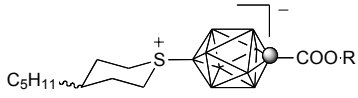
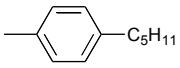
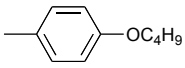
6-CHBT

```
Dipole moment (field-independent basis, Debye):
    X=  4.8601    Y=   0.9100    Z=  0.2509  Tot=   4.9509
Exact polarizability: 410.177  26.651 168.042   3.933  16.227 167.890
diagonal components: 413.2  182.2   150.7
```

ClEster

```
Dipole moment (field-independent basis, Debye):
    X= 0.1233    Y= -0.3247    Z= 1.3299  Tot= 1.3745
Exact polarizability: 454.391  -1.190 275.955  15.441  17.698 257.907
diagonal components: 455.6  286.5  246.2
```

Table S17. Calculated molecular parameters for **3**, **4**, and **11**. [a]

	R		$\mu_{\|\|}$ /D	$\mu_{\perp}$ /D	μ /D	$\alpha_{\|\|}$/ Å^3	$\alpha_{\perp}$/ Å^3	$\Delta\alpha$/ Å^3	α_{avrg} / Å^3
		□–□							
3a		N^+–B^-	13.99	3.31	14.38	95.60	43.79	51.81	61.06
□**c 11**		N^+–B^-	20.23	1.79	20.31	89.82	37.60	52.23	55.01
		C–C	8.10	0.51	8.11	88.34	37.30	51.00	54.35
		 **4**							
4a		*trans*	9.62	2.31	9.89	85.17	43.30	41.87	57.26
		cis	8.49	3.02	9.02	80.67	44.77	35.89	56.73
4b		*trans*	8.89	2.62	9.27	84.83	42.10	42.73	56.34
		cis	7.69	3.45	8.43	80.30	43.64	36.66	55.86

[a] Obtained at the B3LYP/6-31G(d,p) level of theory. Polarizability units were converted from au to Å^3 using the factor 0.1482.

8. Equilibrium data for 4a

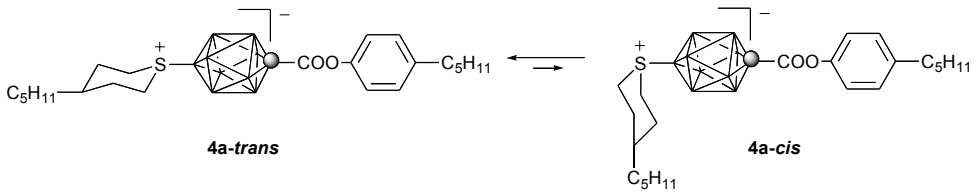


Figure S1. The *trans* and *cis* isomers of **4a**.

Procedure ^{1}H NMR spectra were recorded for a solution of **4a** in $CDCl_3$ at several temperatures on cooling from 328 K. For measurement at temperatures higher than ambient (328K, 318 K, and 308 K) the sample was equilibrated for 10 min before recording the spectrum. For lower temperatures the sample was equilibrated for 30 min. Apparently, this was not long enough to achieve equilibrium at $T = 283$ K and the data point was off the line.

Equilibrium constant at each temperature was obtained by integrating the doublet at 3.72 ppm, ascribed to the equatorial epimer **4a-*trans***, and the multiplet of the axial form, **4a-*cis***, in the range of 3.53-3.63 ppm. The resulting ratio of the two multiplets is shown in Table S18 and the graph as function of 1/T in Figure S2.

Table S18. Ratio of two forms **4a-*trans*** / **4a-*cis*** from NMR data in $CDCl_3$.

T/K	328	318	308	298	293	288
K_{epi}	3.188	3.303	3.475	3.636	3.747	3.820
K_{C5}	16.231	17.538	19.046	20.799	21.784	22.853
K_{CB9}	3.890	3.998	4.186	4.349	4.470	4.534

