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Electronic Supplementary Information for

Mesogenic, Optical, and Dielectric Properties of 5-Substituted 2-[12-(4-pentyloxyphenyl)-p-carboran-1-yl] [1,3]dioxanes

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1. Numerical Analysis of T_{NI} for series 2[n]

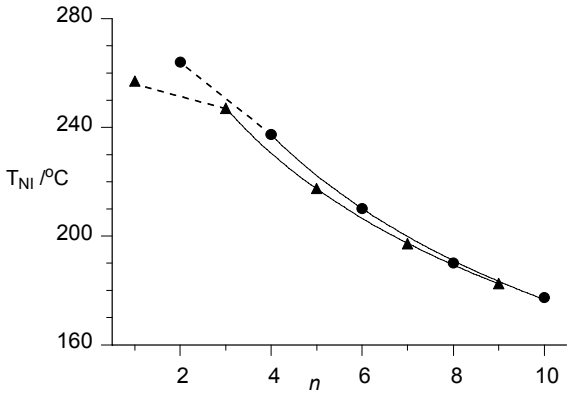
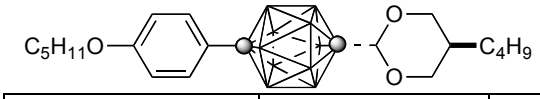


Fig. S1 Nematic-isotropic transition temperatures T_{NI} for **2[n]** as a function of the chain length *n*. Best fit 2-parameter functions of type 1: T_{NI} = 86+exp(5.901–0.441•√n) for odd n excluding **1[1]**, and T_{NI} = 86+exp(5.783-0.405•√n) for even n excluding **1[2]**; r^2 > 0.999. Best fit 2-parameter functions of type 2: T_{NI} = 89•(19.26+ n)/(4.72+n); r^2 > 0.999.

2. Optical Measurements and Order Parameter Calculations

Table S1. Refractive indices of **1[4]** measured at λ = 589 nm as a function of temperature.



Temperature / °C	n_e	n_o	Δn	n_{avrg}
71.5	1.5066	1.680	0.173	1.566
72.6	1.5059	1.678	0.172	1.565
74.8	1.5051	1.676	0.171	1.564
77.5	1.5046	1.674	0.170	1.563
80.1	1.5040	1.673	0.169	1.562
82.2	1.5033	1.671	0.168	1.561
85.0	1.5030	1.6705	0.168	1.561
86.0	1.5024	1.6700	0.1675	1.560

Orientational order parameter *S* was calculated from equation 1 [1]

$$S = \frac{\alpha}{\Delta\alpha} \bullet \frac{n_e^2 - n_o^2}{n_{avrg}^2 - 1} \qquad \text{Eq 1}$$

or by using the Vuks model (Eq 2).[2]

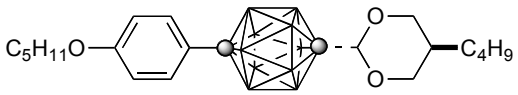
$$S = \frac{3\varepsilon_0 M_w}{\Delta\alpha N_A d} \bullet \frac{n_e^2 - n_o^2}{n_{avrg}^2 + 2} \qquad \text{Eq 2}$$

where $n_{avrg}^2 = (n_e^2 + 2n_o^2)/3$, M_w = 448.6 g/mol, *d* is assumed to be 1.0 g/cm^3, and $\Delta\alpha$ is computed (*vide infra*).

3. Dielectric Data

Dielectric parameters in Table S2 for low concentration solutions of additives **1[4]** to 6-CHBT were obtained from by averaging 5 measurements of each solution in a single cell. Standard deviation of the resulting values ≤ ±0.03. Dielectric permittivity values for the host were obtained by averaging results for 3 cells. All measurements were run at 24 ^{o}C. Error on concentration values ~1.5%

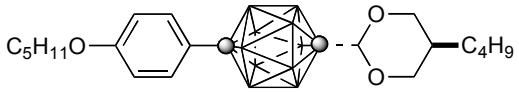
Table S2. Dielectric parameters for **1[4]** as a function of concentration. Average of 5 runs in a single cell**.**



parameter	**Mole fraction**			
	0.00 (host)	0.055	0.107	0.138
V_{TH10} /V	1.55 ±0.02	1.56 ±0.01	1.57 ±0.01	1.62 ±0.01
$\varepsilon_{\|\|}$	12.0 ±0.2	11.65 ±0.03	11.14 ±0.03	10.99 ±0.05
$\varepsilon_{\perp}$	4.0 ±0.1	4.04 ±0.01	4.01 ±0.01	3.99 ±0.03
$\Delta\varepsilon$	8.0 ±0.15	7.60 ±0.03	7.12 ±0.03	7.00 ±0.03

Dielectric parameters for **1[4]** were obtained from 3 cells and each was measured 3 times over the temperature range of 75-105 ^{o}C. The resulting values were averaged and are shown in Table S3. Standard deviation of the resulting values is <±0.1.

Table S3. Dielectric parameters for **1[4]** as a function of temperature. Average of 3 runs for 3 cells. Std for $\varepsilon_{||}$ and $\varepsilon_{\perp}$ is 0.1, and for $\Delta\varepsilon$ is 0.01.



Temperature ^{o}C	Δε	$\varepsilon_{\perp}$	ε||
75	0.42	3.51	3.09
76	0.42	3.50	3.08
77	0.42	3.50	3.08
78	0.41	3.49	3.07
79	0.42	3.49	3.07
80	0.41	3.48	3.07
81	0.41	3.47	3.06
82	0.41	3.46	3.06
83	0.40	3.46	3.05
84	0.41	3.45	3.05
85	0.40	3.45	3.05
86	0.40	3.44	3.05
87	0.40	3.44	3.04
88	0.39	3.42	3.04
89	0.38	3.40	3.05
90	0.38	3.40	3.03
91	0.38	3.40	3.02
92	0.37	3.39	3.02
93	0.34	3.36	3.02
94	0.37	3.37	3.02
95	0.35	3.35	3.01
96	0.33	3.34	3.01
97	0.33	3.34	3.01
98	0.26	3.28	3.03
99	0.11	3.16	3.05
100	0.02	3.09	3.07
101	-0.01	3.06	3.07
102	-0.01	3.06	3.06
103	0.02	3.07	3.06
104	0.000	3.06	3.05
105	0.01	3.07	3.05
106	0.00	3.04	3.04
107	0.03	3.07	3.04
108	0.01	3.05	3.03
109	-0.01	3.02	3.03
110	0.01	3.06	3.03

4. Details for Calculations in the Nematic Phase

The Equations derived from the Maier-Meier theory used in this work were adopted from literature[3,4] and had the following form:

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

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

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

All quantities were in SI units.

• Reaction field factors *F* and *h* for the pure **1[4]** were calculated using the experimental average permittivity and refractive index. For calculations involving extrapolated dielectric parameters for **1[4]**, reaction field factors *F* and *h* were calculated for the pure host 6-CHBT using literature[5] values for $n_{\perp}$ = 1.5212 and $n_{||}$ = 1.6610 and experimental average permittivity. Thus, reaction field parameters *F* and *h* were using the following equations:

$$F = \frac{(2\varepsilon_s+1)(n^2+2)}{3(2\varepsilon_s+n^2)} \qquad h = \frac{3\varepsilon_s}{(2\varepsilon_s+1)}$$

The former is a Dunmur-Toriyama expression for *F*.[6]

	□ °C	ε_{avrg}	$\tilde{n}^2_{avrg}$	*F*	*h*
1[4]	85	3.18	2.44	1.237	1.296
6-CHBT	24	6.27	2.46	1.342	1.289

5. **Quantum-mechanical computational details**

Quantum-mechanical calculations were carried out using Gaussian 98[7] suite of programs. Geometry optimizations for unconstrained conformers of **1[4]** with alkyl chains in the most extended forms were undertaken at the HF/6-31G(d) and B3LYP/3-21G levels of theory using default convergence limits.

6. Dipole moment and polarizability computational results for 1[4]

In all these calculations long molecular axes are oriented along the x axes.

Dipole Moments (D) at the HF/6-31G* level of theory (full geometry optimization)

conformer **A**
Dipole moment (Debye):
X= -1.5463 Y= 1.5440 Z= -0.9778 Tot= 2.3940

conformer **B**
Dipole moment (Debye):
X= -1.7656 Y= -0.7244 Z= 0.2921 Tot= 1.9307

conformer **C** (syn)
Dipole moment (Debye):
X= -1.5956 Y= -0.8343 Z= 1.3418 Tot= 2.2455

conformer **C** (anti)
Dipole moment (Debye):
X= 1.5436 Y= 1.4551 Z= 0.6326 Tot= 2.2137

conformer **D** (syn)
Dipole moment (Debye):
X= -1.8197 Y= 1.0532 Z= 0.1678 Tot= 2.1092

conformer **D** (anti)
Dipole moment (Debye):
X= 1.7613 Y= -0.8804 Z= 0.6423 Tot= 2.0712

conformer **E** (syn)
Dipole moment (Debye):
X= -1.6915 Y= -1.1599 Z= 1.0725 Tot= 2.3145
conformer **E** (anti)
Dipole moment (Debye):
X= -1.5986 Y= -1.5259 Z= 0.4719 Tot= 2.2597

conformer **F** (syn)
Dipole moment (Debye):
X= -1.7397 Y= 0.9756 Z= 0.5976 Tot= 2.0822

conformer **F** (anti)
Dipole moment (Debye):
X= 1.6572 Y= -1.1476 Z= 0.2133 Tot= 2.0270

Electronic polarizabilities (au) at the B3LYP/3-21G level of theory (full geometry optimization) for selected conformers of **1[4]**

conformer A
```
Exact polarizability: 495.325  -3.203 264.271  -0.969 -13.939 247.030
```

conformer B
```
Exact polarizability: 490.525  -3.808 273.499   1.610   9.954 242.280
```

conformer C (anti)
```
Exact polarizability: 495.381   2.107 272.259   0.826   8.426 238.793
```

conformer D (syn)
```
Exact polarizability: 488.053   3.043 281.919  -2.343   1.224 235.836
```

conformer E (anti)
```
Exact polarizability: 492.909   1.313 276.318  -4.785   0.633 236.187
```

conformer F (syn)
```
Exact polarizability: 490.440   3.952 276.147  -4.038  10.508 239.047
```

7. Preparative Details

NMR spectra were obtained at the 270 MHz (^{1}H) or 67.8 MHz (^{13}C) in $CDCl_3$ and referenced to TMS. Elemental analysis was provided by Instrumental Analysis Center for Chemistry, Graduate School of Science, Tohoku University or at Atlantic Microlab, GA. *p*-Carborane was purchased from Katchem s. r. o. (Prague, Czech Republic). Other chemicals were purchased from Aldrich or Tokyo Kasei Ltd.

***trans*-5-Alkyl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxanes (1[n]) and *trans*-5-Aryl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxanes 2[n] and 3[n]. General procedure**. A solution of 12-(4-pentyloxyphenyl)-*p*-carborane-1-carbaldehyde (**4**, 500 mg, 1.50 mmol), appropriate 2-alkyl-1,3-propanediol (**5[n]**, 2.0 equiv.) or 2-aryl-1,3-propanediol (**6[n]** or **7[n]**, 1.3 equiv.) and a catalytic amount of *p*-toluenesulfonic acid in toluene or xylene (5 mL) was refluxed for 18 hr using Dean-Stark water trap. The mixture was poured into saturated aqueous $NaHCO_3$ and extracted with AcOEt. The organic layer was washed with brine, dried ($MgSO_4$) and concentrated under reduced pressure. The crude product was purified by silica gel flash column chromatography (**5[n]**: *n*-hexane/benzene, 8:1; **6[n]** and **7[n]**: *n*-hexane/Et_2O, 15:1) and subsequently recrystallized to give colorless crystalline product.

***trans*-5-Methyl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (1[1]).** Yield 36%, rods (*n*-hexane): mp 137-139 °C; ^{1}H NMR δ (ppm) 0.64 (d, *J* = 6.8 Hz, 3 H), 0.90 (t, *J* = 7.2 Hz, 3 H), 1.27-1.45 (m, 4 H), 1.50-3.75 (brm, 10 H), 1.73 (quint., *J* = 7.0 Hz, 2 H), 1.90-2.05 (m, 1 H), 3.16 (t, *J* = 11.5 Hz, 2 H), 3.87 (t, *J* = 6.6 Hz, 2 H), 3.98 (dd, *J* = 4.9 Hz, 11.9 Hz, 2 H), 4.18 (s, 1 H), 6.65 (d, *J* = 8.9 Hz, 2 H), 7.09 (d, *J* = 8.9 Hz, 2 H). Anal. Calcd. for $C_{18}H_{34}B_{10}O_3$: C, 53.17; H, 8.43. Found: C, 53.35; H, 8.44.

