Electronic Supplementary Information for

How much do coulombic interactions stabilize a mesophase? Ionic pair and non-ionic binary isosteric derivatives of monocarbaborates and carboranes

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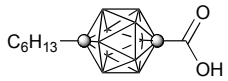
1. Additional synthetic details

4-Undecylphenol (8[11]).[1] A solution of *n*-undecylmagnesium bromide in THF (11.6 mmo1 in 10 mL) was added to a stirred suspension of $PdCl_2(dppf)_2$ (47 mg, 0.2 mmol) and 4-bromophenol (1.00 g, 5.8 mmol) in THF (5 mL) at -78 °C. The mixture was stirred at -78 °C for 15 min, then cooling was removed. After stirring for 3h at 20 °C the mixture was quenched with 5% HCl and extracted with ether. The combined extracts were dried (Na_2SO_4), solvent was evaporated and the crude mixture was passed through a silica gel plug (CH_2Cl_2/hexane, 2:1). The product was further purified by distillation (180 °C / 0.5 mm Hg) to give 0.50 g (35% yield) of phenol **8[11]**, whose ^{1}H NMR was identical with that reported.[1]

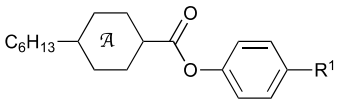
Preparation of [*closo*-1,12-$C_2B_{10}H_{10}$-1-COOH-12-C_6H_{13}] (5[12]).

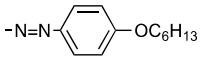


p-Carborane (1.44 g, 10 mmol) was dissolved in dry THF (20 mL), cooled to –80 °C, and 1.8 M *n*-BuLi in hexane (6.0 mL, 10.8 mmol) was added dropwise. After 30 min 1-bromohexane (1.65 g, 10.0 mmol) was added and the mixture was stirred at ambient temperature for 2 hrs. The mixture was cooled to –80 °C and another portion of 1.8 M n-BuLi in hexane (6.0 mL, 10.8 mmol) was added dropwise. After 30 min dry CO_2 gas was passed through the mixture for 40 min. The mixture was evaporated to dryness, dissolved in 2 M KOH and washed with hexanes (2x) to remove 1,12-dihexyl-*p*-carborane. The aqueous layer was acidified and precipitation extracted with ether (3x). The extracts were dried (Na_2SO_4), ether evaporated, and the solid residue dried in vacuum. The crude acid **5[12]** was extracted into hot hexane leaving behind insoluble *p*-carborane-1,12-dicarboxylic acid (0.42 g, 18% yield). Hexane was evaporated and the residue (1.40 g, 51% yield) was purified by sublimation (130 °C /0.3 mm Hg) followed by recrystallization from heptane giving pure acid **5[12]**: mp 126-128 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.84 (t, J = 7.1 Hz, 3H), 1.08-1.25 (m, 8H), 1.5-3.5 (m, 10H), 1.59 (t, J = 7.9 Hz, 2H); {^{1}H}^{11}B NMR (128 MHz, $CDCl_3$) δ –13.5 (5B), –12.7 (5B). Anal. Calc. for $C_9H_{24}B_{10}O_2$: C, 39.68; H, 8.88. Found: C, 39.61; H, 8.98%.

2. Additional DSC data

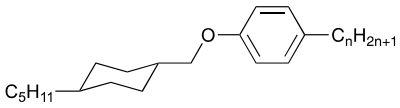
Table S1. Transition temperatures for **2**. [a]



	R	A	Temperature (*enthalpy*)
a		**[10]**	Cr 67 (*23.2*) N 197 (*1.4*) I
		[12]	Cr 92 (*22.7*) N 206 (*1.5*) I
		[Ph][b]	Cr_1 84 Cr_2 91 (*72.8*) N 206 (*1.8*) I
b		**[10]**	Cr_1 104 (*11.9*) Cr_2 115 (*15.3*) N 176 (1.0) I
		[12]	Cr 145 (*16.4*) N 187 (1.2) I
		[Ph]	NA
c	$-OCOC_8H_{17}$	**[10]**	Cr 43 (38.9) (N 37 (0.9)) I
		[12]	Cr 46 (*52.8*) (N 45 (*0.6*)) I
		[Ph]	NA

[a] Cr-crystal, N-nematic, I-isotropic. Temperatures in °C and enthalpies in kJ/mol (in parentheses) obtained on heating at 5 K min^{-1}. [b] ref [2]

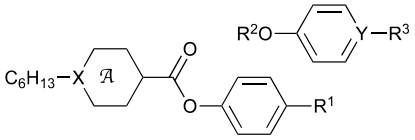
Table S2. Transition temperatures for **[Ph]**. [a]



	n	Temperature (*enthalpy*)
	3	Cr 32 (Sm 10) I [b]
	5	Cr 35 (Sm 31) I [b]
	7	Cr 34 Sm 38 I [b]
c	11	Cr 32 (*26.4*) B 42 (*12.7*) I

[a] Cr-crystal, Sm-smectic, B - soft crystlline (SmB_{cryst}), I-isotropic. Temperatures in °C and enthalpies in kJ/mol (in parentheses) obtained on heating at 5 K min^{-1}. [b] Ref. [3]

Table S3. Transition temperatures for **1-[Pyr]** and **2-[Ph]**. [a]



	X, Y	Temperature (*enthalpy*)
1[10]c–[Pyr]c	N^+, B^-	Cr 126 (12.6) E 163 (11.8) SmA 207 (15.2) I
2[10]c–[Ph]c	C, C	Cr 27 (56.1) (N 26 (2.0)) I
1[12]c–[Pyr]c	N^+, B^-	Cr_1 85 (18.6) X 148 (5.8) E 200 (12.3) SmA 210 (14.5) I
2[12]c–[Ph]c	C, C	Cr 30 (50.2) (N 29 (2.2)) I
2[10]c–[Pyr]a [b]	N^+, B^-	Cr_1 64 (9.2) Cr_2 101 (3.4) X 107 (15.1) I
2[12]c–[Pyr]a [c]	N^+, B^-	Cr 117 (27.4) I
1[12]c–[Pyr]b	N^+, B^-	Cr_1 77 (33.9) Cr_2 132 (8.4) E 172 (24.8) I

[a] Cr-crystal, N-nematic, I-isotropic. Temperatures in ^oC and enthalpies in kJ/mol (in parentheses) obtained on heating at 5 K min^{-1}. [b] ref [4]. [c] ref [5].