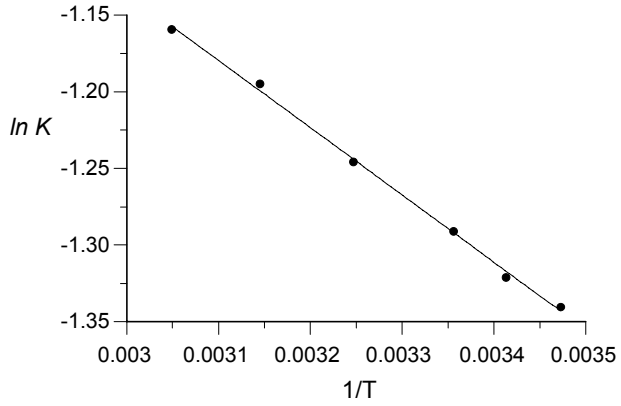
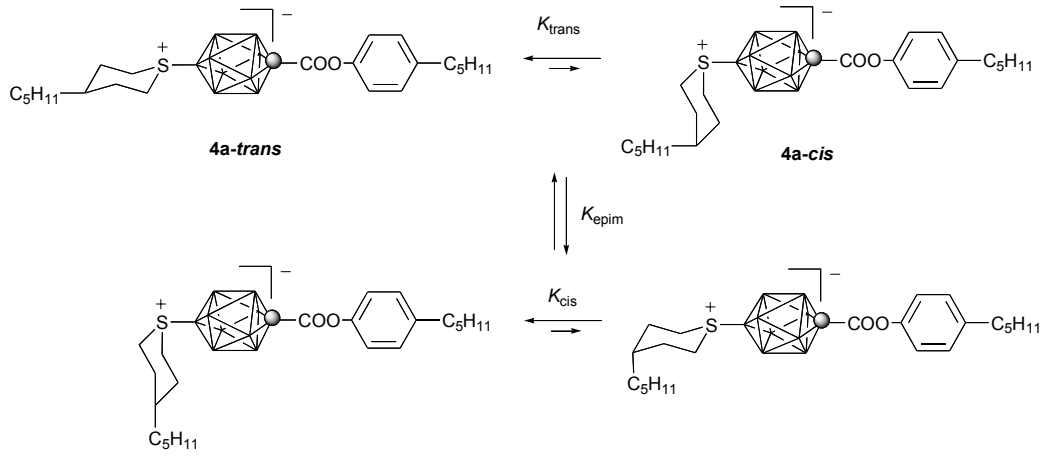


Figure S2. Temperature dependence of equilibrium constant *K* for **4a-*trans*** and **4a-*cis***. Best fit line: *ln*K = -439•1/T + 0.18, $r^2 = 0.999$.

Assuming that:



$$K_{CB9} = \frac{1 - K_{C5} \times K_{epi}}{K_{epi} - K_{C5}}$$

Analysis of the data gives ΔH = +0.87±0.02 kcal/mol and ΔS = +0.36±0.06 cal/molK.

9. Archive files for B3LYP/6-31G(d,p) calculations

3a

GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C25H42B9N1O3\PIOTR\28-Apr-2010
\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck freq=nor
aman #P guess=check\\C7O-Pyr-BC9-COO-Ph-C5, preopt\\0,1\B,0.1610897571
,1.0209289033,1.282461971\B,-0.2697866249,-0.7685568314,1.460863895\B,
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898355303\B,0.8037060271,1.1023196657,-0.4012275294\B,-0.7527389556,0.
1551909934,-0.0080577176\B,0.1884720952,-1.4441209027,-0.145841228\B,1
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7667,-12.7774119157\H,1.0156713407,0.0552229136,-12.8909466329\H,-0.93
83262887,-1.0990435452,-11.8050080363\H,-1.7839803799,0.4355768721,-11
.6933739451\H,0.0475752663,1.3400712494,-10.2292231646\H,0.8953632888,
-0.1948895917,-10.341512148\H,-1.0595523168,-1.3569985338,-9.248986475
5\H,-1.9100164287,0.1804501638,-9.137119792\H,-0.1022755124,1.08495551
02,-7.6631315227\H,0.7575994926,-0.4712722827,-7.7760129679\C,-1.55018
07579,-0.9687842112,-4.5356734085\C,-1.21834326,-0.8866823102,-3.20379
86324\H,-1.8462737641,-1.2940038504,-2.4222454585\H,-2.4672073774,-1.4
528962875,-4.8480586584\H,1.2041828743,0.6459652968,-5.7425736406\H,1.
6539440671,0.7096275982,-3.3066384441\C,1.035343688,-0.064061082,2.084
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644,1.1690551903\H,0.9652356495,2.1594296249,-0.9285024845\H,-1.900272
7302,0.4131077688,-0.2041236162\H,-0.1659724751,-2.5388965668,-0.45751
72908\H,2.6947867853,-0.7939520679,-1.2014742856\H,1.6349528324,-1.354
7610934,6.0133875423\H,1.6041515429,-1.1043554335,8.4734847915\C,0.355
4266473,0.8083694192,9.979045709\C,-0.8319629107,0.056035589,10.612246
3883\C,-0.8810257728,0.1760884265,12.1395280085\C,-2.0610906364,-0.570
5422564,12.7738555359\C,-2.1051647637,-0.4472662824,14.2998258126\H,-1
.1954447899,-0.8530706137,14.7569316812\H,-2.1900091172,0.6003761496,1
4.610563215\H,-2.9583481845,-0.9886326542,14.7215272688\H,-2.999645718
8,-0.190215425,12.3483761762\H,-2.0101096967,-1.6312643035,12.49321258
96\H,0.0587837991,-0.2039882951,12.5654902956\H,-0.9317220943,1.237996
8072,12.4207382747\H,-1.7674184129,0.4371845164,10.1811603992\H,-0.776
9153106,-1.0028416478,10.3260809906\H,1.2897310751,0.4261226895,10.409
5668192\H,0.2964253433,1.8678118961,10.2591988421\H,-0.7876470819,2.44
11409206,8.0970371804\H,-0.7568696249,2.181196846,5.6199459509\O,2.526