***trans*-5-Ethyl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (1[2]).** Yield 41%, prisms (*n*-hexane): mp 116-117 °C; ^{1}H NMR δ (ppm) 0.85 (t, *J* = 7.4 Hz, 3H), 0.91 (t, *J* = 7.0 Hz, 3 H), 1.02 (quint., *J* = 7.3 Hz, 2H), 1.28-1.46 (m, 4H), 1.50-3.75 (brm, 10H), 1.74 (quint., *J* = 7.0 Hz, 2 H), 1.81 (ttt, *J* = 4.5 Hz, 6.8 Hz, 11.3 Hz, 1H), 3.20 (t, *J* = 11.5 Hz, 2H), 3.87 (t, *J* = 6.5 Hz, 2H), 4.06 (dd, *J* = 4.6 Hz, 11.9 Hz, 2H), 4.18 (s, 1H), 6.66 (d, *J* = 8.9 Hz, 2H), 7.10 (d, *J* = 9.2 Hz, 2H). Anal. Calcd. for $C_{19}H_{36}B_{10}O_3$: C, 54.26; H, 8.63. Found: C, 54.52; H, 8.90.

***trans*-5-Propyl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (1[3]).** Yield 34%, prisms (*n*-hexane): mp 86-87 °C; ^{1}H NMR δ (ppm) 0.86 (t, *J* = 7.2 Hz, 3H), 0.91 (t, *J* = 7.0 Hz, 3H), 0.91 (sext, *J* = 7.6 Hz, 2H), 1.22 (quint., *J* = 7.4 Hz, 2H), 1.30-1.44 (m, 4H), 1.50-3.75 (brm, 10H), 1.73 (quint., *J* = 6.9 Hz, 2H), 1.90 (ttt, *J* = 4.8 Hz, 6.8 Hz, 11.3 Hz, 1H), 3.19 (t, *J* = 11.6 Hz, 2H), 3.87 (t, *J* = 6.5 Hz, 2H), 4.03 (dd, *J* = 4.6 Hz, 11.9 Hz, 2H), 4.18 (s, 1 H), 6.65 (d, *J* = 8.9 Hz, 2H), 7.09 (d, *J* = 8.9 Hz, 2H). Anal. Calcd. for $C_{20}H_{38}B_{10}O_3$: C, 55.27; H, 8.81. Found: C, 55.38; H, 8.94.

***trans*-5-Butyl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (1[4]).** Yield 45%, cubes (*n*-hexane/2-propanol): mp 68 °C; ^{1}H NMR δ 0.85-0.99 (m, 2H), 0.85 (t, *J* = 6.9 Hz, 3H), 0.90 (t, *J* = 6.8 Hz, 3H), 1.12-1.42 (m, 8H), 1.50-3.75 (brm, 10 H), 1.73 (quint., *J* = 7.0 Hz, 2H), 1.87 (ttt, *J* = 4.7 Hz, 6.8 Hz, 11.4 Hz, 1H), 3.18 (t, *J* = 11.4 Hz, 2H), 3.86 (t, *J* = 6.5 Hz, 2H), 4.03 (dd, *J* = 4.7 Hz, 11.8 Hz, 2H), 4.17 (s, 1H), 6.34 (d, *J* = 8.9 Hz, 2H), 7.09 (d, *J* = 8.6 Hz, 2H); MS: *m/z* = 448 (M^+), 143 (100 %); HRMS: calcd. for $C_{21}H_{40}B_{10}O_3$: 448.3980. found. 448.3993. Anal. Calcd. for $C_{21}H_{40}B_{10}O_3$: C, 56.22; H, 8.99. Found: C, 55.96; H, 9.03.

***trans*-5-Pentyl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (1[5]).** Yield 51%, cubes (*n*-hexane/2-propanol): mp 89-91 °C; ^{1}H NMR δ 0.85-0.99 (m, 2H), 0.86 (t, *J* = 6.7 Hz, 3H), 0.90 (t, *J* = 6.7 Hz, 3H), 1.16-1.43 (m, 10H), 1.50-3.75 (brm, 10H), 1.73 (quint., *J* = 7.0 Hz, 2H), 1.87 (ttt, *J* = 4.5 Hz, 6.7 Hz, 11.3 Hz, 1H), 3.18 (t, *J* = 11.6 Hz, 2H), 3.86 (t, *J* = 6.5

Hz, 2H), 4.03 (dd, *J* = 4.6 Hz, 11.9 Hz, 2H), 4.17 (s, 1 H), 6.65 (d, *J* = 9.0 Hz, 2H), 7.09 (d, *J* = 9.0 Hz, 2H); MS: *m/z* = 462 (M^+), 69 (100 %); HRMS: calcd. for $C_{22}H_{42}B_{10}O_3$: 462.4137. found. 462.4167. Anal. Calcd. for $C_{22}H_{42}B_{10}O_3$: C, 57.11; H, 9.15. Found: C, 57.20; H, 9.17.

***trans*-5-Hexyl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (1[6]).** Yield 31%, needles (*n*-hexane/2-propanol): mp 62 °C; ^{1}H NMR δ 0.85-0.99 (m, 2H), 0.86 (t, *J* = 6.8 Hz, 3H), 0.90 (t, *J* = 7.0 Hz, 3H), 1.15-1.44 (m, 12H), 1.50-3.75 (brm, 10H), 1.73 (quint., *J* = 6.9 Hz, 2H), 1.87 (ttt, *J* = 4.7Hz, 6.6Hz, 11.3 Hz, 1H), 3.18 (t, *J* = 11.5 Hz, 2H), 3.86 (t, *J* = 6.6 Hz, 2H), 4.03 (dd, *J* = 4.7 Hz, 11.8 Hz, 2H), 4.17 (s, 1H), 6.65 (d, *J* = 8.9 Hz, 2H), 7.09 (d, *J* = 8.9 Hz, 2H); MS: *m/z* = 476 (M^+), 69 (100 %); HRMS: calcd. for $C_{23}H_{44}B_{10}O_3$: 476.4294. found. 476.4299. Anal. Calcd. for $C_{23}H_{44}B_{10}O_3$: C, 57.95; H, 9.30. Found: C, 58.07; H, 9.40.

***trans*-5-Heptyl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (1[7]).** Yield 42%, needles (*n*-hexane/2-propanol): mp 68-69 °C; ^{1}H NMR δ 0.85-0.99 (m, 2 H), 0.87 (t, *J* = 6.8 Hz, 3H), 0.90 (t, *J* = 7.2 Hz, 3H), 1.15-1.45 (m, 14H), 1.50-3.75 (brm, 10H), 1.73 (quint., *J* = 7.0 Hz, 2H), 1.87 (ttt, *J* = 4.7 Hz, 6.5 Hz, 11.3 Hz, 1H), 3.18 (t, *J* = 11.6 Hz, 2H), 3.87 (t, *J* = 6.6 Hz, 2H), 4.03 (dd, *J* = 4.7 Hz, 11.9 Hz, 2 H), 4.17 (s, 1H), 6.65 (d, *J* = 9.0 Hz, 2H), 7.09 (d, *J* = 9.0 Hz, 2H); MS: *m/z* = 490 (M^+), 185 (100 %); HRMS: calcd. for $C_{24}H_{46}B_{10}O_3$: 490.4456. found. 490.4445. Anal. Calcd. for $C_{24}H_{46}B_{10}O_3$: C, 58.74; H, 9.45. Found: C, 58.83; H, 9.55.

***trans*-5-Octyl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (1[8]).** Yield 45%, cubes (*n*-hexane/2-propanol): mp 58 °C; ^{1}H NMR δ 0.85-0.99 (m, 2H), 0.87 (t, *J* = 6.8 Hz, 3H), 0.90 (t, *J* = 7.1 Hz, 3H), 1.15-1.45 (m, 16H), 1.50-3.75 (brm, 10H), 1.73 (quint., *J* = 7.1 Hz, 2 H), 1.87 (ttt, *J* = 4.7 Hz, 6.7 Hz, 11.3 Hz, 1H), 3.18 (t, *J* = 11.5 Hz, 2H), 3.86 (t, *J* = 6.5 Hz, 2 H), 4.03 (dd, *J* = 4.8 Hz, 11.8 Hz, 2H), 4.17 (s, 1H), 6.65 (d, *J* = 9.0 Hz, 2H), 7.09 (d, *J* = 8.9 Hz, 2H); MS: *m/z* = 504 (M^+), 199 (100 %); HRMS: calcd. for $C_{25}H_{48}B_{10}O_3$: 504.4607; found. 504.4605. Anal. Calcd. for $C_{25}H_{48}B_{10}O_3$: C, 59.49; H, 9.59. Found: C, 59.70; H, 9.72.

***trans*-5-Nonyl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (1[9]).** Yield 41%, prisms (*n*-hexane/2-propanol): mp 53 °C; ^{1}H NMR δ 0.85-0.99 (m, 2 H), 0.87 (t, *J* = 6.8 Hz, 3 H), 0.90 (t, *J* = 6.9 Hz, 3H), 1.15-1.45 (m, 18H), 1.50-3.75 (brm, 10 H), 1.73 (quint., *J* = 6.9 Hz, 2H), 1.87 (ttt, *J* = 4.6 Hz, 6.7 Hz, 11.3 Hz, 1H), 3.18 (t, *J* = 11.5 Hz, 2 H), 3.86 (t, *J* = 6.5 Hz, 2 H), 4.03 (dd, *J* = 4.7 Hz, 11.8 Hz, 2H), 4.17 (s, 1H), 6.65 (d, *J* = 8.9 Hz, 2H), 7.09 (d, *J* = 9.0 Hz, 2H); MS: *m/z* = 518 (M^+), 518 (100 %); HRMS: calcd. for $C_{26}H_{50}B_{10}O_3$: 518.4763. found. 518.4745. Anal. Calcd. for $C_{26}H_{50}B_{10}O_3$: C, 60.20; H, 9.71. Found: C, 60.23; H, 9.72.

***trans*-5-Decyl-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (1[10]).** Yield 38%, cubes (*n*-hexane/2-propanol): mp 50-52 °C; ^{1}H NMR δ 0.86-0.99 (m, 2H), 0.88 (t, *J* = 6.9 Hz, 3H), 0.90 (t, *J* = 7.1 Hz, 3H), 1.15-1.45 (m, 20H), 1.50-3.75 (brm, 10H), 1.73 (quint., *J* = 6.8 Hz, 2H), 1.87 (ttt, *J* = 4.6 Hz, 6.7 Hz, 11.3 Hz, 1H), 3.18 (t, *J* = 11.5 Hz, 2H), 3.87 (t, *J* = 6.5 Hz, 2H), 4.03 (dd, *J* = 4.7 Hz, 11.9 Hz, 2H), 4.17 (s, 1H), 6.65 (d, *J* = 9.1 Hz, 2H), 7.09 (d, *J* = 8.9 Hz, 2H); MS: *m/z* = 532 (M^+), 69, 43 (100 %); HRMS: calcd. for $C_{27}H_{52}B_{10}O_3$: 532.4919. found. 532.4909. Anal. Calcd. for $C_{27}H_{52}B_{10}O_3$: C, 60.87; H, 9.84. Found: C, 61.10; H, 10.01.

***trans*-5-(4-Methoxyphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]-dioxane (2[1]).** : Yield 47%, needles (*n*-hexane): mp 128 °C; ^{1}H NMR δ 0.91 (t, *J* = 7.0 Hz, 3H), 1.25-1.45 (m, 4H), 1.50-3.75 (brm, 10H), 1.73 (quint., *J* = 6.8 Hz, 2H), 3.06 (tt, *J* = 4.5, 11.3 Hz, 1H), 3.65 (t, *J* = 11.8 Hz, 2H), 3.77 (s, 3H), 3.87 (t, *J* = 6.6 Hz, 2H), 4.12 (dd, *J* = 4.6 Hz, 11.9 Hz, 2H), 4.34 (s, 1H), 6.66 (d, *J* = 8.9 Hz, 2H), 6.84 (d, *J* = 8.6 Hz, 2H), 7.02 (d, *J* = 8.6 Hz, 2H), 7.10 (d, *J* = 8.6 Hz, 2H): ^{13}C NMR δ 14.0, 22.4, 28.1, 28.9, 39.4, 55.3, 68.0, 72.5, 80.0, 84.6, 98.6, 113.7, 114.3, 128.2, 128.6, 128.7, 128.8, 159.0, 159.2; MS: *m/z* = 498 (M^+), 43, 134 (100 %); HRMS: calcd for $C_{24}H_{38}B_{10}O_4$: 498.3773; found 498.3401. Anal. Calcd. for $C_{24}H_{38}B_{10}O_4$: C, 57.81; H, 7.68. Found: C, 57.65; H, 7.72.