3. Powder XRD measurements

X-ray diffraction experiments were performed with Bruker D8 GADDS (Cu Kα radiation, Göbel mirror, point collimator, Vantec 2000 area detector) equipped with a modified Linkam heating stage and with Bruker D8 Discover system (Cu Kα radiation, Göbel mirror, scintillation counter, Anton Parr DCS350 heating stage). Samples were prepared in a form of a thin film or a droplet on heated surface. XRD data was analyzed using program TOPAS 3 (Bruker). The asymmetric wide angle signal in diffractograms was fitted with two functions type PV (pseudo-Voight).

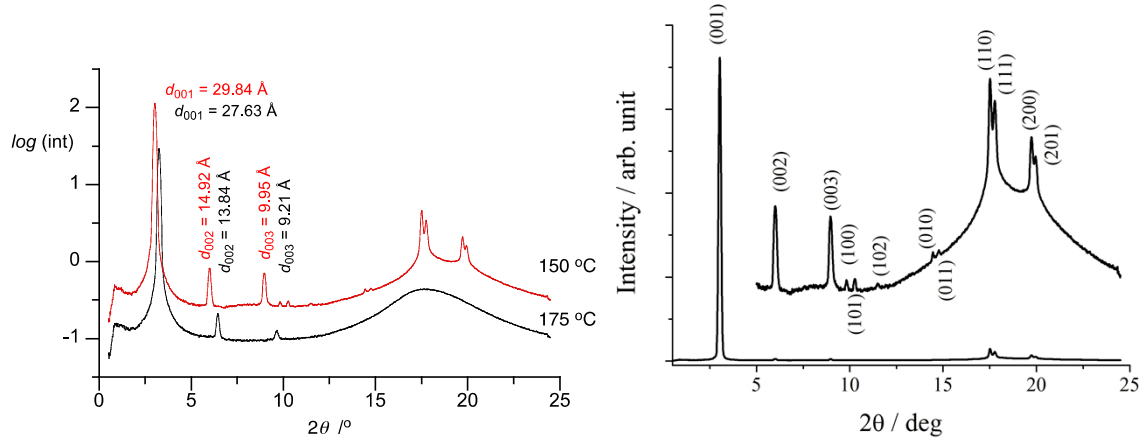
2D patters, integrated intensities and layer spacing as function of temerature, *d*(T), are shown in Figures S1 – S8 for individual materials.

XRD data was analyzed using program TOPAS 3 (Bruker). The asymmetric wide angle signal in diffractograms was fitted with two functions type PV (pseudo-Voight).

Ion pair 1[10]c–[Pyr]c

Table S4. Positions of diffraction signals in the 2D patterns obtained for **1[10]c–[Pyr]c**.

SmA phase, 175 °C			***E phase, 150 °C***		
d_{exp}(Å)	(*hkl*)	d_{calc}(Å)	d_{exp}(Å)	(*hkl*)	d_{calc}(Å)
27.63	(001)		29.84	(001)	
13.84	(002)	13.82	14.92	(002)	14.92
9.23	(003)	9.21	9.95	(003)	9.95
			8.99	(100)	
			8.61	(101)	8.61
5.06	diffused		7.70	(102)	7.70
4.59	diffused		6.12	(010)	
			6.00	(011)	6.00
			5.06	(110)	5.06
			4.99	(111)	4.99
			4.50	(200)	4.50
			4.45	(201)	4.45
			unit cell dimensions: a = 8.99; b = 6.12; c = 29.84		



a) b)

Figure S1. a) A comparison of integrated XRD patterns for SmA (175 °C, black) and E (150 °C, red) phases of **1[10]c–[Pyr]c**, b) integrated XRD pattern in E phase (150 °C) of **1[10]c–[Pyr]c** with full indexing for assumed orthorombic lattice with parameters a = 8.99 Å, b = 6.12 Å and c = 29.84 Å.

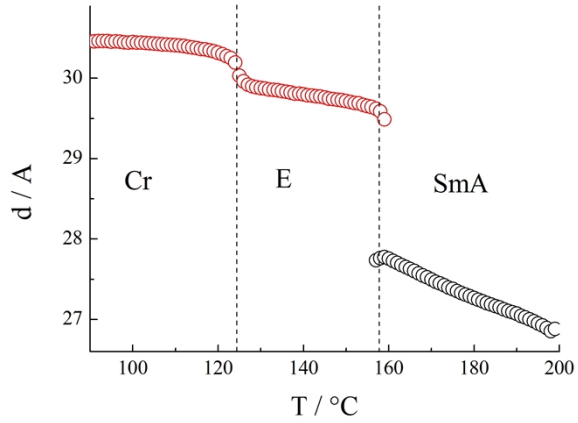


Figure S2. Layer spacing calculated from signal (*001*) for **1[10]c–[Pyr]c** as a function of temperature obtained on heating. Thermal expansion coefficients: κ_A = -24.7±0.2×10^{-3} Å K^{-1} in SmA phase (temperature range 180–160 °C) and κ_E = -8.1±0.1×10^{-3} Å K^{-1} in E phase (temperature range 130—150 °C).

Ion pair 1[12]c–[Pyr]c

Table S5. Positions of diffraction signals in the 2D patterns obtained for **1[12]c–[Pyr]c**.