8847619,-0.2123533045,3.9548795021\\Version=EM64L-G09RevA.02\State=1-A
\HF=-1482.2962516\RMSD=2.830e-09\RMSF=1.820e-06\Dipole=-1.294464,0.103
264,-5.5046155\Quadrupole=-29.3384873,-23.7623603,53.1008477,1.1021013
,-5.2581643,0.3157914\PG=C01 [X(C25H42B9N1O3)]\\

3c

GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C21H31B9N2O3\PIOTR\29-Apr-2010
\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck #P freq=
noraman\\C7O-Pyr-BC9-COO-Ph-CN,C1 start at HF\\0,1\B,0.1751509437,0.84
43810497,1.2914432764\B,-0.1310359595,-0.9737043401,1.4596079266\B,1.6
640440536,-1.3094788716,1.0700680719\B,1.96972465,0.5054790593,0.90065
63054\B,0.806279573,0.9793320342,-0.3911208978\B,-0.6802240028,-0.0760
708831,-0.0021030486\B,0.3710503288,-1.6055072941,-0.1509878985\B,1.85
28945787,-0.5498793455,-0.5518668441\B,0.3551953785,-0.3689685778,-1.2
918120695\N,0.0211669999,-0.4452401699,-2.7803225795\C,0.8188920291,0.
1503678612,-3.6940989579\C,0.5515129845,0.1137842929,-5.0495002509\C,-
0.5925595034,-0.5678861152,-5.4998804684\O,-0.9731751355,-0.6783515329
,-6.7755311435\C,-0.1871236434,-0.0529880605,-7.8142488312\C,-0.877654
3823,-0.3217559618,-9.1409449718\C,-0.1266772235,0.3086151725,-10.3214
068165\C,-0.820339253,0.0663871061,-11.6679716826\C,-0.081226073,0.696
2234913,-12.8545135194\C,-0.7787547898,0.4652128452,-14.2007512648\C,-
0.0356331471,1.0972825435,-15.3812107506\H,0.0583261111,2.1818929831,-
15.2560206843\H,0.9761636439,0.6877187974,-15.4782068981\H,-0.55873955
76,0.9163148899,-16.3254464628\H,-0.8867605615,-0.6144666117,-14.37127
42095\H,-1.7995595132,0.8677862143,-14.1520569261\H,0.0264970122,1.776
8809964,-12.6836302258\H,0.9407855363,0.2939352217,-12.9021526884\H,-0
.9218229593,-1.0151345383,-11.8338329795\H,-1.8436696639,0.464403188,-
11.6234604032\H,-0.0256510467,1.3904678444,-10.1565056329\H,0.89608842
18,-0.0912711835,-10.3629315257\H,-0.9623212941,-1.4057921754,-9.28149
26779\H,-1.8995385785,0.0724228953,-9.0902478079\H,-0.1205952453,1.023
7746178,-7.6134901894\H,0.82616034,-0.4741616242,-7.799715494\C,-1.415
7406304,-1.1890643947,-4.5407259835\C,-1.0845317333,-1.1086580809,-3.2
087969276\H,-1.6844046078,-1.5654027388,-2.4324977401\H,-2.3030548865,
-1.7225269099,-4.858487428\H,1.2300562018,0.6112905472,-5.7287998097\H
,1.6855512379,0.6610520159,-3.2942907107\C,1.1238779741,-0.1834780661,
2.0844336512\C,1.5039857817,-0.1125711477,3.5198366266\O,0.3894644996,
0.1152590316,4.293525743\C,0.4457223687,0.2240370112,5.6725396051\C,1.
3197721265,-0.5042774993,6.4858031719\C,1.2300441201,-0.3609385794,7.8
668143046\C,0.2760870154,0.4958528569,8.4397088507\C,-0.5988313286,1.2
148446581,7.6071469085\C,-0.5118077935,1.0771082112,6.2287222619\H,-0.
3102958413,1.7556227285,1.871971135\H,-0.8662518453,-1.5586671762,2.18
07238423\H,2.3736631902,-2.1628939083,1.4819602471\H,2.9292440693,1.14
20179848,1.1752925688\H,0.8932292224,2.0479416349,-0.9120180815\H,-1.8
432270668,0.1029461445,-0.1927191187\H,0.0939209041,-2.7206194603,-0.4
670829121\H,2.8221325263,-0.7741938882,-1.2086777742\H,2.0612073762,-1
.1564953142,6.0480744771\H,1.9025755422,-0.9181292274,8.5099561632\H,-
1.3389682448,1.8753304986,8.0453598482\H,-1.1772213779,1.618759712,5.5
658324457\O,2.6216072572,-0.2289668715,3.9566761431\C,0.1924645457,0.6
342523789,9.8635230933\N,0.1222283447,0.7471240295,11.0196316198\\Vers
ion=EM64L-G09RevA.02\State=1-A\HF=-1377.9527994\RMSD=5.993e-09\RMSF=2.
373e-06\Dipole=-1.1523129,-0.0985875,-7.9052502\Quadrupole=11.2401085,
13.2361532,-24.4762617,0.5200957,-3.7350331,-5.3530535\PG=C01 [X(C21H3
1B9N2O3)]\\

