Supporting Information for

Inherently chiral calixarenes via direct mercuration of the *partial cone* conformation

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Experimental procedures and characterizations

General Experimental Procedures

All chemicals were purchased from commercial sources and used without further purification. Solvents were dried and distilled using conventional methods. Melting points were measured on Heiztisch Mikroskop – Polytherm A (Wagner & Munz, Germany). NMR spectra were performed on Varian Gemini 300 (^{1}H: 300 MHz, ^{13}C: 75 MHz) or Agilent 400-MR DDR2 (^{1}H: 400 MHz, ^{13}C: 100 MHz. Deuterated solvents used are indicated in each case. Chemical shifts (δ) are expressed in ppm and are referred to the residual peak of the solvent or TMS as an internal standard; coupling constants (J) are in Hz. The mass analyses were performed using ESI technique on Q–TOF (Micromass) spectrometer. Elemental analyses were done on Perkin–Elmer 240, Elementar vario EL (Elementar, Germany) or Mitsubishi TOX–100 instruments. All samples were dried in the desiccator over P_2O_5 under vacuum (1 Torr) at 80 °C for 8 hours. The IR spectra were measured on an FT–IR spectrometer Nicolet 740 or Bruker IFS66 spectrometers equipped with a heatable Golden Gate Diamante ATR–Unit (SPECAC) in KBr. 100 Scans for one spectrum were co–added at a spectral resolution of 4 cm^{-1}. The courses of the reactions were monitored by TLC using TLC aluminium sheets with Silica gel 60 F254 (Merck). The column chromatography was performed using Silica gel 60 (Merck).

General remark:

All organomercurial derivatives are considered potentially hazardous and require special consideration!

4-(Chloromercurio)-25,26,27,28-tetrapropoxycalix[4]arene *partial cone* (2c)

A mixture of calixarene **1** (4.05 g, 6.81 mmol) and mercury(II) trifluoroacetate (2.9 g, 6.81 mmol) were dissolved in chloroform (130 ml). Mixture was stirred overnight at room temperature. Solution of brine (30 ml) was then added and the mixture was stirred vigorously for 30 min. The organic layer was separated, washed with water (50 ml) and dried over magnesium sulfate. Solvent was removed under a reduced pressure to yield the crude product which was purified by column chromatography on silica gel (eluent: CH_2Cl_2:hexane = 1:1 v/v). The fractions containing the title compound were collected, evaporated to dryness and crystallized from dichloromethane : methanol mixture. Product **2c** was

obtained as a white powder in 23% yield (1.32 g), mp: 231.9-235 °C. After several crystallization of a mother liquid another isomer **2e** was obtained as a white powder, mp: 136.1-137.4 °C.

Data for compound 2c:

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.29-7.25 (m, 1H, Ar-**H**), 7.23-7.18 (m, 2H, Ar-**H**), 7.15 (dd, 1H, *J*= 7.4, 1.5 Hz, Ar-**H**), 7.09-6.95 (m, 3H, Ar-**H**), 6.87 (t, 1H, *J*= 7.4 Hz, Ar-**H**), 6.48-6.40 (m, 2H, Ar-**H**), 6.23 (dd, 1H, *J*= 7.4, 1.2 Hz, Ar-**H**), 4.35 (d, 1H, *J*= 14.1 Hz, Ar-**CH_2**-Ar), 4.10 (d, 1H, *J*= 13.7 Hz, Ar-**CH_2**-Ar), 3.84-3.72 (m, 4H, O-**CH_2**), 3.69-3.64 (m, 4H, Ar-**CH_2**-Ar), 3.60-3.51 (m, 2H, O-**CH_2**), 3.26-3.14 (m, 2H, O-**CH_2**), 3.11 (d, 1H, *J*= 13.7 Hz, Ar-**CH_2**-Ar), 2.92 (d, 1H, *J*= 14.1 Hz, Ar-**CH_2**-Ar), 2.06-1.80 (m, 6H, O-CH_2-**CH_2**), 1.41-1.29 (m, 2H, O-CH_2-**CH_2**), 1.15-1.06 (m, 9H, O-CH_2-CH_2-**CH_3**), 0.67 (t, 3H, *J*=7.4 Hz, O-CH_2-CH_2-**CH_3**) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 157.8, 157.6, 157.2, 156.0, 148.8, 139.1, 138.7, 137.5, 134.4, 133.9, 133.8, 133.7, 132.3, 130.7, 130.6, 130.2, 130.1, 129.7, 129.5, 129.3, 128.3, 124.0, 122.1, 122.0, 76.5, 76.3, 75.6, 75.3, 35.7, 35.5, 33.3, 31.2, 24.5, 24.1 (2x), 22.2, 11.2 (2x), 11.1, 9.5 ppm. IR (KBr) ν 1453.7 cm^{-1}. HRMS (ESI$^+$): $C_{40}H_{47}O_4HgCl$, calcd for 851.27613 [(M+Na)$^+$]; found: 851.27655 [(M+Na)$^+$], 867.24942 [(M+K)$^+$].