SmA phase, 205 °C			***E phase, 180 °C***		
d_{exp}(Å)	(*hkl*)	d_{calc}(Å)	d_{exp}(Å)	(*hkl*)	d_{calc}(Å)
26.64	(001)		28.71	(002)	
13.36	(002)	13.32	14.33	(004)	14.35
8.89	(003)	8.88	9.55	(006)	9.57
			9.05	(101)	9.05
5.35	diffused		8.23	(103)	8.26
4.85	diffused		6.46	(011)	6.46
			5.30	(110)	5.30
			5.22	(112)	5.21
			4.58	(200)	4.58
			4.53	(202)	4.52
			unit cell dimensions: a = *9.16*, b = *6.50*, c = *57.42*		

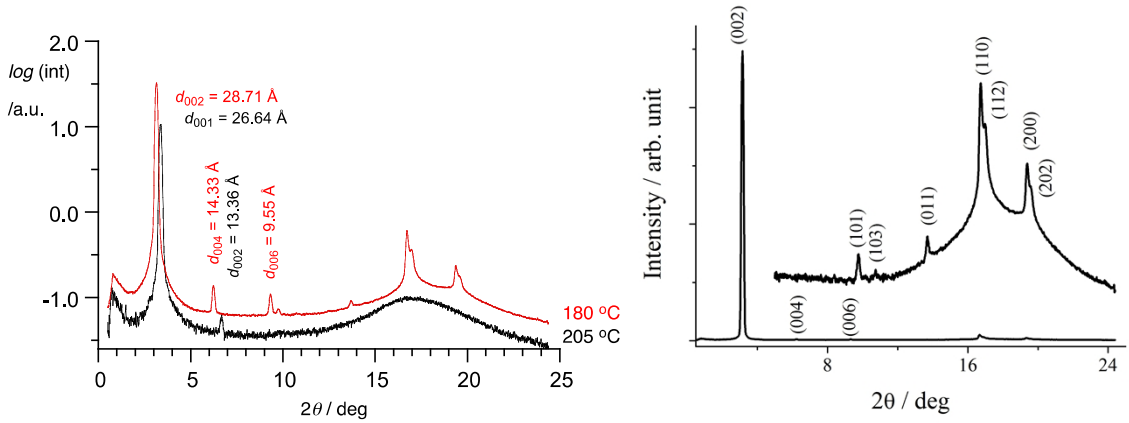


Figure S3. a) A comparison of integrated XRD patterns for **1[12]c–[Pyr]c** of a SmA (205 °C, black) and of E phase (180 °C, red), b) integrated XRD pattern in the E phase of **1[10]c–[Pyr]c** (150 °C) with full indexing for assumed orthorombic lattice with parameters a = 9.16 Å, b = 6.50 Å and c = 57.42 Å. For the enlarged part of the graph the 2D pattern has been integrated only in limited azimuthal angle range to avoid signal overleaping, thus (*004*) and (*006*) peaks are not visible.

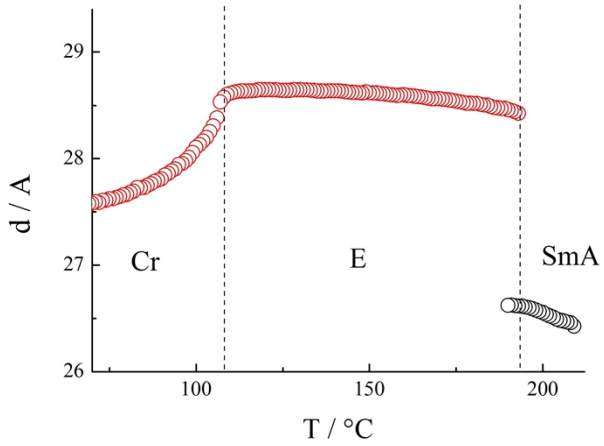


Figure S4. Layer spacing calculated from signal (*001*) for **1[12]c–[Pyr]c** as a function of temperature obtained on cooling. Thermal expansion coefficients: κ_A = -12.1±0.3×10^{-3} Å K^{-1} for SmA phase (temperature range 193–208 °C), and κ_E = -2.5±0.1×10^{-3} Å K^{-1} for E phase (temperature range 140–170 °C).

Ion pair 1[12]c–[Pyr]b

Table S6. Positions of diffraction signals in the 2D patterns obtained for **1[12]c–[Pyr]b**.

E phase, 150 °C

d_{exp}(Å)	(*hkl*)	d_{calc}(Å)
25.26	(001)	
12.67	(002)	12.63
9.11	(100)	
8.56	(101)	8.57
6.44	(010)	
6.23	(011)	6.24
5.25	(110)	5.26
5.15	(111)	5.15
4.56	(200)	4.56
4.49	(201)	4.48

unit cell dimensions:
a = *9.11*, b = *6.44*, c = *25.26*

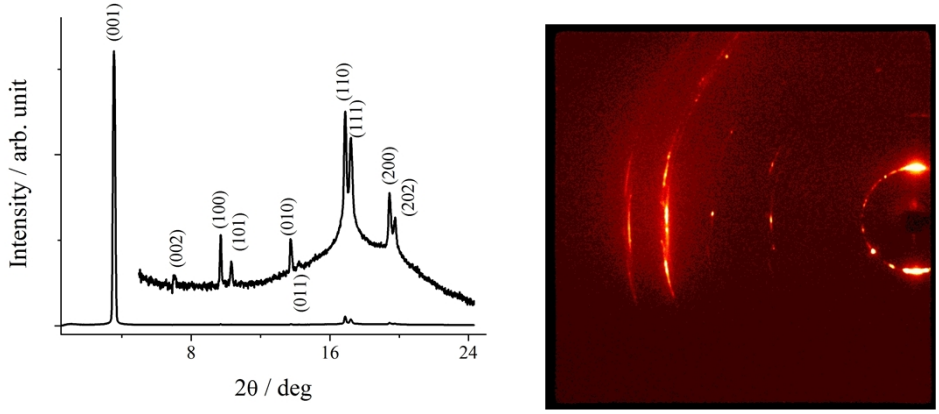


Figure S5. a) Integrated XRD pattern taken at 150 °C in E phase of **1[12]c–[Pyr]b**. Indexing done assuming orthorombic lattice with parameters *a* = 9.11 Å, *b* = 6.44 Å and *c* = 25.62 Å; b) 2D XRD pattern for **1[12]c–[Pyr]b** at 150 °C (E phase). Due to direct Iso – E phase transition well aligned sample could not be obtained.