4a-trans, C5

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)]\\@

4a-cis C5

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)]\\@

4b-trans OBu

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C22H41B9O3S1\PIOTR\02-May-2010
\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)\\
C5-C5S-CB9-COO-PhOC4, trans start at the HF/6-31G* geom\\0,1\B,0.46355
18174,0.0436752712,0.3833844373\B,0.757787962,0.006304845,2.2299754844

\B,2.5789738268,-0.052231853,1.9387537161\B,2.2842100992,-0.0140882,0.
0914011424\C,1.5538310529,0.922007363,1.1743909822\C,1.5916308759,2.41
46268511,1.1462637534\O,1.7988647174,2.9073870505,2.4016671566\C,1.862
6009112,4.2886410298,2.6158234123\C,2.9178273211,4.7494514874,3.391369
1601\C,3.0042794899,6.1032340095,3.727087855\C,2.0220923745,6.99208311
06,3.276022826\O,2.0033091354,8.3321171342,3.5420510383\C,3.0564135641
,8.8889685681,4.3245918305\C,2.7901321065,10.3805329916,4.4706301828\C
,3.8669752867,11.0933000064,5.2976153984\C,3.6004932631,12.5934214,5.4
533987608\H,2.6415085919,12.7749711139,5.9512009783\H,4.3816172081,13.
0771300416,6.0483154548\H,3.5662913106,13.0927580684,4.4788083349\H,3.
9318555658,10.6294453586,6.291206133\H,4.8480893372,10.9436457579,4.82
71180022\H,2.7278689506,10.825471907,3.4699345293\H,1.8063561036,10.51
70357382,4.936295052\H,3.0909804273,8.4033708659,5.3112908967\H,4.0246
572556,8.7133092307,3.8325436343\C,0.9604383002,6.5124991107,2.4938502
113\C,0.8741890995,5.1663999383,2.1640910153\H,0.0562287685,4.80161276
49,1.5560071123\H,0.2088296745,7.2171989011,2.1544518912\H,3.833464470
5,6.444846653,4.334165551\H,3.6674531435,4.0451379997,3.7361307975\O,1
.4545383984,3.0901160698,0.1557226838\H,-0.3881171601,0.5937284705,-0.
227697003\H,0.138854352,0.5222790624,3.0972334058\H,3.4680149708,0.414
9766101,2.5657473941\H,2.9347140276,0.4863940699,-0.7614122352\B,1.259
5933004,-1.4710480604,-0.1656863652\B,0.1690348983,-1.4575414256,1.347
779739\B,1.6770247625,-1.5263440681,2.4461979365\B,2.7703190505,-1.540
761297,0.9322289352\B,1.4341621059,-2.5343363748,1.1234177142\S,1.3837
278234,-4.4165390969,1.1124144311\C,2.510171944,-4.8988658534,-0.26467
78408\C,2.269638754,-6.3525538022,-0.6734257146\C,0.8519599594,-6.6404
029481,-1.2091367044\C,-0.2257447513,-6.2956541156,-0.1613133651\C,-0.
2129123659,-4.8346139436,0.2917698189\C,0.7556038759,-8.104162433,-1.6
812812479\C,-0.5356811834,-8.4772537653,-2.422765854\C,-0.5157549677,-
9.9115292444,-2.9671078966\C,-1.8055740103,-10.308820998,-3.6956055789
\C,-1.7730449099,-11.7399813026,-4.2396657526\H,1.0699764411,-1.875287
2588,-1.2726371\H,-0.9485585707,-1.8349399987,1.5147167366\H,1.8365970
534,-1.9793782426,3.534607454\H,3.8585026172,-1.9884463768,0.744957781
3\H,2.3309745409,-4.1950577308,-1.0817523194\H,3.519616458,-4.73461438
64,0.1177412473\H,2.4840380354,-7.014902605,0.1757461955\H,3.005651872
3,-6.596285203,-1.4491286488\H,0.6876446728,-5.9905399492,-2.082801703
1\H,-1.221374584,-6.4895992923,-0.5740493153\H,-0.1159662491,-6.955111
2975,0.7101103264\H,-0.3349909186,-4.1360358897,-0.5402064095\H,-0.983
3169977,-4.6227290302,1.035904155\H,1.6085876993,-8.3057739171,-2.3433
145759\H,0.8843010068,-8.7690290833,-0.814684302\H,-1.4020874884,-8.36
4013854,-1.7581391049\H,-0.6938686922,-7.7757318519,-3.2542248635\H,0.
3373368645,-10.0284458053,-3.6504203\H,-0.3376097432,-10.6119377376,-2
.1386342606\H,-2.6569067482,-10.196296383,-3.0106797594\H,-1.985841170
3,-9.6067793655,-4.5209009769\H,-2.7056506558,-11.9935730745,-4.753428
6474\H,-0.9530057009,-11.8738261779,-4.9541694377\H,-1.629385629,-12.4
676725572,-3.432968403\\Version=EM64L-G09RevA.02\State=1-A\HF=-1710.77
89609\RMSD=8.093e-09\RMSF=4.110e-06\Dipole=0.035077,-3.628231,-0.37618
43\Quadrupole=-16.9661819,36.2918382,-19.3256563,12.1177017,5.5023035,
26.4950087\PG=C01 [X(C22H41B9O3S1)]\\@