***trans*-5-(4-Ethoxyphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]-dioxane (2[2]).** Yield 72%, needles (*n*-hexane): mp 171°C; ^{1}H NMR δ 0.91 (t, *J* = 7.0 Hz, 3H), 1.25-1.45 (m, 4H), 1.39 (t, *J* = 6.9 Hz, 3H), 1.50-3.75 (brm, 10H), 1.73 (quint., *J* = 6.8 Hz, 2H), 3.05 (tt, *J* = 4.5, 11.3 Hz, 1H), 3.64 (t, *J* = 11.6 Hz, 2H), 3.87 (t, *J* = 6.5 Hz, 2H), 3.99 (q, *J* = 7.0 Hz, 2H), 4.12 (dd, *J* = 4.7 Hz, 12.0 Hz, 2H), 4.34 (s, 1H), 6.66 (d, *J* = 8.9 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 7.00 (d, *J* = 8.6 Hz, 2H), 7.10 (d, *J* = 8.9 Hz, 2H); MS: *m/z* = 512 (M^+), 43, 120, 148 (100 %); HRMS: calcd for $C_{25}H_{40}B_{10}O_4$: 512.3929; found 512.3918. Anal. Calcd. for $C_{25}H_{40}B_{10}O_4$: C, 58.57; H, 7.86; Found: C, 58.68; H, 7.81.

***trans*-5-(4-Propoxyphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]-dioxane (2[3])**. Yield 72%, needles (*n*-hexane): mp 161 °C; ^{1}H NMR δ 0.91 (t, *J* = 7.0 Hz, 3H), 1.01 (t, *J* = 7.4 Hz, 3H), 1.25-1.45 (m, 4H), 1.50-3.75 (brm, 10H), 1.73 (quint., *J* = 6.8 Hz, 2H), 1.75 (sext., *J* = 7.0 Hz, 2H), 3.05 (tt, *J* = 4.4, 11.3 Hz, 1H), 3.64 (t, *J* = 11.6 Hz, 2H), 3.87 (t, *J* = 6.5 Hz, 4H), 4.12 (dd, *J* = 4.6 Hz, 11.9 Hz, 2H), 4.34 (s, 1H), 6.66 (d, *J* = 8.6 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 2H), 7.01 (d, *J* = 8.6 Hz, 2H), 7.10 (d, *J* = 8.6 Hz, 2H); MS: *m/z* = 526 (M^+), 43, 120,

162 (100 %); HRMS: calcd for $C_{26}H_{42}B_{10}O_4$: 526.4086; found 526.4097. Anal. Calcd. for $C_{26}H_{42}B_{10}O_4$: C, 59.29; H, 8.04; Found: C, 59.45; H, 8.09.

***trans*-5-(4-Butoxyphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]-dioxane (2[4])**. Yield 34%, needles (*n*-hexane): mp 139-140 °C; ^{1}H NMR δ 0.91 (t, *J* = 7.0 Hz, 3H), 0.96 (t, *J* = 7.4 Hz, 3H), 1.25-1.45 (m, 4H), 1.50-3.75 (brm, 10H), 1.47 (sext., *J* = 7.5 Hz, 2H), 1.73 (quint., *J* = 6.2 Hz, 2H), 1.74 (quint., *J* = 6.8 Hz, 2H), 3.05 (tt, *J* = 4.6, 11.3 Hz, 1H), 3.64 (t, *J* = 11.6 Hz, 2H), 3.87 (t, *J* = 6.2 Hz, 2H), 3.92 (t, *J* = 6.5 Hz, 2H), 4.12 (dd, *J* = 4.7 Hz, 11.7 Hz, 2H), 4.34 (s, 1H), 6.66 (d, *J* = 8.9 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 2H), 7.00 (d, *J* = 8.9 Hz, 2H), 7.10 (d, *J* = 8.9 Hz, 2H); MS: *m/z* = 540 (M^+), 43, 120, 176 (100 %); HRMS: calcd for $C_{27}H_{44}B_{10}O_4$: 540.4243; found 540.4239. Anal. Calcd. for $C_{27}H_{44}B_{10}O_4$: C, 59.97; H, 8.20. Found: C, 60.15; H, 8.24.

***trans*-5-(4-Pentyloxyphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]-dioxane (2[5])**. Yield 42%, needles (*n*-hexane): mp 144 °C; ^{1}H NMR δ 0.91 (t, *J* = 6.9 Hz, 3H), 0.92 (t, *J* = 6.6 Hz, 3H), 1.25-1.45 (m, 8H), 1.50-3.75 (brm, 10H), 1.68-1.82 (m, 4H), 3.05 (tt, 4.5, 11.6 Hz, 1H), 3.64 (t, *J* = 11.8 Hz, 2H), 3.87 (t, *J* = 6.5 Hz, 2H), 3.90 (t, *J* = 6.6 Hz, 2H), 4.11 (dd, *J* = 4.7 Hz, 11.7 Hz, 2H), 4.34 (s, 1 H), 6.66 (d, *J* = 8.9 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 7.00 (d, *J* = 8.6 Hz, 2H), 7.10 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR δ 14.0, 22.4, 28.09, 28.12, 28.8, 28.9, 39.3, 67.85, 67.89, 72.4, 79.9, 84.5, 113.5, 114.6, 128.0, 128.3, 128.4, 158.3, 158.9; MS: *m/z* = 554 (M^+), 43, 120, 190 (100 %); HRMS: calcd. for $C_{28}H_{46}B_{10}O_4$: 554.4399; found: 554.4401. Anal. Calcd. for $C_{28}H_{46}B_{10}O_4$: C, 60.62; H, 8.36. Found: C, 60.59; H, 8.19.

***trans*-5-(4-Hexyloxyphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]-dioxane (2[6])**. Yield 59%, needles (*n*-hexane): mp 145 °C; ^{1}H NMR δ 0.89 (t, *J* = 6.5 Hz, 3H), 0.91 (t, *J* = 6.8 Hz, 3H), 1.25-1.45 (m, 10H), 1.50-3.75 (brm, 10H), 1.65-1.82 (m, 4H), 3.05 (tt, 4.7, 11.5 Hz, 1H), 3.64 (t, *J* = 11.6 Hz, 2H), 3.87 (t, *J* = 6.8 Hz, 2H), 3.90 (t, *J* = 6.5 Hz, 2H), 4.11 (dd, *J* = 4.7 Hz, 11.7 Hz, 2H), 4.34 (s, 1H), 6.65 (d, *J* = 8.9 Hz, 2H), 6.82 (d, *J* = 8.9 Hz, 2H), 7.00 (d, *J* = 8.9 Hz, 2H), 7.10 (d, *J* = 9.2 Hz, 2H); ^{13}C NMR δ 14.08, 14.10, 22.5, 22.6, 25.8, 28.2, 28.9, 29.2, 31.6, 39.4, 67.9, 68.0, 72.5, 80.0, 84.5, 98.5, 113.6, 114.7, 128.0, 128.4, 128.5, 158.3, 159.0; MS: *m/z* = 568 (M^+), 43, 120 (100 %); HRMS: calcd. for $C_{29}H_{48}B_{10}O_4$: 568.4556; found: 568.4573. Anal. calcd. for $C_{29}H_{48}B_{10}O_4$: C, 61.24; H, 8.51. Found: C, 61.38; H, 8.52.

***trans*-5-(4-Heptyloxyphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]-dioxane (2[7])**. Yield 56%, needles (*n*-hexane): mp 146 °C; ^{1}H NMR δ 0.88 (t, *J* = 6.5 Hz, 3H), 0.91 (t, *J* = 6.9 Hz, 3H), 1.20-1.50 (m, 12H), 1.50-3.75 (brm, 10H), 1.65-1.82 (m, 4H), 3.05 (tt, 4.8, 11.2 Hz, 1H), 3.64 (t, *J* = 11.0 Hz, 2H), 3.87 (t, *J* = 7.2 Hz, 2H), 3.90 (t, *J* = 7.4 Hz, 2H), 4.11 (dd, *J* = 4.3 Hz, 11.0 Hz, 2H), 4.34 (s, 1H), 6.65 (d, *J* = 8.9 Hz, 2H), 6.81 (d, *J* = 8.7 Hz, 2H), 7.00 (d, *J* = 8.7 Hz, 2H), 7.10 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR δ 159.0, 158.4, 128.6, 128.4, 128.1, 114.7, 113.6, 98.6, 84.6, 80.0, 72.5, 68.0, 67.9, 39.5, 31.8, 29.3, 29.1, 28.9, 28.2, 26.1, 22.7, 22.5, 14.2, 14.1; MS: *m/z* = 582 (M^+), 120, 218 (100 %); HRMS: calcd for $C_{30}H_{50}O_4$: 582.4713; found 582.4718. Anal. Calcd. for $C_{30}H_{50}B_{10}O_4$: C, 61.82; H, 8.65. Found: C, 61.98; H, 8.66.

***trans*-5-(4-Octyloxyphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]-dioxane (2[8])**. Yield 42%, needles (*n*-hexane): mp 124-125 °C; ^{1}H NMR δ 0.88 (t, *J* = 7.0 Hz, 3H), 0.91 (t, *J* = 7.0 Hz, 3H), 1.25-1.45 (m, 14H), 1.50-3.75 (brm, 10H), 1.73 (quint., *J* = 6.9 Hz, 2H), 1.75 (quint., *J* = 6.5 Hz, 2H), 3.05 (tt, *J* = 4.5, 11.4 Hz, 1H), 3.64 (t, *J* = 11.8 Hz, 2H), 3.87 (t, *J* = 6.6 Hz, 2H), 3.90 (t, *J* = 6.6 Hz, 2H), 4.11 (dd, *J* = 4.2 Hz, 11.6 Hz, 2H), 4.34 (s, 1H), 6.66 (d, *J* = 8.9 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 7.00 (d, *J* = 8.6 Hz, 2H), 7.10 (d, *J* = 8.9 Hz, 2H); MS: *m/z* = 597 (M^+), 43, 120 (100 %); HRMS: calcd for $C_{31}H_{52}B_{10}O_4$: 596.4869; found 596.4906. Anal. Calcd. for $C_{31}H_{52}B_{10}O_4$: C, 62.38; H, 8.78. Found: C, 62.56; H, 8.76.

***trans*-5-(4-Nonyloxyphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]-dioxane (2[9])**. Yield 49%, needles (*n*-hexane); mp 124-126 °C; ^{1}H NMR δ 0.88 (t, *J* = 7.0 Hz, 3H), 0.91 (t, *J* = 7.0 Hz, 3H), 1.25-1.45 (m, 16H), 1.50-3.75 (brm, 10H), 1.65-1.82 (m, 4H), 3.05 (tt, *J* = 4.6, 11.3 Hz, 1H), 3.64 (t, *J* = 11.7 Hz, 2H), 3.87 (t, *J* = 6.6 Hz, 2H), 3.90 (t, *J* = 6.5 Hz, 2H), 4.11 (dd, *J* = 5.0 Hz, 11.7 Hz, 2H), 4.34 (s, 1H), 6.66 (d, *J* = 8.9 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 7.00 (d, *J* = 8.6 Hz, 2H), 7.10 (d, *J* = 8.6 Hz, 2H); MS: *m/z* = 611 (M^+), 43, 120, 246 (100 %). Anal. Calcd. for $C_{32}H_{54}B_{10}O_4$: C, 62.92; H, 8.91. Found: C, 62.93; H, 8.92.

***trans*-5-(4-Decyloxyphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]-dioxane (2[10])**. Yield 45%, needles (*n*-hexane): mp 125-126 °C; ^{1}H NMR δ 0.88 (t, *J* = 7.0 Hz, 3H), 0.91 (t, *J* = 7.0 Hz, 3H), 1.25-1.45 (m, 18H), 1.50-3.75 (brm, 10H), 1.65-1.82 (m, 4H), 3.05 (tt, *J* = 4.7, 11.5 Hz, 1H), 3.64 (t, *J* = 11.6 Hz, 2H), 3.87 (t, *J* = 6.5 Hz, 2H), 3.90 (t, *J* = 6.5 Hz, 2H), 4.12 (dd, *J* = 4.7 Hz, 12.0 Hz, 2H), 4.34 (s, 1H), 6.66 (d, *J* = 8.9 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 6.99 (d, *J* = 8.6 Hz, 2H), 7.10 (d, *J* = 9.2 Hz, 2H); MS: *m/z* = 625 (M^+), 43, 69, 120 (100

%); HRMS: calcd for $C_{33}H_{56}B_{10}O_4$: 624.5182; found 624.5218. Anal. Calcd. for $C_{33}H_{56}B_{10}O_4$: C, 63.43; H, 9.03. Found: C, 63.62; H, 9.06.