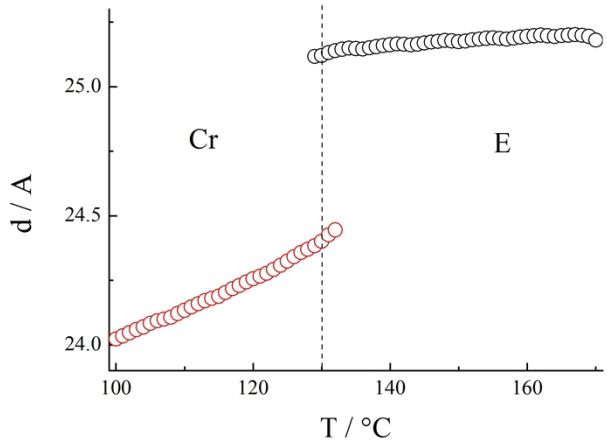


Figure S6. Layer spacing calculated from signal (*001*) for **1[12]c–[Pyr]b** as a function of temperature obtained on cooling. Thermal expansion coefficient: $\kappa_E = +1.9\pm0.1\times10^{-3}$ Å K^{-1} for E phase (temperature range 130—160 °C)

Ion pair [Pyr]c–Br

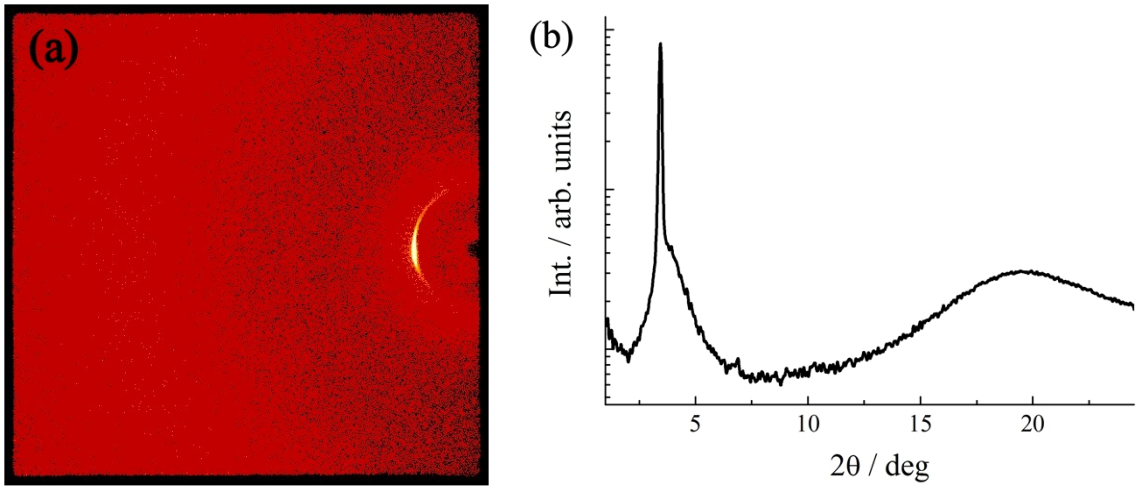


Figure S7. a) 2D XRD pattern for **[Pyr]c–Br** at 155 °C and b) intensity vs. diffraction angle obtained by integration of the 2D pattern over azimuthal angle. Note that due to low thermal stability of the material SmA phase coexists with the isotropic liquid.

[Ph]c

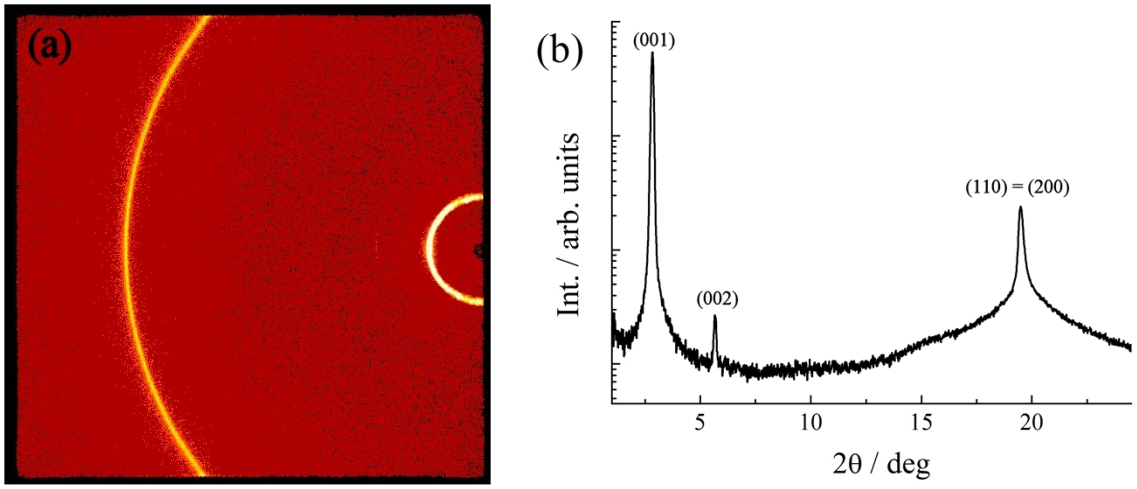


Figure S8. a) 2D XRD pattern for powder sample of **[Ph]c** in B phase (SmB_{cry}) at 29 °C and b) intensity vs. diffraction angle obtained by integration of the 2D pattern over azimuthal angle.