4b-cis OBu

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C22H41B9O3S1\PIOTR\02-May-2010
\0\\#P B3LYP/6-31G(d,p) Fopt Geom(NoAngle, noDistance) freq(noraman)\\
C5-C5S-CB9-COO-PhOC4, cis, start at the HF/6-31G* geom\\0,1\B,-0.52898
22902,0.2007802507,0.152963204\B,-0.5287053234,-0.1713257799,1.9576386
468\B,-1.2758780604,-1.8503172235,1.6125692094\B,-1.2756500259,-1.4778
954851,-0.1950012519\C,-0.052378044,-1.1874127393,0.8070991226\C,1.294
2442986,-1.8203771212,0.6761066949\O,2.2717532217,-0.9077519544,0.9401

181054\C,3.6244693537,-1.258322278,0.8727912646\C,4.1434073331,-2.4238
765581,1.4429658196\C,5.5140651457,-2.6453589822,1.4010631179\C,6.3747
95117,-1.7133734643,0.8023696978\O,7.7026267558,-2.0347306536,0.820900
3692\C,8.6334161804,-1.1296499453,0.2326899385\C,10.0252418975,-1.7256
273011,0.3893149991\C,11.1201492714,-0.8322969124,-0.2062501748\C,12.5
224039821,-1.4286490773,-0.0522580288\C,5.8447867341,-0.5460586055,0.2
409882346\C,4.4658705591,-0.3258400584,0.279663262\O,1.4870980442,-2.9
751437268,0.3819697591\H,0.2324259558,0.8313580856,-0.4987515824\H,0.2
318249696,0.1491347521,2.8060168243\H,-1.1063507371,-2.8771114969,2.17
69779415\H,-1.1069642812,-2.196719098,-1.1198626667\H,3.4846765392,-3.
1501617242,1.9000531758\H,5.9439368024,-3.5432172459,1.8321566555\H,8.
3926006797,-0.9792780251,-0.8302314372\H,8.5726615635,-0.1501852554,0.
7302049037\H,10.216272154,-1.8941979463,1.4562750062\H,10.040725089,-2
.7114789204,-0.0914203622\H,10.9122032581,-0.6591380268,-1.2707783387\
H,11.0886533916,0.1547945327,0.2745493027\H,12.5959855044,-2.40048032,
-0.5526787964\H,13.2840476007,-0.772414999,-0.4850191361\H,12.77393962
5,-1.5808301408,1.0031847741\H,6.4846247015,0.1933481377,-0.2245890495
\H,4.0374788536,0.5751525269,-0.1464194098\B,-2.2784949788,0.024428046
9,-0.2856631456\B,-1.746629409,0.9400782199,1.2464464778\B,-2.27903578
43,-0.5082126834,2.2920432448\B,-2.8011672846,-1.4333888641,0.75593982
93\B,-3.2350488019,0.1597491449,1.0862212333\S,-4.8615224761,1.0949317
682,1.2714962555\C,-5.8712970141,0.7506377877,-0.2343644699\C,-6.35196
18217,-0.6932866628,-0.360078613\C,-7.1837471899,-1.1971569586,0.83586
33252\C,-6.3495393165,-1.1754358117,2.1316126933\C,-5.8649270973,0.213
4960643,2.5448064076\C,-7.7425568619,-2.6014660157,0.5332811466\C,-8.7
58806789,-3.1412385476,1.5488474046\C,-9.3584753861,-4.490523353,1.131
6971962\C,-10.3669958387,-5.0517239411,2.1414286376\C,-10.9615706141,-
6.3971694398,1.7152121112\H,-2.6551246779,0.4118625217,-1.3480843104\H
,-1.7110080262,2.1046465655,1.4869302926\H,-2.6540590853,-0.5737818736
,3.4213855229\H,-3.6116657218,-2.2867968373,0.5778462287\H,-6.70637263
96,1.456182404,-0.1766523792\H,-5.2272011525,1.0446315238,-1.066160010
5\H,-5.4907334648,-1.3511821714,-0.5136866952\H,-6.9578141982,-0.74501
82543,-1.2736768274\H,-8.039400466,-0.5142799984,0.9680565406\H,-6.946
6062947,-1.5532601167,2.9691512848\H,-5.4903098386,-1.8460257844,2.026
316038\H,-6.6989508067,0.8899491281,2.7578861759\H,-5.2168123016,0.177
8903028,3.4233276497\H,-8.2201111523,-2.5726523575,-0.4556431612\H,-6.
904501971,-3.3067657329,0.4426973775\H,-8.2889367992,-3.2549522452,2.5
343900167\H,-9.5690339875,-2.4090528536,1.678431006\H,-9.8468813633,-4
.3839114019,0.1525950812\H,-8.5474106645,-5.2181459498,0.9871387439\H,
-9.8773865757,-5.161122659,3.1186277002\H,-11.1762968432,-4.3233136977
,2.2878903457\H,-11.6765681001,-6.7707998164,2.4550817877\H,-11.487787
513,-6.3127793329,0.7576315931\H,-10.1798395128,-7.1556903371,1.595796
4692\\Version=EM64L-G09RevA.02\State=1-A\HF=-1710.7773814\RMSD=5.467e-
09\RMSF=2.685e-06\Dipole=-3.1075895,1.1521199,0.0654864\Quadrupole=45.
3375618,-23.486911,-21.8506507,-2.1190815,-5.6800082,-3.89053\PG=C01 [
X(C22H41B9O3S1)]\\@