***trans*-5-(4-pentylphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (3[5])**. Yield 51%, needles (*n*-hexane): mp 144 °C; ^{1}H NMR δ 0.88 (t, *J* = 6.8 Hz, 3H), 0.91 (t, *J* = 7.0 Hz, 3H), 1.29-1.42 (m, 8H), 1.50-3.75 (brm, 10H), 1.57 (quint., *J* = 7.7 Hz, 2H), 1.73 (quint., *J* = 6.8 Hz, 2H), 2.55 (t, *J* = 7.7 Hz, 2H), 3.08 (tt, 4.7, 11.5 Hz, 1H), 3.67 (t, *J* = 11.6 Hz, 2H), 3.87 (t, *J* = 6.5 Hz, 2H), 4.14 (dd, *J* = 4.6 Hz, 11.9 Hz, 2H), 4.35 (s, 1H), 6.66 (d, *J* = 8.9 Hz, 2H), 7.00 (d, *J* = 8.1 Hz, 2H), 7.10 (d, *J* = 8.9 Hz, 2H), 7.11 (d, *J* = 7.8 Hz, 2H); ^{13}C NMR δ 14.1, 22.5, 22.6, 28.2, 28.9, 31.1, 31.5, 35.5, 39.9, 67.9, 72.3, 80.0, 84.6, 98.5, 113.6, 127.3, 128.0, 128.5, 128.6, 133.7, 142.1, 158.9; MS: *m/z* = 538 (M^+), 117, 174 (100 %); HRMS: calcd. for $C_{28}H_{46}B_{10}O_3$: 538.4450; found: 538.4473. Anal. Calcd. for $C_{28}H_{46}B_{10}O_3$: C, 62.42; H, 8.61. Found: C, 62.47; H, 8.40.

***trans*-5-(4-Hexylphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (3[6])**. Yield 62%, needles (*n*-hexane): mp 148 °C; ^{1}H NMR δ 0.87 (t, *J* = 6.5 Hz, 3H), 0.91 (t, *J* = 6.9 Hz, 3H), 1.20-1.45 (m, 10H), 1.50-3.75 (brm, 10H), 1.47-1.62 (m, 2H), 1.73 (quint., *J* = 6.9 Hz, 2H), 2.55 (t, *J* = 7.7 Hz, 2H), 3.08 (tt, 4.6, 11.3 Hz, 1H), 3.67 (t, *J* = 11.6 Hz, 2H), 3.87 (t, *J* = 6.5 Hz, 2H), 4.14 (dd, *J* = 4.5 Hz, 12.0 Hz, 2H), 4.35 (s, 1H), 6.66 (d, *J* = 8.9 Hz, 2H), 7.00 (d, *J* = 8.1 Hz, 2H), 7.10 (d, *J* = 9.2 Hz, 2H), 7.11 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR δ 14.1, 14.2, 22.5, 22.6, 28.2, 28.9, 29.0, 31.4, 31.7, 35.6, 39.9, 67.9, 72.3, 80.0, 84.5, 98.5, 113.6, 127.2, 128.0, 128.5, 128.6, 133.7, 142.1, 159.0; MS: *m/z* = 552 (M^+), 43, 117, 188 (100 %); HRMS: calcd. for $C_{29}H_{48}B_{10}O_3$: 552.4607; found: 552.4612. Anal. Calcd. for $C_{29}H_{48}B_{10}O_3$: C, 63.01; H, 8.75. Found: C, 62.81; H, 8.56.

***trans*-5-(4-Heptylphenyl)-2-[12-(4-pentyloxyphenyl)-*p*-carboran-1-yl)[1,3]dioxane (3[7]).** Yield 52%, needles (*n*-hexane): mp 155 °C; ^{1}H NMR δ 0.87 (t, *J* = 6.8 Hz, 3H), 0.91 (t, *J* = 7.2 Hz, 3H), 1.20-1.45 (m, 12H), 1.50-3.75 (brm, 10H), 1.47-1.62 (m, 2H), 1.73 (quint., *J* = 6.6 Hz, 2H), 2.55 (t, *J* = 7.7 Hz, 2H), 3.08 (tt, 4.6, 11.6 Hz, 1H), 3.67 (t, *J* = 11.6 Hz, 2H), 3.87 (t, *J* = 6.6 Hz, 2H), 4.14 (dd, *J* = 4.6 Hz, 11.9 Hz, 2H), 4.35 (s, 1H), 6.66 (d, *J* = 8.9 Hz, 2H), 7.00 (d, *J* = 8.4 Hz, 2H), 7.10 (d, *J* = 8.9 Hz, 2H), 7.11 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR δ 14.1, 14.2, 22.5, 22.7, 28.2, 28.9, 29.2, 29.3, 31.5, 31.8, 35.6, 39.9, 67.9, 72.3, 80.0, 84.5, 98.5, 113.6, 127.2, 128.0, 128.5, 128.7, 133.7, 142.1, 159.0; MS: *m/z* = 566 (M^+), 43, 117, 202 (100 %);

HRMS: calcd. for $C_{30}H_{50}B_{10}O_3$: 566.4763; found: 566.4746. Anal. Calcd. for $C_{30}H_{50}B_{10}O_3$: C, 63.57; H, 8.89. Found: C, 63.59; H, 8.72.

12-(4-Pentyloxyphenyl)-*p*-carborane-1-carbaldehyde (4). To a stirred solution of 1-(4-pentyloxyphenyl)-*p*-carborane[8] (**13**, 1.00 g, 3.27 mmol) in anhydrous Et_2O (10 mL) was added dropwise a 1.6 M solution of n-BuLi (2.51 mL, 3.92 mmol) at 0 °C under argon atmosphere and the reaction mixture was stirred at room temperature for 30 min. Then HCO_2Et (0.32 mL, 3.92 mmol) was added at -78 °C and the reaction mixture was stirred at room temperature for 24 hr. The mixture was poured into water and the whole was extracted with AcOEt. The organic layer was washed with brine, dried ($MgSO_4$), and concentrated. The crude product was purified by silica gel column chromatography (hexane/CH_2Cl_2, 15:1) to give 0.802 g (74% yield) of aldehyde **4** as colorless powder (*n*-hexane): mp 59 ºC; ^{1}H NMR δ 0.91 (t, *J* = 7.1 Hz, 3H), 1.29-1.45 (m, 4H), 1.50-3.75 (brm, 10H), 1.74 (quint., J = 6.9 Hz, 2H), 3.88 (t, *J* = 6.5 Hz, 2H), 6.67 (d, *J* = 9.1 Hz, 2H), 7.11 (d, *J* = 8.9 Hz, 2H), 8.88 (s, 1H). Anal. Calcd. for $C_{14}H_{26}B_{10}O_2$: C, 50.27; H, 7.84. Found: C, 50.46; H, 7.77.

2-Alkyl-1,3-propanediols (5[n]), 2-(4-Alkyloxyphenyl)-1,3-propanediols (6[n]), and 2-(4-alkylphenyl)-1,3-propanediols (7[n]). General procedure. To a solution of corresponding diethyl alkylmalonate (**8[n]**) or diethyl arylmalonate (**9[n]** or **10[n]**) in dry THF was added $LiAlH_4$ (4.0 equiv.) in small potion at 0 °C and the reaction mixture was stirred at ambient temperature for 12-24 hr under argon. Then, the reaction mixture was poured into ice water and added 10 % HCl. The whole was extracted with Et_2O and the organic layer was washed with brine, dried ($MgSO_4$) and concentrated. The crude product **5[n]** was purified by silica gel column chromatography (hexane/AcOEt, 1:1) to give the corresponding 2-alkyl-1,3-propanediol as a colorless oil. The crude 2-aryl-1,3-propanediols were recrystallized from *n*-hexane to give pure colorless products.

2-Butyl-1,3-propanediol (5[4]).[9,10] Yield 73%, oil: ^{1}H NMR δ 0.90 (t, *J* = 6.9 Hz, 3 H), 1.20-1.40 (m, 6 H), 1.70-1.85 (m, 1 H), 2.34 (brs, 2 H), 3.66 (dd, *J* = 7.6, 10.5 Hz, 2 H), 3.83 (dd, *J* = 3.8, 10.5 Hz, 2 H); MS: *m/z* = 132 (M^+), 84 (100); HRMS: calcd. for $C_7H_{16}O_2$: 132.1150; found: 132.1126.

2-Pentyl-1,3-propanediol (5[5]).[11,12] Yield 54%, oil (lit.[11] bp 100-106 °C/0.2 mm Hg): ^{1}H NMR δ 0.89 (t, *J* = 6.8 Hz, 3H), 1.16-1.40 (m, 8H), 1.71-1.84 (m, 1H), 2.37 (brs, 2H), 3.66 (dd, *J* = 7.7, 10.5 Hz, 2H), 3.82 (dd, *J* = 3.8, 10.5 Hz, 2H); ^{13}C NMR δ 14.13, 22.62, 26.95,

27.73, 32.12, 42.03, 66.8; MS: *m/z* = 147 (M^+), 55 (100); HRMS: calcd. for $C_8H_{18}O_2$: 146.1307; found: 146.1307.

2-Hexyl-1,3-propanediol (5[6]).[11,13] Yield 44%; oil (lit.[11] mp 30-32 °C); ^{1}H NMR δ 0.88 (t, *J* = 6.6 Hz, 3H), 1.20-1.40 (m, 10H), 1.70-1.85 (m, 1H), 2.15 (t, *J* = 5.0 Hz, 2H), 3.66 (ddd, *J* = 4.6, 7.4, 10.5 Hz, 2H), 3.82 (ddd, *J* = 4.1, 5.3, 10.2 Hz, 2 H); ^{13}C NMR δ 14.2, 22.7, 27.2, 27.8, 29.6, 31.8, 42.0, 66.8.

2-Heptyl-1,3-propanediol (5[7]).[10] Yield 44%; oil (lit.[10] mp 32-32.1 °C); ^{1}H NMR δ 0.88 (t, *J* = 6.8 Hz, 3H), 1.14-1.40 (m, 12H), 1.65-1.85 (m, 1H), 2.32 (brs, 2H), 3.65 (dd, *J* = 7.6, 10.5 Hz, 2H), 3.82 (dd, *J* = 3.8, 10.5 Hz, 2H); ^{13}C NMR δ 14.2, 22.7, 27.3, 27.8, 29.3, 29.9, 31.9, 42.0, 66.8; MS: *m/z* = 174(M^+), 55(100); HRMS: calcd. for $C_{10}H_{22}O_2$: 174.1620; found: 174.1593. Anal. Calcd. for $C_{10}H_{22}O_2$: C, 68.92; H, 12.72. Found: C, 68.80; H, 12.63.

2-Octyl-1,3-propanediol (5[8]).[13] Yield 68%; leaflets; mp 40-41 °C; ^{1}H NMR δ 0.88 (t, *J* = 6.6 Hz, 3H), 1.20-1.35 (m, 14H), 1.70-1.85 (m, 1H), 2.22 (brs, 2H), 3.66 (dd, *J* = 7.6, 10.5 Hz, 2H), 3.83 (dd, *J* = 3.5, 10.5 Hz, 2H); ^{13}C NMR δ 14.2, 22.7, 27.3, 27.8, 29.4, 29.6, 30.0, 31.9, 42.0, 66.8; MS: *m/z* = 188 (M^+), 41, 55 (100 %); HRMS: calcd. for $C_{11}H_{24}O_2$: 188.1776; found: 188.1806. Anal. Calcd. for $C_{11}H_{24}O_2$: C, 70.16; H, 12.85. Found: C, 70.23; H, 13.07.

2-Nonyl-1,3-propanediol (5[9]). Yield 63%; leaflets: mp 44-45 °C; ^{1}H NMR δ 0.88 (t, *J* = 6.5 Hz, 3H), 1.20-1.40 (m, 16H), 1.70-1.85 (m, 1H), 2.22 (brs, 2H), 3.66 (dd, *J* = 7.6, 10.5 Hz, 2H), 3.83 (dd, *J* = 3.8, 10.5 Hz, 2H); MS: *m/z* = 203 (M^+), 43 (100 %); HRMS: calcd. for $C_{12}H_{26}O_2$: 202.1933; found: 202.1915. Anal. calcd. for $C_{12}H_{26}O_2$: C, 71.23; H, 12.95. Found: C, 71.44; H, 13.23.

2-Decyl-1,3-propanediol (5[10]).[14] Yield 66%; needles: mp 57 °C (lit.[14] mp 60 °C); ^{1}H NMR δ 0.88 (t, *J* = 7.0 Hz, 3H), 1.20-1.30 (m, 18H), 1.70-1.85 (m, 1H), 2.24 (brs, 2H), 3.66 (dd, *J* = 7.8, 10.5 Hz, 2H), 3.82 (dd, *J* = 3.8, 10.5 Hz, 2H); MS: *m/z* = 216 (M^+), 32, 43, 57 (100 %); HRMS: calcd. for $C_{13}H_{28}O_2$: 216.2089; found: 216.2108. Anal. calcd. for $C_{13}H_{28}O_2$: C, 72.17; H, 13.04. Found: C, 72.26; H, 13.33.

2-(4-Methoxyphenyl)-1,3-propanediol (6[1]).[15,16] Yield 67%: mp 83-85 °C (lit.[16] mp 83-85 °C); ^{1}H NMR δ 2.45 (br s, 2H), 3.07 (tt, *J* = 5.7 Hz, 7.4 Hz, 1H), 3.80 (s, 3H), 3.91 (dd, *J* = 5.7, 10.8 Hz, 2H), 3.98 (dd, *J* = 7.4, 10.9 Hz, 2H), 6.88 (d, *J* = 8.9 Hz, 2H), 7.16 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR δ 49.0, 55.3, 66.1, 114.3, 129.0, 131.1, 158.8.