Table S7. Positions of diffraction signals in the 2D patterns taken for for **[Ph]c**

B phase, 42 °C	***B phase, 35 °C***	***B phase, 29 °C***
d_{exp}(Å) (*hkl*) d_{calc}(Å)	d_{exp}(Å) (*hkl*) d_{calc}(Å)	d_{exp}(Å) (*hkl*) d_{calc}(Å)
31.14 (001)	31.16 (001)	31.19 (001)
15.56 (002) 15.07	15.55 (002) 15.08	15.57 (002) 15.09
4.57 (110)=(200)	4.56 (110)=(200)	4.55 (110)=(200)
4.53 diff	4.52 diff	4.50 diff

4. Additional molecular models

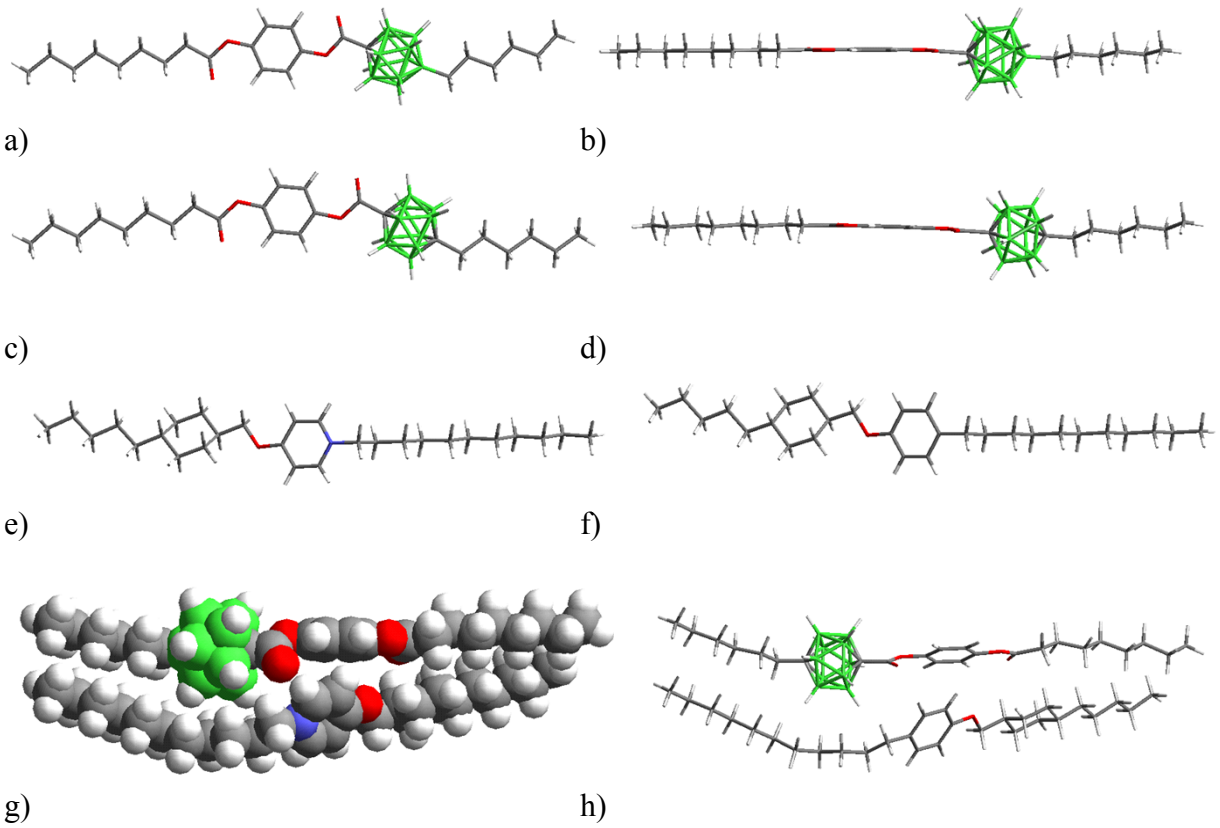


Figure S9. Equilibrium ground state geometry obtained at the M06-2x/3-21G* level of theory for a,b) **1[12]c** anion, c,d) **2[12]c**, e) **[Pyr]c** cation, f) **[Ph]c**, g) ion pair **1[12]c–[Pyr]c**, h) non-ion pair **2[12]c–[Ph]c**.