11

GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C23H31B8N1O3\PIOTR\30-Apr-2010
\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck #P freq=
noraman\\C7O-Ph-B2C8-COO-Ph-CN,C1 start at CB9 geom\\0,1\B,0.136423891
9,0.852107281,1.275160331\B,-0.1442258457,-0.9711404781,1.4124466537\B
,1.6494568553,-1.2729778128,1.0048992154\B,1.9280625698,0.5483164929,0
.8581187716\B,0.742767574,1.0171624548,-0.4195444702\B,-0.7119005827,-
0.0557613047,-0.0362569928\B,0.3503910199,-1.5579509966,-0.2202143218\
B,1.8014856331,-0.4854059035,-0.6139011502\C,0.3273814218,-0.307947037
8,-1.2412675264\C,-0.0138497116,-0.3676936037,-2.6898848681\C,0.785060

0236,0.2733891087,-3.640964305\C,0.4781973722,0.2238901211,-5.00098830
01\C,-0.6531103558,-0.4808448465,-5.4315683712\O,-1.0486348678,-0.5966
181135,-6.7280151452\C,-0.2600987867,0.0190990815,-7.7488140097\C,-0.9
225190233,-0.2708615215,-9.0877047627\C,-0.1468601909,0.3286396692,-10
.267095522\C,-0.8078885315,0.0562744846,-11.6240050855\C,-0.030904768,
0.6409131373,-12.8095382603\C,-0.6924083795,0.3749623712,-14.167320677
4\C,0.092340617,0.9576680268,-15.346386464\H,0.1979786449,2.0446014615
,-15.2541237045\H,1.1009414321,0.5323116319,-15.4002282587\H,-0.405614
8833,0.7523159934,-16.2994401327\H,-0.8103946264,-0.708343455,-14.3057
015191\H,-1.7087616375,0.791614471,-14.1619464975\H,0.0848710204,1.725
3083267,-12.6696422022\H,0.9876314648,0.2268310119,-12.8162949279\H,-0
.918858073,-1.0284926031,-11.761384686\H,-1.8273772152,0.4668207973,-1
1.6184694914\H,-0.0447296655,1.4140192644,-10.1263953035\H,0.875747112
1,-0.0743864748,-10.2759135708\H,-1.0099152311,-1.3575890965,-9.206951
8217\H,-1.9446931748,0.1262248329,-9.0662646955\H,-0.1985764239,1.1024
739184,-7.5715038742\H,0.7625139443,-0.3843054223,-7.7239383075\C,-1.4
630211659,-1.1277632313,-4.4848643125\C,-1.1453223516,-1.0701409005,-3
.1362742472\H,-1.7817774553,-1.576884048,-2.4175788472\H,-2.3355620434
,-1.6696670732,-4.8336734477\H,1.1216665914,0.7329289989,-5.7077732866
\H,1.6648533843,0.8225257236,-3.3200929801\C,1.1050554627,-0.173402855
4,2.0383159461\C,1.5043282621,-0.1167704885,3.4785402966\O,0.400373180
2,0.0620668131,4.2618305683\C,0.4743074422,0.1657032234,5.6478580119\C
,1.3761492856,-0.5510041588,6.437880239\C,1.307964723,-0.4154913537,7.
8212935673\C,0.34795972,0.4209792883,8.4131657785\C,-0.5552965968,1.12
70976718,7.6006392119\C,-0.4903643318,0.9973633468,6.2196777828\H,-0.3
608374495,1.7488729476,1.863065247\H,-0.8694229456,-1.5798236387,2.119
8525699\H,2.3744137957,-2.1271978152,1.3798940927\H,2.880949641,1.1943
005791,1.1229135928\H,0.7865387928,2.0593273871,-0.9768440246\H,-1.857
9956569,0.1063073592,-0.2789607715\H,0.0799618866,-2.6390762943,-0.615
9208934\H,2.7189339266,-0.6871446363,-1.3322518267\H,2.1215310506,-1.1
885277824,5.9850501592\H,2.0018172293,-0.9624048249,8.4501567192\H,-1.
299712611,1.7712747513,8.0551555825\H,-1.1779333065,1.5294199336,5.571