2-(4-Ethoxyphenyl)-1,3-propanediol (6[2]).[17] Yield 32% for 2 steps from *p*-ethoxyiodobenzene **11[2]**): mp 75-76 °C; ^{1}H NMR δ 1.41 (t, *J* = 7.0 Hz, 3H), 1.93 (br s, 2H), 3.06 (tt, *J* = 5.8 Hz, 7.4 Hz, 1H), 3.87-4.01 (m, 4H), 4.02 (q, *J* =7.0 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 7.15 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR δ 14.8, 48.9, 63.4, 66.1, 114.8, 128.9, 131.0, 158.0; MS: *m/z* = 196 (M^+), 165 (100 %). Anal. Calcd for $C_{11}H_{16}O_3$: C, 67.32; H, 8.22. Found: C, 67.22; H, 8.09.

2-(4-Propoxyphenyl)-1,3-propanediol (6[3]). Yield 30% for 2 steps from *p*-propoxyiodobenzene **11[3]**: mp 68-69 °C; ^{1}H NMR δ 1.03 (t, *J* = 7.4 Hz, 3H), 1.80 (sext., *J* = 7.1 Hz, 2H), 1.89 (t, *J* = 5.6 Hz, 2H), 3.06 (tt, *J* = 5.9 Hz, 7.4 Hz, 1H), 3.85-4.02 (m, 4H), 3.90 (t, *J* =6.5 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 7.15 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR δ 10.5, 22.5, 48.8, 66.0, 69.5, 114.7, 128.9, 131.0, 158.2; MS: *m/z* = 210 (M^+), 179 (100 %). Anal. calcd for $C_{12}H_{18}O_3$: C, 68.54; H, 8.63. Found: C, 68.43; H, 8.86.

2-(4-Butoxyphenyl)-1,3-propanediol (6[4]).[13] Yield 51%; rods: mp 71-72 °C (lit.[13] mp 70-72 °C); ^{1}H NMR δ 0.97 (t, *J* = 7.4 Hz, 3H), 1.49 (q., *J* = 7.5 Hz, 2H), 1.76 (quint., *J* = 7.0 Hz, 2H), 2.00 (br s, 2H), 3.05 (tt, *J* = 5.9 Hz, 7.3 Hz, 1H), 3.87-4.01 (m, 4H), 3.94 (t, *J* = 6.5 Hz, 2H), 6.87 (d, *J* = 8.9 Hz, 2H), 7.14 (d, *J* = 8.6 Hz, 2H); MS: *m/z* = 224 (M^+), 193 (100); HRMS: calcd for $C_{13}H_{20}O_3$: 224.1412; found 224.1413.

2-(4-Pentyloxyphenyl)-1,3-propanediol (6[5]). Yield 69%; leaflets: mp 59 °C; ^{1}H NMR δ 0.93 (t, *J* = 7.2 Hz, 3H), 1.30-1.49 (m, 4H), 1.77 (quint., *J* = 7.0 Hz, 2H), 2.53 (br s, 2H), 3.02 (tt, *J* = 5.7 Hz, 7.6 Hz, 1H), 3.80-4.00 (m, 4H),3.92 (t, *J* = 6.5 Hz, 2H), 6.85 (d, *J* = 8.9 Hz, 2H), 7.11 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR δ 14.1, 22.5, 28.2, 29.0, 48.9, 66.1, 68.0, 114.7, 128.8, 130.8, 158.1; MS: *m/z* = 238 (M^+), 43 (100 %); HRMS: calcd for $C_{14}H_{22}O_3$: 238.1569; found 238.1587. Anal. Calcd for $C_{14}H_{22}O_3$: C, 70.56; H, 9.30. Found: C, 70.35; H, 9.46.

2-(4-Hexyloxyphenyl)-1,3-propanediol (6[6]). Yield 73%; leaflets: mp 60 °C; ^{1}H NMR (270 MHz, $CDCl_3$) δ 0.90 (t, *J* = 6.9 Hz, 3H), 1.25-1.58 (m, 6H), 1.77 (quint., *J* = 7.0 Hz, 2H), 1.94 (br s, 2H), 3.06 (tt, *J* = 5.7 Hz, 7.6 Hz, 1H), 3.85-4.01 (m, 4H),3.93 (t, *J* = 6.6 Hz, 2H), 6.87 (d, *J* = 8.9 Hz, 2H), 7.14 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR δ 14.1, 22.6, 25.7, 29.3, 31.6, 48.8, 66.0, 68.0, 114.6, 128.8, 130.9, 158.0; MS: *m/z* = 252 (M^+), 221 (100 %); HRMS: calcd for $C_{15}H_{24}O_3$: 252.1725; found 252.1716. Anal. Calcd for $C_{15}H_{24}O_3$: C, 71.39; H, 9.59. Found: C, 71.32; H, 9.71.

2-(4-Heptyloxyphenyl)-1,3-propanediol (6[7]). Yield 71%; prisms: mp 58-60 °C; ^{1}H NMR δ 0.89 (t, *J* = 6.5 Hz, 3H), 1.25-1.50 (m, 8H), 1.77 (quint., *J* = 6.9 Hz, 2H), 1.97 (br s, 2H), 3.06 (tt, *J* = 5.7 Hz, 7.6 Hz, 1H), 3.85-4.01 (m, 4H),3.93 (t, *J* = 6.5 Hz, 2H), 6.86 (d, *J* = 8.9 Hz, 2H), 7.14 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR δ 14.1, 22.6, 26.0, 29.1, 29.3, 31.8, 48.9, 66.0, 68.0, 114.7, 128.8, 130.9, 158.1; MS: *m/z* = 266 (M^+), 235 (100 %); HRMS: calcd for $C_{16}H_{26}O_3$: 266.1882; found 266.1866. Anal. Calcd for $C_{16}H_{26}O_3$: C, 72.14; H, 9.84. Found: C, 72.15; H, 10.01.

2-(4-Octyloxyphenyl)-1,3-propanediol (6[8]). Yield 44%; cubes: mp 61-62 °C; ^{1}H NMR δ 0.89 (t, *J* = 6.8 Hz, 3H), 1.25-1.45 (m, 10H), 1.77 (quint., *J* = 7.0 Hz, 2H), 1.94 (br s, 2H), 3.06 (tt, *J* = 5.7 Hz, 7.3 Hz, 1H), 3.87-4.00 (m, 6H), 6.87 (d, *J* = 8.9 Hz, 2H), 7.14 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR δ 14.0, 22.6, 26.0, 29.18, 29.24, 29.3, 31.8, 48.9, 66.1, 68.0, 114.8, 128.9, 130.9, 158.3; MS: *m/z* = 280 (M^+), 249 (100 %); Anal. Calcd for $C_{17}H_{28}O_3$: C, 72.82; H, 10.06. Found: C, 72.95; H, 10.19.

2-(4-Nonyloxyphenyl)-1,3-propanediol (6[9]). Yield 40%; cubes: mp 64-65 °C; ^{1}H NMR δ 0.88 (t, *J* = 6.6 Hz, 3H), 1.20-1.50 (m, 12H), 1.77 (quint., *J* = 7.0 Hz, 2H), 1.99 (br s, 2H), 3.06 (tt, *J* = 5.9 Hz, 7.4 Hz, 1H), 3.82-4.00 (m, 6H), 6.87 (d, *J* = 8.6 Hz, 2H), 7.14 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR δ 14.1, 22.6, 26.0, 29.2, 29.3, 29.4, 29.5, 31.9, 49.0, 66.2, 68.1, 114.9, 129.0, 130.9, 158.4; MS: *m/z* = 294 (M^+), 263 (100 %). Anal. Calcd for $C_{18}H_{30}O_3$: C, 73.43; H, 10.27. Found: C, 73.73; H, 10.40.

2-(4-Decyloxyphenyl)-1,3-propanediol (6[10]). Yield 50%; cubes: mp 69-70 °C; ^{1}H NMR δ 0.88 (t, *J* = 6.6 Hz, 3H), 1.25-1.50 (m, 14H), 1.77 (quint., *J* = 6.9 Hz, 2H), 1.97 (br s, 2H), 3.06 (tt, *J* = 5.9 Hz, 7.3 Hz, 1H), 3.82-4.00 (m, 6H), 6.87 (d, *J* = 8.9 Hz, 2H), 7.14 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR δ 14.1, 22.6, 26.0, 29.2, 29.3, 29.4, 29.52, 29.53, 31.8, 48.8, 66.1, 68.0, 114.7, 128.9, 130.9, 158.2. Anal. Calcd for $C_{19}H_{32}O_3$: C, 73.98; H, 10.46. Found: C, 73.88; H, 10.54.

2-(4-Pentylphenyl)-1,3-propanediol (7[5]).[18] Yield 62%; leaflets (*n*-hexane); mp 71 °C (lit.[18] mp 71.1-73.5 °C) ^{1}H NMR δ 0.89 (t, *J* = 6.8 Hz, 3H), 1.26-1.34 (m, 4H), 1.60 (quint., *J* = 7.5 Hz, 2H), 1.96 (t, *J* = 5.5 Hz, 2H), 2.57 (t, *J* = 7.8 Hz, 2H), 3.08 (tt, *J* = 5.7 Hz, 7.6 Hz, 1H), 3.88-4.04 (m, 4H), 7.14 (s, 4H); MS: *m/z* = 222 (M^+), 174 (100 %); ^{13}C NMR δ 14.0, 22.5, 31.1,

31.5, 35.5, 49.5, 66.1, 127.9, 128.8, 136.3, 142.0; HRMS: calcd for $C_{14}H_{22}O_2$: 222.1620; found 222.1639. Anal. Calcd for $C_{14}H_{22}O_2$: C, 75.63; H, 9.97. Found: C, 75.45; H, 10.22.

2-(4-Hexylphenyl)-1,3-propanediol (7[6]).[13] Yield 56%; prisms: mp 68 °C (lit.[13] mp 72-74 °C); ^{1}H NMR δ 0.88 (t, *J* = 6.8 Hz, 3H), 1.20-1.30 (m, 6H), 1.55-1.65 (m, 2H), 1.94 (t, *J* = 5.6 Hz, 2H), 2.58 (t, *J* = 7.8 Hz, 2H), 3.08 (tt, *J* = 5.7 Hz, 7.6 Hz, 1H), 3.88-4.04 (m, 4H), 7.14 (s, 4H); ^{13}C NMR δ 14.2, 22.7, 29.1, 31.5, 31.7, 35.6, 49.3, 65.9, 127.7, 128.6, 136.2, 141.7; MS: *m/z* = 236 (M^+), 188 (100 %); HRMS: calcd for $C_{15}H_{24}O_2$: 236.1776; found 236.1769. Anal. Calcd for $C_{15}H_{24}O_2$: C, 76.23; H, 10.24. Found: C, 76.04; H, 10.44.

2-(4-Heptylphenyl)-1,3-propanediol (7[7]). Yield 72%; prisms: mp 69-70 °C; ^{1}H NMR δ 0.88 (t, *J* = 6.8 Hz, 3H), 1.25-1.35 (m, 8H), 1.59 (quint., *J* = 7.6 Hz, 2H), 1.93 (t, *J* = 5.4 Hz, 2H), 2.57 (t, *J* = 7.7 Hz, 2H), 3.09 (tt, *J* = 5.7 Hz, 7.6 Hz, 1H), 3.88-4.04 (m, 4H), 7.14 (s, 4H); ^{13}C NMR δ 14.2, 22.7, 29.2, 29.4, 31.5, 31.9, 35.6, 49.3, 66.0, 127.7, 128.7, 136.2, 141.7; MS: *m/z* = 250 (M^+), 202 (100 %); HRMS: calcd for $C_{16}H_{26}O_2$: 250.1933; found 250.1940. Anal. Calcd for $C_{16}H_{26}O_2$: C, 76.75; H, 10.47. Found: C, 76.60; H, 10.68.

Diethyl Arylmalonates 9[n] and 10[n]. General procedure. A double neck flask was charged sequentially with CuI (20 mol %), 2-phenylphenol (40 mol %) and Cs_2CO_3 (1.5 equiv.). The flask was evacuated and backfilled with argon (3 times). The aryl iodide was added followed by diethyl malonate (2.0 equiv) and anhydrous 1,4-dioxane. The reaction mixture was refluxed for 17 hr. Then the reaction mixture was cooled and filtrated through Celite. The filtrate was washed with saturate aqueous NH_4Cl followed by brine, dried over $MgSO_4$ and concentrated. The crude product purified by silica gel flash column chromatography (*n*-hexane/AcOEt, 15:1) to give diethyl arylmalonate as a colorless oil.