5. Archive files for M06-2x/3-21G* calculations

1[12]c

```
1\1\GINC-OCTOPUS\FOpt\RM062X\3-21G*\C23H44B11O4(1-)\PIOTR\06-Feb-2014\
 0\\#P M062x/3-21G* FOpt(RCFC) Geom(NoAngle, noDistance) fcheck #P freq
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0969,-9.4733183\Quadrupole=31.4337765,34.3638653,-65.7976418,-0.057991
5,4.3630623,4.9050063\PG=C01 [X(C23H44B11O4)]\\@

2[12]c

1\1\GINC-OCTOPUS\FOpt\RM062X\3-21G*\C24H44B10O4\PIOTR\05-Feb-2014\0\\#
P M062x/3-21G* FOpt Geom(NoAngle, noDistance) fcheck freq=noraman\\C6-
C2B10-COO-PhOOCC8, C1 in vacuum\\0,1\B,0.9420839569,-1.4911576678,5.12
81225163\B,1.636184128,0.134322576,4.8832265067\B,-0.6723783633,-1.295
3880737,5.879286574\B,0.4512844224,1.3360845713,5.4759624036\C,0.61205
82436,-0.2032680884,6.2312402271\B,-0.9811954282,0.4521530492,6.082790
5128\B,-1.0123134881,1.2076308474,4.4877947995\B,0.6160978336,1.012363
1941,3.7381630584\B,-1.7083492493,-0.4273303848,4.7347099331\B,0.91884
93056,-0.7443093427,3.5266089166\B,-0.5178410875,-1.6373672184,4.14573
41\C,-0.6632148716,-0.0871405767,3.4130313622\C,-1.3202923819,-0.02060
87299,2.0699237252\C,-0.6240113218,0.1140321081,-0.2971499472\C,-1.890
6783894,0.1212401557,-0.8791865578\C,-1.9833612123,0.1451336947,-2.267
226494\C,-0.8361139737,0.1616143723,-3.0584852889\C,0.4299647014,0.161
7395544,-2.469577628\C,0.5245773891,0.1369245082,-1.0819227024\C,1.292

8046797,-0.2876415574,7.6016692348\C,0.4131439932,0.149382261,8.786680
3146\C,1.1664674805,-0.0159680433,10.1208953339\C,0.297176272,0.386156
463,11.3270019297\C,1.0414498091,0.2198402356,12.6657234781\C,0.152041
3932,0.6113441929,13.8615350385\C,-0.1202186066,0.1783613372,-5.428526
2247\C,-0.7878624295,0.1282914504,-6.7807127577\C,0.2498606248,0.19694
18789,-7.9072437679\C,-0.4004560538,0.0637917679,-9.2953227686\C,0.640
4081263,0.1592199616,-10.4264839377\C,0.0058030601,0.0064720699,-11.82
15817365\C,1.0481765263,0.1129384808,-12.9505476715\C,0.4203683146,-0.
0444405376,-14.3486032234\C,1.4792247147,0.0672135699,-15.4627135234\O
,-0.3667981136,0.0784213575,1.0946128627\O,-1.0895684389,0.1700167204,
-4.4419077506\O,-2.5245086567,-0.0450626932,1.8818316104\O,1.080421579
3,0.213683163,-5.2151531631\H,-0.8967318414,-2.5983066056,3.5778511599
\H,1.4860251529,-1.1390643863,2.5756355937\H,-2.8566427874,-0.60658955
94,4.5588029568\H,0.9724187493,1.7782751814,2.9196451169\H,-1.70595782
55,2.0925557738,4.1381550575\H,-1.5749367801,0.8463835097,7.0200936363
\H,-0.1618705379,1.6572011484,13.7762786157\H,0.8271543112,2.306597075
1,6.0327408386\H,-0.7470748824,-0.013746364,13.8862307041\H,0.68340126
56,0.4878874077,14.8097364609\H,-1.0389325151,-2.0618388653,6.69833905
18\H,1.3647204673,-0.8235308853,12.7690740045\H,1.9449912849,0.8419522
023,12.6551086549\H,-0.0195618902,1.4319224618,11.215698366\H,2.788654
6742,0.3134904408,5.0591469497\H,-0.6114475362,-0.2306899962,11.339427
1393\H,1.4805226385,-1.0624512824,10.2350401691\H,1.6354393774,-2.3851
218203,5.4607555249\H,2.0756387505,0.6001219492,10.1071774036\H,0.1174
14491,1.1983568702,8.6618566186\H,-0.5021538455,-0.455554603,8.8067187
837\H,1.6100924695,-1.3261140723,7.7556310683\H,2.1957964555,0.3337762
468,7.5741558734\H,-2.7733892847,0.1039607695,-0.2621989115\H,-2.94606
41594,0.1480788374,-2.7595610724\H,1.3111738111,0.1783734937,-3.088161
4919\H,1.4867524171,0.1325362165,-0.5880056998\H,-1.5028516485,0.95696
49822,-6.8400857394\H,-1.3708745654,-0.7998540892,-6.8322374894\H,0.79
13554382,1.1478398125,-7.8398538864\H,0.9894140711,-0.5986879539,-7.76
38616833\H,-0.9226362958,-0.9003864057,-9.3644041474\H,-1.1529927059,0
.8526394344,-9.4283319309\H,1.1532375848,1.1286501292,-10.3646089623\H
,1.4004078538,-0.6208968023,-10.28633174\H,-0.7593758597,0.7821323207,
-11.9599608771\H,-0.5002759126,-0.966555572,-11.8862696186\H,1.5523169
311,1.0871408641,-12.8875408422\H,1.8157907974,-0.6599888041,-12.81001
93855\H,-0.0814383499,-1.0184096475,-14.4099279234\H,-0.3473950813,0.7
268946802,-14.4866167409\H,1.0288752492,-0.0481186988,-16.4533281508\H
,1.9743324367,1.0434204939,-15.4196943081\H,2.2433211388,-0.7077775149
,-15.3390214414\\Version=EM64L-G09RevC.01\State=1-A\HF=-1481.9099988\R
MSD=6.321e-09\RMSF=6.465e-06\Dipole=0.1499808,-0.0273145,-0.1176637\Qu
adrupole=-14.1055897,-12.3094443,26.415034,-0.4476052,12.7555662,-0.06
8749\PG=C01 [X(C24H44B10O4)]\\

[Pyr]c

1\1\GINC-OCTOPUS\FOpt\RM062X\3-21G*\C28H50N1O1(1+)\PIOTR\05-Feb-2014\0
\\#P M062x/3-21G* FOpt(RCFC) Geom(NoAngle, noDistance) fcheck #P freq=
noraman\\C5ChxCH2OPyrC11 cation, C1 in vacuum start at DFT\\1,1\C,-0.8
114380488,-2.0470914012,1.0968750138\C,0.4944766858,-1.6753160623,1.26
94138234\C,1.2095725262,-1.089861147,0.198304579\C,0.5348227672,-0.911