8837099\O,2.6366122399,-0.2100290572,3.8786638338\C,0.2872233073,0.552
0844964,9.8392924607\N,0.2360473697,0.6590123697,10.9966245219\\Versio
n=EM64L-G09RevA.02\State=1-A\HF=-1374.5328652\RMSD=2.982e-09\RMSF=2.08
5e-06\Dipole=-0.3736445,0.0756333,-3.1692468\Quadrupole=13.419546,16.4
551556,-29.8747015,-1.4531795,-5.8452064,-6.4948542\PG=C01 [X(C23H31B8
N1O3)]\\

6CHBT

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C19H27N1S1\PIOTR\09-May-2010\0
\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck freq=noram
an\\4-Hexylcyclohexylphenyl-1-isothiocyanate, 6-CHBT, C1 start at HF\\
0,1\C,-0.9412681378,-0.3756718308,0.3573326814\C,-1.049428754,-0.38736
84514,1.8716136304\C,0.0867306483,-0.498501298,2.6896350004\C,-0.01330
75305,-0.5128627337,4.0760080209\C,-1.2756551715,-0.4143094322,4.68315
37814\C,-2.4240289862,-0.3013531469,3.8862540705\C,-2.2983906142,-0.28
92743634,2.5003380005\N,-1.3840764575,-0.4290236128,6.0524069071\C,-0.
3497043384,-1.688404424,-0.2034917928\C,-0.2721945,-1.6673261285,-1.73
62766906\C,0.5221534893,-0.4637862389,-2.2761329979\C,-0.0616224387,0.
8430628558,-1.7063309478\C,-0.1383228878,0.8324769201,-0.1722396849\C,
-1.479944101,-0.4424808401,7.2343074406\S,-1.6087833483,-0.4613967047,
8.8250089395\C,0.5697868401,-0.4821334123,-3.8146944967\C,1.4886852666
,0.5647814505,-4.4594130249\C,1.5689571718,0.435071313,-5.9859022067\C
,2.4677068002,1.4874349189,-6.6463030074\C,2.5467411822,1.3566652551,-
8.1722388334\C,3.4380314819,2.4168108633,-8.8258491039\H,-1.9624816685

,-0.2846693123,-0.040334062\H,1.0714786772,-0.5765858346,2.2382995519\
H,0.870655018,-0.5999657345,4.6985783144\H,-3.3968035484,-0.2251793551
,4.3599275587\H,-3.1944532489,-0.2017642178,1.8916866359\H,0.657645727
8,-1.8362253341,0.2095931685\H,-0.9508411828,-2.5399803614,0.136004647
8\H,-1.2913526992,-1.6350759684,-2.1496051584\H,0.1762692713,-2.601193
3158,-2.0974591811\H,1.5567165395,-0.555854293,-1.9062086062\H,0.53255
23161,1.7041476694,-2.0314819852\H,-1.0711419446,0.9895493745,-2.11943
22173\H,0.8790810471,0.8001124364,0.2412466836\H,-0.5892006525,1.76328
73718,0.1911966645\H,0.8951485664,-1.4808087949,-4.1388952075\H,-0.451
2506254,-0.3580836555,-4.2052115655\H,1.1434937749,1.5756970618,-4.207
0298287\H,2.4985927467,0.4731451267,-4.0341711933\H,1.9331673265,-0.56
90294215,-6.2462798507\H,0.556565765,0.5071998599,-6.4087411647\H,2.10
15950189,2.4915705957,-6.3881084603\H,3.4807271638,1.4183588082,-6.224
2273404\H,2.9181580242,0.3556136844,-8.4304818739\H,1.5338477984,1.420
6040002,-8.5927807045\H,3.0712810392,3.4276709584,-8.6141743871\H,4.46
67874509,2.3555946479,-8.4527374397\H,3.4720816842,2.2970820446,-9.913
5896846\\Version=EM64L-G09RevA.02\State=1-A\HF=-1193.2960565\RMSD=3.12
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.4358691,9.5300465,-23.9659156,-1.1166665,6.2300772,1.6734078\PG=C01 [
X(C19H27N1S1)]\\@