Diethyl (4-Methoxyphenyl)malonate (9[1]).[19] Yield 70%; ^{1}H NMR δ 1.26 (t, *J* = 7.0 Hz, 6H), 3.80 (s, 1H), 4.12-4.29 (m, 4H), 4.55 (s, 1H), 6.89 (d, *J* = 8.9 Hz, 2 H), 7.33 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR δ 14.0, 55.2, 57.1, 61.7, 114.0, 124.9, 130.4, 159.5, 168.4.

Diethyl (4-Ethoxyphenyl)malonate (9[2]).[17,19] Isolation of **9[2]** from 2-phenylphenol was not achieved with any solvent system. Therefore the mixture was used in the reduction of malonate **9[2]** with $LiAlH_4$ without further purification.

Diethyl (4-Propoxyphenyl)malonate (9[3]).[19] Isolation of **9[3]** from 2-phenylphenol was not achieved with any solvent system. Therefore the mixture was used in the reduction of malonate **9[3]** with $LiAlH_4$ without further purification.

Diethyl (4-Butoxyphenyl)malonate (9[4]).[19] Yield 30%: ^{1}H NMR δ 0.93 (t, *J* = 6.9 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 6H), 1.33-1.49 (m, 4H), 1.78 (quint., *J* = 6.8 Hz, 2H), 3.94 (t, *J* = 6.6 Hz, 2H), 4.12-4.29 (m, 4H), 4.54 (s, 1H), 6.87 (d, *J* = 8.6 Hz, 2H), 7.30 (d, *J* = 8.6 Hz, 2H).

Diethyl (4-Pentyloxyphenyl)malonate (9[5]).[19] Yield 38%: ^{1}H NMR δ 0.93 (t, *J* = 6.9 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 6H), 1.33-1.49 (m, 4H), 1.78 (quint., *J* = 6.8 Hz, 2H), 3.94 (t, *J* = 6.6 Hz, 2H), 4.12-4.29 (m, 4H), 4.54 (s, 1H), 6.87 (d, *J* = 8.6 Hz, 2H), 7.30 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR δ 14.1, 22.5, 28.2, 29.0, 57.2, 61.7, 67.9, 114.4, 124.5, 130.2, 158.9, 168.3; MS: *m/z* = 322 (M^+), 179 (100); HRMS: calcd for $C_{18}H_{26}O_5$: 322.1780; found 322.1796.

Diethyl (4-Hexyloxyphenyl)malonate (9[6]).[19] Yield 56%: ^{1}H NMR δ 0.90 (t, *J* = 6.8 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 6H), 1.27-1.52 (m, 6H), 1.77 (quint., *J* = 7.0 Hz, 2H), 3.94 (t, *J* = 6.6 Hz, 2H), 4.12-4.29 (m, 4H), 4.54 (s, 1H), 6.87 (d, *J* = 8.6 Hz, 2H), 7.3 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR δ 14.1, 22.7, 25.8, 29.3, 31.6, 57.2, 61.7, 68.0, 114.4, 124.5, 130.2, 158.9, 168.3; MS: *m/z* = 336 (M^+), 179 (100); HRMS: calcd for $C_{19}H_{28}O_5$: 336.1937; found 336.1921.

Diethyl (4-Heptyloxyphenyl)malonate (9[7]).[19] Yield 59%: ^{1}H NMR δ 0.89 (t, *J* = 6.8 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 6H), 1.24-1.52 (m, 8H), 1.77 (quint., *J* = 7.0 Hz, 2H), 3.94 (t, *J* = 6.5 Hz, 2H), 4.12-4.29 (m, 4H), 4.54 (s, 1H), 6.87 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR δ 14.1, 14.2, 22.7, 26.1, 29.1, 29.3, 31.8, 57.2, 61.7, 68.0, 114.4, 124.5, 130.2, 158.9, 168.3; MS: *m/z* = 350 (M^+), 179 (100); HRMS: calcd for $C_{20}H_{30}O_5$: 350.2093; found 350.2071.

Diethyl (4-Octyloxyphenyl)malonate (9[8]).[19] Yield 60%: (lit.[19] mp 26-27 ^{o}C); ^{1}H NMR δ 0.89 (t, *J* = 6.8 Hz, 3H), 1.26 (t, *J* = 7.0 Hz, 6H), 1.23-1.52 (m, 10H), 1.77 (quint., *J* = 6.9 Hz, 2H), 3.94 (t, *J* = 6.6 Hz, 2H), 4.15-4.29 (m, 4H), 4.54 (s, 1H), 6.87 (d, *J* = 8.9 Hz, 2H), 7.3 (d, *J* = 8.9 Hz, 2H); MS: *m/z* = 364 (M^+), 179 (100); HRMS: calcd for $C_{21}H_{32}O_5$: 364.2250; found 364.2241.

Diethyl (4-Nonyloxyphenyl)malonate (9[9]).[19] Yield 67%: ^{1}H NMR δ 0.88 (t, *J* = 6.6 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 6H), 1.20-1.50 (m, 12H), 1.77 (quint., *J* = 7.0 Hz, 2H), 3.94 (t, *J* = 6.6 Hz, 2H), 4.11-4.29 (m, 4H), 4.54 (s, 1H), 6.87 (d, *J* = 8.6 Hz, 2H), 7.30 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR δ 14.0, 14.1, 22.7, 26.0, 29.2, 29.4, 29.5, 31.9, 57.2, 61.7, 68.0, 114.6, 124.7, 130.3,

159.1, 168.5; MS: *m/z* = 378 (M^+), 179 (100); HRMS: calcd for $C_{22}H_{34}O_5$: 378.2406; found 378.2394.

Diethyl (4-Decyloxyphenyl)malonate (9[10]).[19] Yield 66%, rods (*n*-hexane): mp 38 °C; (lit.[19] mp 38-39 °C); ^{1}H NMR δ 0.88 (t, *J* = 6.6 Hz, 3H), 1.26 (t, *J* = 7.0 Hz, 6H), 1.20-1.50 (m, 14H), 1.77 (quint., *J* = 6.9 Hz, 2H), 3.94 (t, *J* = 6.5 Hz, 2H), 4.11-4.29 (m, 4H), 4.54 (s, 1H), 6.87 (d, *J* = 8.6 Hz, 2H), 7.30 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR δ 14.0, 14.1, 22.7, 26.1, 29.26, 29.31, 29.39, 29.56, 29.58, 31.9, 57.2, 61.7, 68.0, 114.6, 124.7, 130.3, 159.1, 168.5; MS: *m/z* = 392 (M^+), 179 (100); HRMS: calcd for $C_{23}H_{36}O_5$: 392.2563; found 392.2554. Anal. Calcd for $C_{23}H_{36}O_5$: C, 70.38; H, 9.24. Found: C, 70.50; H, 9.47.

Diethyl (4-Pentylphenyl)malonate (10[5]).[19] Yield 46%: ^{1}H NMR δ 0.89 (t, *J* = 6.8 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 6H), 1.22-1.30 (m, 4H), 1.61 (quint., *J* = 7.6 Hz, 2H), 2.59 (t, *J* = 7.7 Hz, 2H), 4.11-4.29 (m, 4H), 4.57 (s, 1H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR δ 14.0, 22.5, 31.0, 31.5, 35.6, 57.6, 61.6, 128.4, 128.9, 129.8, 142.7, 168.1; MS: *m/z* = 306 (M^+), 233 (100); HRMS: calcd for $C_{18}H_{26}O_4$: 306.1831; found 306.1825.

Diethyl (4-Hexylphenyl)malonate (10[6]).[19] Yield 36%: ^{1}H NMR δ 0.88 (t, *J* = 6.6 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 6H), 1.26-1.40 (m, 6H), 1.60 (quint., *J* = 7.6 Hz, 2H), 2.59 (t, *J* = 7.7 Hz, 2H), 4.12-4.29 (m, 4H), 4.57 (s, 1H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR δ 13.9, 14.0, 22.5, 28.9, 31.2, 31.6, 35.5, 57.5, 61.5, 128.3, 128.8, 129.8, 142.6, 197.9; MS: *m/z* = 320 (M^+), 247 (100); HRMS: calcd for $C_{19}H_{28}O_4$: 320.1988; found 320.1966.

Diethyl (4-Heptylphenyl)malonate (10[7]). Yield 38%: ^{1}H NMR δ 0.88 (t, *J* = 6.8 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 6H), 1.23-1.35 (m, 8H), 1.60 (quint., *J* = 7.8 Hz, 2H), 2.59 (t, *J* = 7.7 Hz, 2H), 4.12-4.29 (m, 4H), 4.57 (s, 1H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR δ 14.1, 14.2, 22.7, 29.2, 29.4, 31.4, 31.9, 35.7, 57.6, 61.7, 128.5, 128.9, 129.8, 142.8, 168.1; MS: *m/z* = 334 (M^+), 262 (100); HRMS: calcd for $C_{20}H_{30}O_4$: 334.2144; found 334.2157.