Data for compound 2e:

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.24 (dd, 1H, *J*= 7.4, 1.6 Hz, Ar-**H**), 7.20 (dd, 1H, *J*= 7.4, 1.6 Hz, Ar-**H**), 7.13 (dd, 1H, *J*= 7.4, 1.6 Hz, Ar-**H**), 7.07 (dd, 1H, *J*= 7.4, 1.6 Hz, Ar-**H**), 6.99-6.92 (m, 2H, Ar-**H**), 6.91-6.84 (m, 2H, Ar-**H**), 6.49 (t, 1H, *J*= 7.4 Hz, Ar-**H**), 6.30-6.26 (m, 1H, Ar-**H**), 6.05 (bs, 1H, Ar-**H**), 4.07 (d, 1H, *J*= 13.3 Hz, Ar-**CH_2**-Ar), 4.07 (d, 1H, *J*= 13.7 Hz, Ar-**CH_2**-Ar), 3.86-3.50 (m, 10H, O-**CH_2** + Ar-**CH_2**-Ar), 3.35-3.25 (m, 2H, O-**CH_2**), 3.06 (d, 1H, *J*= 13.7 Hz, Ar-**CH_2**-Ar), 3.02 (d, 1H, *J*= 13.7 Hz, Ar-**CH_2**-Ar), 2.04-1.81 (m, 6H, O-CH_2-**CH_2**), 1.43-1.29 (m, 2H, O-CH_2-**CH_2**), 1.15-1.04 (m, 9H, O-CH_2-CH_2-**CH_3**), 0.70 (t, 3H, *J*=7.4 Hz, O-CH_2-CH_2-**CH_3**) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 157.5, 157.0, 156.8, 155.8, 140.8, 137.2, 136.6, 135.9, 135.3, 135.1, 134.0, 133.6, 133.3, 133.2, 132.2, 130.6, 130.1, 129.3 (2x), 128.9, 128.4, 122.3, 121.8, 121.4, 76.4, 76.1, 75.5, 74.8, 35.6, 35.5, 30.7, 30.5, 24.3, 23.8 (2x), 22.3, 10.9 (2x), 9.3 (2x) ppm. IR (KBr) ν 1454.4 cm^{-1}. HRMS (ESI$^+$): $C_{40}H_{47}O_4HgCl$, calcd for 851.27613 [(M+Na)$^+$]; found: 851.27570 [(M+Na)$^+$], 867.24860 [(M+K)$^+$].

6,10-bridged-25,26,27,28-tetrapropoxycalix[4]arene *partial cone* (3)

Organomercurial derivative **2c** (0.11 g, 0.14 mmol), triphenylarsine (0.0083 g, 0.027 mmol), palladium acetate (0.0031 g, 0.014 mmol) and cesium carbonate (0.089 g, 0.27 mmol) were added to an oven-dried 10 ml Schlenk flask under argon. All compounds were then dried under vacuum for one hour. Flask was then filled with argon. Dry deoxygenated toluene (5 ml bubbled with argon) was added and the reaction mixture was stirred overnight at 110 °C (conversion was monitored by TLC).

The reaction mixture was cooled down to room temperature and the solvent was removed under reduced pressure. The residue was dissolved in 30 ml of dichloromethane and filtered over short pad of silica gel. The resulting solution was washed with water (30 ml) and dried over magnesium sulfate. Solvent was removed under reduced pressure to yield the crude product which was purified by preparative TLC (eluent: hexane:CH_2Cl_2 = 5:1 v/v). The title compound was obtained as a white powder in 88% yield (0.071 g), mp: 120.0-122.3 °C.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.16 (dd, 1H, *J*= 7.4, 1.6 Hz, Ar-**H**), 7.03 (d, 1H, *J*= 7.7 Hz, Ar-**H**), 6.97 (dd, 1H, *J*= 7.3, 1.7 Hz, Ar-**H**), 6.89 (dd, 1H, *J*= 7.5, 1.5 Hz, Ar-**H**), 6.87-6.78 (m, 3H, Ar-**H**), 6.77-6.72 (m, 2H, Ar-**H**), 6.65 (d, 1H, *J*= 8.2 Hz, Ar-**H**), 4.27 (d, 1H, *J*= 12.9 Hz, Ar-**CH_2**-Ar), 4.02-3.93 (m, 2H, O-**CH_2**), 3.91-3.81 (m, 3H, O-**CH_2** + Ar-**CH_2**-Ar), 3.71-3.53 (m, 5H, O-**CH_2** + Ar-**CH_2**-Ar), 3.34-3.32 (m, 2H, O-**CH_2**), 3.30 (d, 1H, *J*= 13.0 Hz, Ar-**CH_2**-Ar), 3.24 (d, 1H, *J*= 18.6 Hz, Ar-**CH_2**-Ar), 3.16-3.08 (m, 1H, O-**CH_2**), 1.83-1.69 (m, 5H, O-CH_2-**CH_2**), 1.46-1.18 (m, 3H, O-CH_2-**CH_2**), 1.05 (dt, 6H, *J*= 7.38, 3.0 Hz, O-CH_2-CH_2-**CH_3**), 0.76 (t, 3H, *J*= 7.5 Hz, O-CH_2-CH_2-**CH_3**), 0.63 (t, 3H, *J*= 7.4 Hz, O-CH_2-CH_2-**CH_3**) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 157.4, 157.2, 156.9, 156.5, 147.0, 145.6, 138.6, 138.4, 138.1, 134.3, 134.0, 132.7, 132.6, 130.6 (2x), 130.3, 130.2, 128.7, 127.3, 126.6, 122.6, 120.9, 117.8, 116.0, 75.5, 73.9, 73.7, 72.2, 39.1, 37.8, 33.7, 32.7, 23.7, 23.6, 23.2, 22.4, 10.9 (2x), 10.1, 9.8 ppm. IR (KBr) ν 1453.4 cm^{-1}. HRMS (ESI$^+$): $C_{40}H_{48}O_4$, calcd for 591.34689 [(M+H)$^+$]; found: 591.34576 [(M+H)$^+$], 613.32874 [(M+K)$^+$].