ClEster

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C29H45Cl1O2\PIOTR\09-May-2010\
0\\#P B3LYP/6-31G(d,p) FOpt SCF=Direct Geom=(NoDistance,NoAngle) fchec
k freq=noraman\\C7-BCO-COO-PhClC7, C1\\0,1\C,2.0608573378,2.7217946572
,-0.0005276028\C,3.5834697016,2.7261871537,0.2974421457\C,4.2156402845
,1.3425170947,0.0064034497\C,3.778586512,0.9260459706,-1.4185602077\C,
2.2428697351,0.6965537234,-1.4796652618\C,1.5804295746,1.270244319,-0.
1980690172\C,5.7492162031,1.448344164,0.1404177714\C,6.5638443793,0.15
4212787,-0.0054018187\C,8.0746553487,0.3928910356,0.1209836404\C,8.912
8370349,-0.8820242662,-0.033970203\C,10.4216870268,-0.6435842533,0.099
641048\C,11.2627430835,-1.9154943392,-0.0650175353\C,12.7676951801,-1.
6676138932,0.0740315975\C,3.6068844536,0.3310858541,1.0067640214\C,2.0
549307636,0.4215692557,1.0118691254\C,0.067495433,1.2363564413,-0.3237
442341\O,-0.3697609483,-0.0545093761,-0.5514276485\C,-1.7235312142,-0.
3039698725,-0.7127110139\C,-2.4708454263,0.3051236593,-1.7206087374\C,
-3.8077924556,-0.0358874418,-1.9013902319\C,-4.430179881,-0.9929062261
,-1.0886668232\C,-3.6705233374,-1.6020551501,-0.0844603954\C,-2.332691
4966,-1.259594571,0.1050967007\C,-5.8948941316,-1.3323743729,-1.259502
1878\C,-6.8279379614,-0.4082669761,-0.4515781106\C,-8.3108711068,-0.76
32418476,-0.6099348892\C,-9.2452798762,0.154639638,0.1878387228\C,-10.
7286105117,-0.2066330219,0.0439032877\C,-11.6640801104,0.7117221253,0.
8398354512\C,-13.1429823066,0.3409573542,0.6947844165\Cl,-1.4151463153
,-2.0466624915,1.3760123916\O,-0.6802774436,2.1798726473,-0.2512706702
\H,1.8332959839,3.3001738389,-0.9022843034\H,1.4946449291,3.1891993996
,0.8096683224\H,4.0866818592,3.4927726168,-0.303641097\H,3.7694833981,
2.9865158915,1.3468585622\H,4.2997343341,0.0142641459,-1.7276466045\H,
4.078027758,1.7103780779,-2.1247291141\H,1.8173015073,1.1789167937,-2.
3670605023\H,2.0065157887,-0.3685700832,-1.5568982845\H,5.9744157004,1
.8922949259,1.1210711692\H,6.1077438417,2.1741834717,-0.6040318092\H,6
.3588875197,-0.3147208941,-0.9768391778\H,6.2541198218,-0.5735116293,0
.75584059\H,8.3904703537,1.1277456159,-0.6333021593\H,8.2890368167,0.8
518476257,1.0967124194\H,8.5942696531,-1.619759337,0.7163686585\H,8.70
26421621,-1.3370133985,-1.0125415429\H,10.739975466,0.0990970131,-0.64
61264095\H,10.6332821952,-0.1948708524,1.0808848094\H,11.054131871,-2.
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842,-2.3218813369\H,-6.660034829,0.6313650763,-0.7624653756\H,-6.54753
83465,-0.4558807747,0.6090043908\H,-8.4701341253,-1.8048990332,-0.2964
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upole=9.6474017,-8.3024963,-1.3449054,3.5108279,2.9231587,-1.3732053\P
G=C01 [X(C29H45Cl1O2)]\\@

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