8. Archive files for HF/6-31G(d) calculations

1[4] conformer A

```
1\1\GINC-MONSTER\FOpt\RHF\6-31G(d)\C21H40B10O3\PIOTR\19-Jan-2006\0\\#P
  HF/6-31G* FOPT GEOM(NOANGLE, NODISTANCE) FCHECK\\1-(4-Pentyloxyphenyl
 )-12-(5-butyldiox[1,3]an-2-yl)-p-carborane C1, high diople\\0,1\B,-1.3
 438728076,1.5369720748,-0.9756788801\B,-1.3385317418,1.5107808833,0.80
 88764064\B,0.3544845693,1.5422741868,-1.5346191225\B,0.3597738665,1.52
 50901984,1.357533908\B,1.4095111305,1.5348144331,-0.0897124037\B,1.123
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56186,-0.0958915598\B,-0.5839434151,0.0384246785,-1.5418149409\C,-0.11
0209294,-0.7956498126,-0.0996541587\C,-0.1307704136,-2.3137654166,-0.0
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44690186,-0.7767756898\C,-0.1940983094,-5.1254116481,-0.0616793762\O,-
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0.5809735002\C,-0.7585343562,-8.7050736769,0.3325138074\C,-1.730893769
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,1.1630266627\H,3.9528038586,10.6279363341,-0.4881332809\\Version=x86-
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1[4] conformer B

1\1\GINC-MONSTER\FOpt\RHF\6-31G(d)\C21H40B10O3\PIOTR\27-Dec-2005\0\\#P
HF/6-31G* FOPT GEOM(NOANGLE, NODISTANCE) FCHECK\\1-(4-Pentyloxyphenyl
)-12-(5-butyldiox[1,3]an-2-yl)-p-carborane C1, low diople 2\\0,1\B,-1.
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30868\B,-1.7057561861,-0.508316736,0.8828046402\B,-1.2831451764,1.2753
55434,-1.3544417075\B,-1.5645949494,-0.4305065035,-0.8989497764\B,0.06
85257623,0.1294590235,-1.3005045511\B,-0.1972776774,-0.962054415,0.084
323624\B,0.2659578459,1.7796848965,-0.6570962522\B,0.1248683006,1.7019
895601,1.1241074831\B,-0.1600389437,0.0036156486,1.5830608396\C,0.8356
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\H,-1.7713429907,1.7226598466,-2.3275122567\H,-2.2293731045,-1.1266338
637,-1.5721919829\H,0.7160362424,-0.2241317374,-2.2194759509\H,0.22922
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0.085939\PG=C01 [X(C21H40B10O3)]\\@

1[4] conformer C (syn)

1\1\GINC-MASTER\FOpt\RHF\6-31G(d)\C21H40B10O3\PIOTR\12-Mar-2006\0\\#P
HF/6-31G* FOPT GEOM(NOANGLE,NODISTANCE) FCHECK\\1-(4-Pentyloxyphenyl)-
12-(5-butyldiox[1,3]an-2-yl)-p-carborane, C syn\\0,1\B,-1.1922237088,1
.5779882698,-0.5745565968\B,-1.1756492613,1.5850882104,1.2112355875\B,
0.5009260436,1.5206172235,-1.1464560194\B,0.5220973276,1.5535554332,1.
7478270118\B,1.5642248134,1.5023979031,0.2909167211\B,1.2286066741,0.0
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764458\B,-0.4873895865,0.0472828015,-1.119083472\C,-0.0284448839,-0.77
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2190029848,-3.0196920315,0.3633290434\C,-1.2274867779,-4.4089497622,0.
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,-0.6228415802,-8.7033341557,0.4153528143\C,-1.7993757666,-9.680595959
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\C,1.1555659498,-3.0179069389,0.3490023347\C,0.0662915744,2.3511695365
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11152\H,1.92919703,10.5402015811,-3.5733649965\H,0.1796452415,10.62672
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[X(C21H40B10O3)]\\@

1[4] conformer C (anti)

1\1\GINC-MONSTER\FOpt\RHF\6-31G(d)\C21H40B10O3\PIOTR\20-Jan-2006\0\\#P
HF/6-31G* FOPT GEOM(NOANGLE, NODISTANCE) FCHECK\\1-(4-Pentyloxyphenyl
)-12-(5-butyldiox[1,3]an-2-yl)-p-carborane C1\\0,1\B,-1.3485541483,1.5
920553864,-0.8064069107\B,-1.3448028169,1.5926036764,0.9794914137\B,0.
3482875609,1.5260806834,-1.366301707\B,0.3487841142,1.5484346075,1.528
1465928\B,1.401068913,1.4959615783,0.0786033435\B,1.0495784416,0.01809
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46858,0.0736565587,1.5431712459\B,-1.6889718543,0.1078680061,0.0971499
798\B,-0.6494050844,0.0589170313,-1.351442962\C,-0.2060837605,-0.77269
42681,0.1019767679\C,-0.2273209162,-2.290732724,0.111369139\C,-1.41093
44177,-3.008724801,0.1150047514\C,-1.4282303627,-4.3979386255,0.123844
9539\C,-0.2371068197,-5.1030279278,0.1294609467\O,-0.135502453,-6.4443
36446,0.1382441107\C,-1.2924981041,-7.2436042947,0.1408653196\C,-0.850
8336829,-8.6961599625,0.1499204877\C,-2.033565282,-9.6660285235,0.1535
297388\C,-1.6008160316,-11.1333830943,0.1626454224\C,-2.7821106045,-12
.1026148698,0.1662434742\C,0.9630566736,-4.3973365845,0.1259218084\C,0
.9636367188,-3.0218535769,0.1168946525\C,-0.0915181567,2.3541266091,0.
0784568207\C,-0.08610771,3.8867201681,0.1042781161\O,-0.2613872515,4.3
687071069,-1.1773881783\C,-0.2840781625,5.7737079448,-1.2406863169\C,0
.9917411013,6.3645371149,-0.6444713372\C,1.185888328,5.7352199367,0.73
41749121\O,1.0998629672,4.3326626092,0.6516584147\C,0.9304637314,7.895
0893764,-0.6121743177\C,2.2346469879,8.5784374574,-0.1901437919\C,2.15
78936174,10.1042538126,-0.2740930679\C,3.4554074313,10.7901776003,0.15
15068839\H,-2.1463564548,2.232305477,-1.388425298\H,-2.1324329023,2.25

26338555,1.5590578369\H,0.6823576368,2.1122389,-2.3278860907\H,0.67911
17518,2.1606885528,2.4775938736\H,2.4303601889,2.0618101571,0.07301553
33\H,1.838269547,-0.6166038905,1.5892125031\H,1.8305040576,-0.64128827
98,-1.3933960361\H,-0.9711020853,-0.529514512,2.5009674986\H,-2.735040
5516,-0.4302709123,0.1010623349\H,-0.9845493166,-0.5604285585,-2.29637
53424\H,-2.3532832457,-2.4991937132,0.1107058536\H,-2.3746356904,-4.90
21376346,0.1260909002\H,-1.8938467896,-7.0207809515,1.017820737\H,-1.8
908836967,-7.0308056017,-0.7405849166\H,-0.2249764297,-8.8720997271,-0
.7201603052\H,-0.2278425571,-8.8621136733,1.0240155477\H,-2.6605438454
,-9.4734797476,1.0226877181\H,-2.6576704074,-9.4834566968,-0.719834529
5\H,-0.9755222682,-11.3285326227,-0.705598069\H,-0.9783899006,-11.3185
698399,1.03512415\H,-3.4083848643,-11.954764377,1.0415021004\H,-3.4054
826455,-11.9648078429,-0.7127156098\H,-2.4434981205,-13.1338760901,0.1
727074056\H,1.8850212672,-4.9481095599,0.1301289278\H,1.907788377,-2.5
137049246,0.114011606\H,-0.9129431887,4.2267973473,0.7261783602\H,-0.3
908510644,6.029091614,-2.285472413\H,-1.1599619902,6.1470795316,-0.709
4328482\H,1.8215094537,6.0464241669,-1.2703579953\H,0.4316870764,6.106
1914422,1.4291162552\H,2.1595932129,5.9478935293,1.1486955843\H,0.6590
347519,8.2480572245,-1.6052837386\H,0.1261889596,8.2121675627,0.050365
0368\H,2.4932825689,8.2954625079,0.8275804656\H,3.0467972092,8.2240597
954,-0.8220728248\H,1.9124641128,10.3961316407,-1.2928391644\H,1.34048
50986,10.4586877043,0.3502687267\H,3.3704077699,11.8698036495,0.078916
578\H,3.7092857102,10.5469292719,1.1793279261\H,4.2865368754,10.480844
6158,-0.4757527915\\Version=x86-Linux-G98RevA.9\HF=-1290.0278314\RMSD=
4.239e-09\RMSF=2.721e-06\Dipole=-0.5014528,0.7072214,0.0829819\PG=C01
[X(C21H40B10O3)]\\@

1[4] conformer D (syn)

1\1\GINC-MONSTER\FOpt\RHF\6-31G(d)\C21H40B10O3\PIOTR\26-Dec-2005\0\\#P
HF/6-31G* FOPT GEOM(NOANGLE, NODISTANCE) FCHECK\\1-(4-Pentyloxyphenyl
)-12-(5-butyldiox[1,3]an-2-yl)-p-carborane C1, low diople\\0,1\B,-2.16
18110219,0.6405207905,-1.244594003\B,-1.0717900276,2.0552574276,-1.244
0264367\B,-1.1680322643,-0.8275122366,-1.4777299876\B,0.5912808653,1.4
709399098,-1.4972261681\B,0.5379139102,-0.3150802916,-1.6318713353\B,1
.021597631,0.4572568505,-0.1143470548\B,-0.0683648863,-0.957912405,-0.
1003140931\B,0.0301514776,1.9182330968,0.1289236848\B,-1.6722571938,1.
4018462194,0.2770960995\B,-1.7349209431,-0.3755196321,0.1419523537\C,-
0.3885776608,0.4223885309,0.8840002957\C,-0.1889132693,0.2799861806,2.
3823315824\C,-1.0169660392,0.9264673062,3.3018499262\C,-0.8271369972,0
.7913325261,4.6584260837\C,0.2049531763,-0.0004387398,5.152905838\O,0.
3095786338,-0.069926043,6.4922387571\C,1.3210813515,-0.8459152897,7.08
57928595\C,1.17537929,-0.7213799967,8.591887144\C,2.2302241682,-1.5295
306676,9.3493257116\C,2.0934944168,-1.411824973,10.8685131323\C,3.1471
225526,-2.2190578243,11.6255612015\C,1.0380498402,-0.6503183595,4.2577
741584\C,0.8333861316,-0.5041025747,2.8923730337\C,-0.7470572471,0.671
4347628,-2.2145570156\C,-0.9400088581,0.8534887259,-3.7242197946\O,-1.
9200767249,-0.0104791759,-4.1699415298\C,-2.1716079919,0.1042533315,-5
.5491088818\C,-0.8929417456,-0.1173997091,-6.3542044367\C,0.1813683541
,0.7962967403,-5.7664457438\O,0.2589493956,0.6306297225,-4.3707637023\
C,-1.1342024393,0.1100403469,-7.8500181399\C,0.048374946,-0.2570901426
,-8.7515133299\C,-0.2747821366,-0.1135529096,-10.240144135\C,0.9043787
435,-0.4735509509,-11.1430005199\H,-3.2279831607,0.7255008157,-1.73571
82475\H,-1.4255479481,3.0579674907,-1.7551410436\H,-1.5738482677,-1.72
7643823,-2.1140355877\H,1.3424469192,2.0923269883,-2.1567762721\H,1.26
00725799,-0.8754745382,-2.369624842\H,2.0921113023,0.3939817297,0.3728
228656\H,0.2735262494,-1.9704699344,0.3949667813\H,0.4404242635,2.8099
938928,0.7811731345\H,-2.4124129304,1.9737807524,0.9901680224\H,-2.486
0051812,-0.9911222762,0.8095893004\H,-1.8230130302,1.5452405199,2.9629

60628\H,-1.4709283265,1.2935077293,5.3561312732\H,1.2217971154,-1.8824
526758,6.7759216668\H,2.2962317871,-0.4904835142,6.7647794265\H,1.2447
609846,0.3289235906,8.859754433\H,0.1790198731,-1.0517868783,8.8708062
974\H,2.1599427103,-2.5782203612,9.0648846501\H,3.2246755858,-1.198840
359,9.0538376658\H,2.1648971353,-0.3651076099,11.1552494716\H,1.101254
6208,-1.7430715311,11.1662787327\H,3.078819519,-3.2763148517,11.385372
1222\H,4.15070945,-1.8876833347,11.3742519808\H,3.0241528369,-2.115541
976,12.6990440946\H,1.845267309,-1.2699717958,4.5958292588\H,1.4975887
344,-1.0220040036,2.228709821\H,-1.258841938,1.8776020625,-3.912818990
5\H,-2.9232525998,-0.6362059653,-5.7835125188\H,-2.5883979838,1.089104
0541,-5.7615652986\H,-0.5773526554,-1.1442004027,-6.1882375179\H,-0.04
04622984,1.8387217361,-5.997765459\H,1.1658263976,0.5690398742,-6.1464
096887\H,-1.9971815051,-0.480647013,-8.1514748389\H,-1.4075514603,1.15
06827672,-8.019384479\H,0.9064726475,0.3684280432,-8.5167116936\H,0.35
1666638,-1.2820762526,-8.5467225855\H,-1.1243696112,-0.7467992613,-10.
486043818\H,-0.5868033731,0.9085289047,-10.4440760727\H,0.643675891,-0
.3642123217,-12.1909330484\H,1.7593153349,0.1671493045,-10.946452248\H
,1.2191366996,-1.5012521342,-10.985884692\\Version=x86-Linux-G98RevA.9
\HF=-1290.0278142\RMSD=4.154e-09\RMSF=3.459e-06\Dipole=0.2924159,-0.11
93644,-0.7673615\PG=C01 [X(C21H40B10O3)]\\@

1[4] conformer D (anti)

1\1\GINC-MONSTER\FOpt\RHF\6-31G(d)\C21H40B10O3\PIOTR\11-Mar-2006\0\\#P
 HF/6-31G* FOPT GEOM(NOANGLE,NODISTANCE) FCHECK\\1-(4-Pentyloxyphenyl)
-12-(5-butyldiox[1,3]an-2-yl)-p-carborane C1, second orien\\0,1\B,-1.8
919797049,0.740116357,-1.2540825875\B,-0.785899756,2.1422491725,-1.266
0277216\B,-0.9172064234,-0.7395926159,-1.4933511225\B,0.8680745794,1.5
384874343,-1.5329947689\B,0.7930726003,-0.2470507728,-1.663727046\B,1.