5857503,-1.0271718649\C,-0.7777704114,-1.3071229925,-1.1407432996\N,-1
.4426606092,-1.8695520181,-0.1000173764\O,2.4757887881,-0.7483031948,0
.4332879423\C,-2.8964519786,-2.2199296651,-0.2463585874\C,-3.783261093
7,-0.9897080967,0.0006667471\C,-5.2709776313,-1.3688464884,-0.14523432
99\C,-6.1976637276,-0.1503679537,0.03725781\C,-7.681140411,-0.55444232
59,-0.0625146636\C,-8.6332465202,0.6516678827,0.0477137439\C,-10.11006
22225,0.2157638021,-0.0079233184\C,-11.0849810339,1.406146454,0.062114
0149\C,-12.5550012231,0.9464169353,0.0268146876\C,-13.5463175826,2.124

1113948,0.0842190531\C,-15.0068351305,1.6330506417,0.0548628716\C,3.29
87847407,-0.0770965192,-0.6107895954\C,6.7247020144,-0.9655980262,0.97
99129351\C,5.3244961168,-1.1992009717,0.3796292786\C,4.6705404772,0.14
50551224,0.0086769946\C,5.5648229528,0.9105854787,-0.9876055098\C,6.96
61254518,1.1399736898,-0.3831753147\C,7.6401356998,-0.1927530917,0.005
9219715\C,9.0220561666,0.0399923373,0.6499931616\C,10.04205891,0.72390
91681,-0.2812235695\C,11.4257008205,0.8580095227,0.3840960456\C,12.445
1507429,1.567666022,-0.5274592802\C,13.8169496655,1.7130680161,0.15895
70468\H,-1.3946776618,-2.4964653766,1.8892151894\H,0.9956811665,-1.821
0210877,2.2147517742\H,1.0251702166,-0.4740695698,-1.8843834809\H,-1.3
337635527,-1.188634271,-2.0618542503\H,-3.1142496512,-3.0136676158,0.4
73181452\H,-3.0389519006,-2.6140365094,-1.2565203218\H,-3.5946933429,-
0.5988238233,1.0078868395\H,-3.5288303071,-0.2031842006,-0.7208456895\
H,-5.4455349761,-1.8029564092,-1.1389815134\H,-5.5298843792,-2.1332771
274,0.5989995267\H,-6.011553504,0.311297228,1.0159846698\H,-5.97068393
36,0.599665581,-0.7318061098\H,-7.9137282931,-1.272338234,0.735515382\
H,-7.8559001381,-1.0625624976,-1.02059793\H,-8.4470614719,1.1833801191
,0.9905565611\H,-8.4300475066,1.3535757952,-0.7721682899\H,-10.2880272
717,-0.3414087,-0.9378917744\H,-10.3149436254,-0.4685625925,0.82658596
2\H,-10.9047465922,1.9737722798,0.9851037738\H,-10.8961844994,2.083216
3237,-0.7818617463\H,-12.7435610562,0.2739487024,0.8747665053\H,-12.73
22086038,0.3700180147,-0.8915619015\H,-13.36757803,2.7022764066,0.9994
744804\H,-13.3622731398,2.7925477821,-0.7660691992\H,-15.1983767748,1.
0658562077,-0.8624996055\H,-15.2034854134,0.9766677755,0.9094048067\H,
-15.7095832228,2.4700535415,0.0948698649\H,3.3660626195,-0.7395395089,
-1.4825303434\H,2.8096603004,0.8663195632,-0.8798905197\H,5.4193663322
,-1.805632069,-0.5334187874\H,4.6832271064,-1.738515177,1.0841659521\H
,6.6297381237,-0.3827729942,1.9073427704\H,7.1854428565,-1.9264097564,
1.2367441389\H,5.6644622492,0.3170345157,-1.907821317\H,5.1079858859,1
.8729407897,-1.2506862291\H,7.5848192169,1.6820433061,-1.1048742306\H,
6.8764825669,1.7632978967,0.5183405552\H,7.7707676205,-0.7955734837,-0
.9058951841\H,4.5431479669,0.74861135,0.9168103058\H,9.4308512684,-0.9
298969373,0.9662255693\H,8.8918720553,0.6487110414,1.5563883025\H,10.1
394689033,0.1411756589,-1.2076010135\H,9.6884972309,1.7251668917,-0.55
69052432\H,11.3235531362,1.4239390413,1.3201744536\H,11.8052840862,-0.
1387885339,0.64513721\H,12.0571934152,2.5585366363,-0.7946743337\H,12.
5540009245,0.9973673389,-1.4584418975\H,14.5328514718,2.2238932743,-0.
4915164114\H,13.7194675218,2.2905360574,1.0846002881\H,14.2238097049,0
.7283125931,0.4118209784\\Version=EM64L-G09RevC.01\State=1-A\HF=-1219.
6602605\RMSD=9.812e-09\RMSF=3.090e-06\Dipole=-0.6730766,-2.081574,-0.5
243299\Quadrupole=34.7320377,-17.613684,-17.1183537,9.0135428,-1.95136
51,-2.4784235\PG=C01 [X(C28H50N1O1)]\\@

[Ph]c

1\1\GINC-OCTOPUS\FOpt\RM062X\3-21G*\C29H50O1\PIOTR\05-Feb-2014\0\\#P M
062x/3-21G* FOpt Geom(NoAngle, noDistance) fcheck #P freq=noraman\\C5C
hxCH2OPhC11, C1 in vacuum\\0,1\C,0.7771909316,1.441184039,0.4786369772
\C,0.3382772908,1.1044842658,-0.7937685967\C,0.7329950336,-0.104228723
1,-1.3805256314\C,1.5732602629,-0.9648802845,-0.6754357405\C,2.0077178
254,-0.6150712754,0.6058712331\C,1.6228137201,0.5856358946,1.200383782
7\O,0.2423690426,-0.3548484751,-2.6514713837\C,2.0323206382,0.91944066
31,2.6201976404\C,0.9463504986,0.4561296385,3.620266564\C,1.3355158166
,0.7331786725,5.083869596\C,0.2431054843,0.2741501464,6.0683368078\C,0
.6351966121,0.5138986548,7.5385909532\C,-0.461690376,0.0521690347,8.51
65629501\C,-0.0705721827,0.2762472851,9.9895950704\C,-1.171201876,-0.1
873906509,10.9624871466\C,-0.7849702264,0.0335216122,12.4370964407\C,-
1.8889448193,-0.4284078353,13.4074064191\C,-1.4905825287,-0.1965823084

,14.877927679\C,0.6364303411,-1.5883309821,-3.3169328344\C,-0.30302543
1,-0.2851884465,-6.8493988722\C,0.3701689729,-0.3094511136,-5.46458235
99\C,-0.0434846443,-1.5687788024,-4.6828676847\C,0.3230061039,-2.82971
3697,-5.4854660354\C,-0.3453515117,-2.8053250315,-6.8764734135\C,0.050