299169413,0.5224037634,-0.1521185704\B,0.1932710217,-0.8801488003,-0.1
25589567\B,0.3267122747,1.99514097,0.0972482515\B,-1.3800514637,1.4985
413514,0.2617123102\B,-1.4642467837,-0.2782497725,0.1304859925\C,-0.10
22697071,0.5055449512,0.858922466\C,0.109228146,0.363652466,2.35567898
96\C,-0.702542818,1.0218753904,3.2813616293\C,-0.5019926443,0.88708427
72,4.6364291263\C,0.5249485776,0.0838848268,5.1231375131\O,0.640925549
5,0.0157469872,6.4616034838\C,1.6483650926,-0.7712524605,7.0475279092\
C,1.5178517074,-0.6421291757,8.5546285402\C,2.5697541835,-1.4614699633
,9.304096409\C,2.4482461331,-1.339263722,10.824222204\C,3.4989473915,-
2.1576632383,11.5733073378\C,1.3419904439,-0.577697381,4.2218030847\C,
1.1266571118,-0.4316672231,2.8580234089\C,-0.4857574011,0.7530702268,-
2.2367636022\C,-0.6899355908,0.9346565867,-3.7450209343\O,-1.683377763
1,0.0810196156,-4.1802322855\C,-1.9546364562,0.1935522773,-5.556879104
8\C,-0.68477455,-0.0433579292,-6.372810408\C,0.4038415788,0.8591248516
,-5.7959664002\O,0.5007598884,0.6973033698,-4.4020590758\C,-0.87028296
65,0.2029260611,-7.8735935202\C,-1.8193940302,-0.7770298494,-8.5699190
375\C,-1.8911538547,-0.5583891557,-10.0825689129\C,-2.8415044573,-1.53
04975193,-10.7804570949\H,-2.9614953933,0.836388826,-1.7357895857\H,-1
.132742688,3.1480059898,-1.7758967822\H,-1.3390437453,-1.6361824155,-2
.1242159927\H,1.6203197615,2.1500399887,-2.2004364642\H,1.5020866239,-
0.8169945717,-2.4068919375\H,2.3732314793,0.4478115721,0.3255578508\H,
0.5279535981,-1.8956460568,0.3685800836\H,0.7531081863,2.883263812,0.7
440930142\H,-2.1072404137,2.080086583,0.980326141\H,-2.2163591537,-0.8
840071235,0.8059343297\H,-1.5041135033,1.6497064426,2.9485709179\H,-1.
1332900733,1.3983589693,5.3389266928\H,1.5338105402,-1.8071004946,6.74
06363608\H,2.6247655581,-0.428199438,6.7169890892\H,1.6022684602,0.407
7685033,8.8197563508\H,0.5201710522,-0.9600044098,8.8432212937\H,2.484
3131331,-2.5097740901,9.0223968039\H,3.5653785107,-1.1433136715,8.9989
556545\H,2.5347988537,-0.2929402592,11.1082099692\H,1.454849204,-1.658
0053336,11.1316229008\H,3.4157928273,-3.2144747921,11.3358557695\H,4.5

041127605,-1.8388398816,11.3122596785\H,3.3869793665,-2.0506538672,12.
6476513139\H,2.1447749856,-1.2063387826,4.5537637369\H,1.7785527167,-0
.9587570886,2.1894107178\H,-0.9987233704,1.9620084191,-3.9327150685\H,
-2.7202643985,-0.5374297609,-5.7681345492\H,-2.3612164056,1.1831720642
,-5.7683460266\H,-0.3759501076,-1.0724123656,-6.2081060457\H,0.1929108
817,1.9036925467,-6.026518084\H,1.3771029235,0.6163176464,-6.198501070
7\H,-1.2221823728,1.2212387756,-8.03342979\H,0.10461972,0.1426343523,-
8.3536558872\H,-1.4944723642,-1.7961443713,-8.3690608786\H,-2.82047597
51,-0.6877757996,-8.1544847966\H,-2.2071119636,0.4629215589,-10.284299
2897\H,-0.8950277859,-0.6592723178,-10.5078122141\H,-2.8688793902,-1.3
519719244,-11.8507224555\H,-2.5331212026,-2.5603234228,-10.6246251462\
H,-3.8547463617,-1.4286248146,-10.4023070548\\Version=x86-Linux-G98Rev
A.9\HF=-1290.0278144\RMSD=7.589e-09\RMSF=2.471e-06\Dipole=0.244015,-0.
135667,-0.7655564\PG=C01 [X(C21H40B10O3)]\\@

1[4] conformer E (syn)

1\1\GINC-MONSTER\FOpt\RHF\6-31G(d)\C21H40B10O3\PIOTR\13-Mar-2006\0\\#P
HF/6-31G* FOPT GEOM(NOANGLE,NODISTANCE) FCHECK\\1-(4-Pentyloxyphenyl)
-12-(5-butyldiox[1,3]an-2-yl)-p-carborane C1, E syn\\0,1\B,-0.81503353
59,1.63460455,-0.7209614215\B,-1.107945316,0.4773025708,-2.0478396899\
B,-1.4314990183,0.9098054945,0.7975577046\B,-1.9180079428,-0.952287529
,-1.3614050998\B,-2.1121314179,-0.6911553533,0.4018763094\B,-0.8051109
92,-1.7080856758,-0.2167807189\B,-0.496356495,-0.5624718502,1.11460985
23\B,-0.1808117025,-0.9930811992,-1.7267566556\B,0.4961917219,0.608759
5613,-1.3302441396\B,0.2979653531,0.8760845688,0.4252363708\C,0.600745
5374,-0.7004883706,-0.2143612464\C,1.9690569366,-1.3104925072,0.032558
1426\C,2.1356169381,-2.6752480933,0.275202969\C,3.3805248819,-3.218248
5743,0.4985792578\C,4.5156877666,-2.4132677388,0.4888854969\O,5.686135
3847,-3.0358201218,0.7172414909\C,6.8879611597,-2.3057526315,0.7283456
057\C,8.0178991366,-3.2798694574,1.0101315002\C,9.384610183,-2.5940816
332,1.0463645323\C,10.5316047142,-3.5659995325,1.3296677523\C,11.89714
22836,-2.8812584903,1.3659434854\C,4.3723940329,-1.0566122314,0.251211
3476\C,3.1098297375,-0.5240627289,0.0274479377\C,-2.1937037791,0.61407
9694,-0.7185741152\C,-3.5467654682,1.2655479539,-1.0258512648\O,-3.684
2846383,2.4150923422,-0.2743032892\C,-4.8949617932,3.0944846841,-0.506
9116004\C,-6.0843032102,2.1707418076,-0.2489392595\C,-5.8406910721,0.8
82839826,-1.0326545524\O,-4.560618016,0.3669461111,-0.7610206313\C,-7.
4330690498,2.7967624326,-0.6181838121\C,-7.8381206647,3.9970001914,0.2
428377114\C,-9.2358602134,4.5214951438,-0.0922627602\C,-9.6415912989,5
.7227467421,0.7607238262\H,-0.9243563808,2.7904041229,-0.9145835348\H,
-1.4293987649,0.8800780569,-3.1091227366\H,-1.9372967986,1.5873807214,
1.6129614909\H,-2.7582240554,-1.5065824326,-1.9714098668\H,-3.07232458
31,-1.0838608593,0.9526482455\H,-0.7363099435,-2.8682886324,-0.0369322
75\H,-0.1759314194,-0.9613632177,2.1763402619\H,0.3408373799,-1.674284
4195,-2.5347293065\H,1.4581747741,0.9940416601,-1.8901741059\H,1.13365
36836,1.4344665068,1.039434902\H,1.2876699841,-3.3295266792,0.29215944
74\H,3.4961070904,-4.2697559429,0.6840772648\H,7.033302065,-1.81810906
31,-0.2315516577\H,6.8460556263,-1.5361346006,1.4940044618\H,7.8208148
438,-3.7723107109,1.9579446091\H,8.0065426389,-4.0520249103,0.24635900
93\H,9.5670535474,-2.0939203221,0.0965409378\H,9.3814898603,-1.8144768
886,1.8065004873\H,10.3523128706,-4.0658057818,2.2788628952\H,10.53767
84454,-4.3449826559,0.5706689424\H,12.1203418132,-2.4003886804,0.41773
32955\H,11.9335343272,-2.1190577947,2.1391678743\H,12.688970536,-3.595
4990473,1.5685994616\H,5.2202405506,-0.4002735409,0.2357555296\H,3.036
490533,0.5305633174,-0.1522530941\H,-3.5740511484,1.5281680001,-2.0824
175014\H,-4.8871464295,3.9475122471,0.1544877595\H,-4.9158276861,3.460
3651631,-1.5340902173\H,-6.0784530463,1.9152389939,0.80752633\H,-5.939
1538903,1.0651645238,-2.1030959105\H,-6.5444405661,0.1100345254,-0.757

4962436\H,-7.4211155494,3.0923562713,-1.6664363067\H,-8.2015565081,2.0
31125784,-0.5301985404\H,-7.8026283085,3.7140914008,1.2931731111\H,-7.
1210191802,4.8052570024,0.1194612782\H,-9.2749534992,4.795973105,-1.14
42802432\H,-9.9612368233,3.722024265,0.0416733191\H,-10.6368377845,6.0
696710535,0.5014618575\H,-9.6439428261,5.4705775733,1.8172863902\H,-8.
9552710457,6.5531306285,0.6211735334\\Version=x86-Linux-G98RevA.9\HF=-
1290.0277798\RMSD=5.941e-09\RMSF=2.528e-06\Dipole=-0.3883696,0.7764904
,-0.2745952\PG=C01 [X(C21H40B10O3)]\\@

1[4] conformer E (anti)

1\1\GINC-MONSTER\FOpt\RHF\6-31G(d)\C21H40B10O3\PIOTR\26-Dec-2005\0\\#P
HF/6-31G* FOPT GEOM(NOANGLE, NODISTANCE) FCHECK\\1-(4-Pentyloxyphenyl
)-12-(5-butyldiox[1,3]an-2-yl)-p-carborane C1, high dipole\\0,1\B,-0.7
205093936,1.8900722869,-0.6462302222\B,-1.0008098274,0.7406251569,-1.9
826406295\B,-1.3335837177,1.1481562282,0.8653797348\B,-1.7997269546,-0
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1[4] conformer F (syn)

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21H40B10O3)]\\@

1[4] conformer F (anti)

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12-(5-butyldiox[1,3]an-2-yl)-p-carborane, F anti\\0,1\B,-1.6359929423,1.459169056,-0.7359838319\B,-1.6497467218,1.5095467901,1.048227881\B,0.0701392396,1.5078054294,-1.2821891957\B,0.0378546045,1.606374039,1.6082675248\B,1.1056161513,1.5969679906,0.1678736555\B,0.8589279392,0.1231049324,1.1124858832\B,0.8774502497,0.0536964841,-0.6694249543\B,-0.8380543309,0.0627392642,1.6580081361\B,-1.8721610766,-0.0232604323,0.2073900467\B,-0.8118408529,-0.0254634583,-1.2309964872\C,-0.3273743017,-0.7863080219,0.2428341625\C,-0.2903035786,-2.3038361605,0.272890734\C,0.6819162856,-3.0009955575,0.9694945657\C,0.714513368,-4.3897080572,0.9951732552\C,-0.2443141464,-5.1155501586,0.309749372\O,-0.3089547189,-6.4584928001,0.2658111643\C,0.6430113197,-7.2373667123,0.9474564686\C,0.3037260215,-8.6974674907,0.7065005352\C,1.2789371738,-9.6464631823,1.4049916194\C,0.9471270421,-11.1212049431,1.1693656411\C,1.9211656116,-12.0695798397,1.8670143174\C,-1.2290774339,-4.4309460586,-0.3972535675\C,-1.2480125484,-3.0556029593,-0.4129658089\C,-0.4483971998,2.3384479192,0.1349340712\C,-0.5584245217,3.8672550286,0.1190022921\O,-0.7531457521,4.300209942,-1.1770195954\C,-0.8864179241,5.6972282661,-1.2864740525\C,0.3339065423,6.3986131542,-0.6921211331\C,0.5568026681,5.8222599523,0.704448187\O,0.5835615904,4.4164109294,0.6667195035\C,0.1974450693,7.923960288,-0.6461935466\C,0.1437263519,8.6027717372,-2.0181720389\C,0.1140723015,10.129561672,-1.9227983402\C,0.0546684049,10.8106600721,-3.2894677719\H,-2.471045372,2.0211584597,-1.3459635162\H,-2.4884946086,2.1245824519,1.6050756975\H,0.3612768022,2.091227989,-2.2592393295\H,0.3147506567,2.2658020589,2.5430657349\H,2.0889834988,2.2392886281,0.1603634691\H,1.7033359712,-0.4013681961,1.7413979725\H,1.7144093065,-0.5588879779,-1.2291227828\H,-1.128002634,-0.5376353794,2.6298210107\H,-2.8571896808,-0.6686764409,0.2263789424\H,-1.0867763147,-0.6803158645,-2.1705986094\H,1.4416546695,-2.4749682449,1.5114426375\H,1.4908349136,-4.8773097908,1.5514674421\H,1.6393066882,-7.0098665835,0.5787698928\H,0.6164716575,-7.0082516286,2.0091125981\H,-0.7090689754,-8.8785409609,1.0545879437\H,0.3055368692,-8.8801528325,-0.3641617015\H,2.2919232748,-9.4487523485,1.0580518921\H,1.2782914181,-9.4471519993,2.4754507146\H,-0.0639428295,-11.3214956764,1.5165753964\H,0.9486623176,-11.3230895252,0.1006438908\H,2.9375868268,-11.9166089917,1.5153939803\H,1.9171444656,-11.9150033454,2.9423024153\H,1.6599359299,-13.1066406791,1.6813633388\H,-1.9706644946,-4.9977242975,-0.9284857052\H,-2.021529271,-2.564031486,-0.9695121657\H,-1.4162248646,4.160206052,0.7226463702\H,-1.004262161,5.9013983399,-2.3398392843\H,-1.7941174031,6.017844003,-0.7739607325\H,1.1952171097,6.1281203863,-1.2974469393\H,-0.2311629876,6.1524565422,1.3818412214\H,1.5062602433,6.1333174778,1.1167567655\H,-0.6911546073,8.1917873091,-0.0760995272\H,1.0431533424,8.3269624915,-0.0922116138\H,1.0074710962,8.2959916745,-2.6049729946\H,-0.7333960261,8.2682828451,-2.5672557373\H,-0.7439783686,10.4367550734,-1.3286721101\H,0.9956273701,10.4731926696,-1.3860916878\H,0.0370626197,11.8912334694,-3.1887656731\H,0.9170346742,10.5489240514,-3.895883053\H,-0.835750413,10.5151415416,-3.8370618052\\Version=x86-Linux-G98RevA.9\HF=-1290.0278185\RMSD=4.868e-09\RMSF=2.465e-06\Dipole=0.2242145,0.7098069,0.2861259\PG=C01 [X(C21H40B10O3)]\\@

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