5952843,-1.5430189976,-7.672514271\C,-0.6488240321,-1.4968909516,-9.04
60300927\C,-0.2491415686,-2.6456195354,-9.9925022732\C,-0.9020134352,-
2.5024990971,-11.3808646403\C,-0.52192367,-3.6549479064,-12.3300477148
\C,-1.1905624349,-3.5009199867,-13.7098672914\H,0.4649632913,2.3809325
566,0.9230162581\H,-0.3103380135,1.7556394158,-1.3647180337\H,1.895080
2649,-1.9028364875,-1.1075148548\H,2.6589841138,-1.293347449,1.1481326
683\H,2.1846852172,2.000620468,2.7275804626\H,2.9804767302,0.423804553
1,2.8634536367\H,0.0047600726,0.9683856978,3.3826249708\H,0.7741498152
,-0.6186892693,3.4810916115\H,2.2739154971,0.2108395166,5.3158814687\H
,1.5181519759,1.8079162164,5.2187009516\H,-0.6898538909,0.8107343208,5
.8487695598\H,0.0471000238,-0.7958860323,5.9167245421\H,0.832986375,1.
5832092087,7.6929362221\H,1.5663937946,-0.0259054922,7.7582152805\H,-1
.3908691911,0.5970940932,8.3011610969\H,-0.6644340359,-1.0152170245,8.
354812883\H,0.8576300415,-0.2699511493,10.2059188159\H,0.1323139833,1.
3432969489,10.1530028495\H,-2.0990558852,0.3590990538,10.7451477926\H,
-1.3744546635,-1.2541801791,10.7973436873\H,-0.5806000419,1.1000327349
,12.6029317324\H,0.1416858562,-0.5141741204,12.6566816873\H,-2.8139328
147,0.1171996527,13.1827490155\H,-2.0901212548,-1.4940296608,13.240812
4961\H,-0.5773442302,-0.7519684195,15.1169309326\H,-1.2995166887,0.867
2420572,15.0559477682\H,-2.2809660518,-0.5240674894,15.5600526953\H,1.
7282827469,-1.6213731114,-3.43920256\H,0.3165412649,-2.458933634,-2.72
81781371\H,1.4627585911,-0.3223797891,-5.5915423907\H,0.1093220614,0.5
724714892,-4.8737110745\H,-1.3947958389,-0.2484471696,-6.7226648252\H,
-0.001608805,0.6126738789,-7.4026976148\H,1.4148396626,-2.8626204251,-
5.6117676508\H,0.0198469384,-3.7312246409,-4.938003474\H,-0.0679579644
,-3.7073140028,-7.4324130241\H,-1.4381102701,-2.8080272035,-6.75367074
41\H,1.140042991,-1.558880449,-7.8302448405\H,-1.1294943744,-1.5440901
863,-4.5218288536\H,-0.4084662512,-0.5402883406,-9.5317212068\H,-1.736
9076781,-1.5162200911,-8.8886471721\H,0.8436038414,-2.6595486186,-10.1
054843028\H,-0.546926845,-3.6093082728,-9.5608966479\H,-1.9941318588,-
2.4748060932,-11.2655904455\H,-0.5974643016,-1.5472182972,-11.82996943
27\H,-0.8231365007,-4.607562364,-11.8760919363\H,0.5687036074,-3.67978
06506,-12.4466508282\H,-0.9220070421,-4.3259333855,-14.3767160229\H,-2
.2805438226,-3.4850345984,-13.6031868054\H,-0.879935565,-2.5617115717,
-14.1802166312\\Version=EM64L-G09RevC.01\State=1-A\HF=-1203.3251035\RM
SD=6.158e-09\RMSF=6.289e-06\Dipole=0.1544927,-0.447625,-0.0462231\Quad
rupole=-3.1834315,0.8101887,2.3732428,-2.8377523,0.3759875,4.0704832\P
G=C01 [X(C29H50O1)]\\@

2[12]c–[Ph]c

1\1\GINC-OCTOPUS\FOpt\RM062X\3-21G*\C53H94B10O5\PIOTR\07-Feb-2014\0\\#
P M062x/3-21G* FOpt Geom(NoAngle, noDistance) fcheck freq=noraman\\C6-
C2B10-COO-PhOOCC8 - C5-Chx-CH2OPh-C11, C1 antiparalel in vacuum\\0,1\B
,-5.9118572848,-2.1942463327,-2.3806032445\B,-5.1921620031,-2.82343597
55,-0.8697146885\B,-6.4677719426,-0.5209947974,-2.0772503898\B,-5.3102
684155,-1.5449599982,0.3706971716\C,-6.527045096,-1.7251659525,-0.8396
223692\B,-6.0985385332,-0.124489734,-0.3795332459\B,-4.3399568563,-0.1
678195885,-0.1574643651\B,-3.7795024424,-1.8461666439,-0.4633893619\B,
-5.059553642,0.4702790399,-1.675742466\B,-4.1484836322,-2.2472291361,-
2.1730701673\B,-4.9456313525,-0.813041297,-2.9231488386\C,-3.754030001
9,-0.6453466565,-1.6952013783\C,-2.4424818851,-0.0764533037,-2.1355982
499\C,-0.0573349815,-0.6283396144,-2.0136254347\C,0.3846606617,0.08726
7941,-3.1228395189\C,1.7549400948,0.2479202423,-3.3061899214\C,2.66063

87508,-0.2865585772,-2.3910443565\C,2.2109609979,-0.9813890047,-1.2673
148081\C,0.841129786,-1.1519785875,-1.091549124\C,-7.8683827457,-2.295
2715966,-0.3659597193\C,-9.0852810576,-1.9432489823,-1.2445321477\C,-1
0.2844033074,-2.8401372625,-0.8770652276\C,-11.5309622345,-2.554006463
,-1.7351128331\C,-12.646458614,-3.591949585,-1.5012668644\C,-13.880106
4507,-3.314045079,-2.3810929394\C,5.1010703389,-0.5918510225,-2.080690
486\C,6.3597073124,-0.1685961604,-2.8019731491\C,7.5531630527,-1.06847
08958,-2.4350460365\C,8.8926623916,-0.3343507519,-2.6179041325\C,10.10
38635766,-1.2284420863,-2.2930212034\C,11.4153203146,-0.4221518853,-2.
2660206946\C,12.6552555413,-1.3035982783,-2.0290685206\C,13.9444812854
,-0.4692099407,-1.907926493\C,15.1912959205,-1.3599375819,-1.748603101
\O,-1.4219827913,-0.8957885033,-1.7412858104\O,4.0080707554,-0.0613191
536,-2.7289820633\O,-2.3088896552,0.9603662872,-2.7668757923\O,5.04058
82882,-1.2721001446,-1.0646779821\H,-4.6891800054,-0.5282397419,-4.036
2940437\H,-3.3914292308,-2.884760904,-2.8099188959\H,-4.8875790518,1.5
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