8-benzyl-6,10-bridged-25,26,27,28-tetrapropoxycalix[4]arene *partial cone* (4)

Calixarene **4** (0.090 g, 0.15 mmol) was added to an oven-dried 10 ml Schlenk flask under argon. Anhydrous 2-methyltetrahydrofuran (5 ml) was added to the flask by syringe to form colorless solution. The solution was cooled down to -78 °C and stirred for 20 minutes. The solution of *n*-butyllithium (1.6 M, 0.4 ml, 0.62 mmol) was added dropwise to the flask resulted in the yellow colour of the solution. The mixture was stirred 15 minutes at -78 °C, then 30 minutes at room temperature (solution turn red), and again cooled down to -78 °C. Benzyl bromide (0.10 g, 0.61 mmol) was added dropwise and solution was stirred for 10 minutes at -78 and then 3 hours at room temperature. The reaction was quenched by a careful addition of water (3 ml). The mixture was extracted with dichloromethane (30 ml), the separated organic layers were washed with water (30 ml) and dried over magnesium sulfate. Solvent was removed under reduced pressure to yield the crude product that was purified by preparative TLC (eluent: CH_2Cl_2:hexane = 2:3 v/v). The title compound was obtained as a white powder in 70% yield (0.073 g), mp: 65.0-67.0 °C.

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.24-7.13 (m, 5H, Ar-**H**), 7.05 (d, 1H, *J*= 7.8 Hz, Ar-**H**), 6.98 (dd, 1H, *J*= 7.4, 1.6 Hz, Ar-**H**), 6.94 (dd, 1H, *J*= 7.5, 1.2 Hz, Ar-**H**), 6.86-6.72 (m, 4H, Ar-**H**), 6.64 (d, 1H, *J*= 8.2 Hz, Ar-**H**), 4.19-4.13 (m, 1H, Ar-**CH_2**-Ar), 4.10-4.02 (m, 2H, O-**CH_2**), 3.84 (d, 1H, *J*= 14.1

Hz, Ar-**CH_2**-Ar), 3.70-3.61 (m, 3H, O-**CH_2** + Ar-**CH_2**-Ar), 3.56-3.48 (m, 2H), 3.42-3.26 (d, 4H), 3.20-3.03 (m, 3H), 1.92-1.53 (m, 6H, O-CH_2-**CH_2**), 1.41-1.30 (m, 1H, O-CH_2-**CH_2**), 1.26-1.15 (m, 1H), 1.15-1.08 (m, 1H), 1.05 (t, 3H, *J*= 7.43 Hz, O-CH_2-CH_2-**CH_3**), 0.97 (t, 3H, *J*= 7.4 Hz, O-CH_2-CH_2-**CH_3**), 0.74 (t, 3H, *J*= 7.4 Hz, O-CH_2-CH_2-**CH_3**), 0.58 (t, 3H, *J*= 7.4 Hz, O-CH_2-CH_2-**CH_3**) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 157.2, 156.9, 156.5, 156.3, 146.1, 144.8, 144.3, 142.8, 140.6, 137.9, 134.1, 134.0, 132.8, 131.9, 131.8, 130.9, 130.5, 130.0, 129.8, 128.9, 128.5, 128.1, 127.7, 125.7, 122.6, 121.1, 118.7, 117.1, 77.3, 74.9, 73.5, 71.9, 46.1, 42.9, 39.0, 38.3, 33.0, 29.3, 23.8, 23.6, 23.1, 21.9, 10.6, 10.0, 9.6 ppm. IR (KBr) ν 1452.5 cm^{-1}. HRMS (ESI^+): $C_{47}H_{52}O_4$, calcd for 703.37578 [$(M+Na)^+$]; found: 698.42109 [$(M+NH_4^+)^+$], 703.37616 [$(M+Na)^+$], 719.34932 [$(M+K)^+$].

Compound 2c

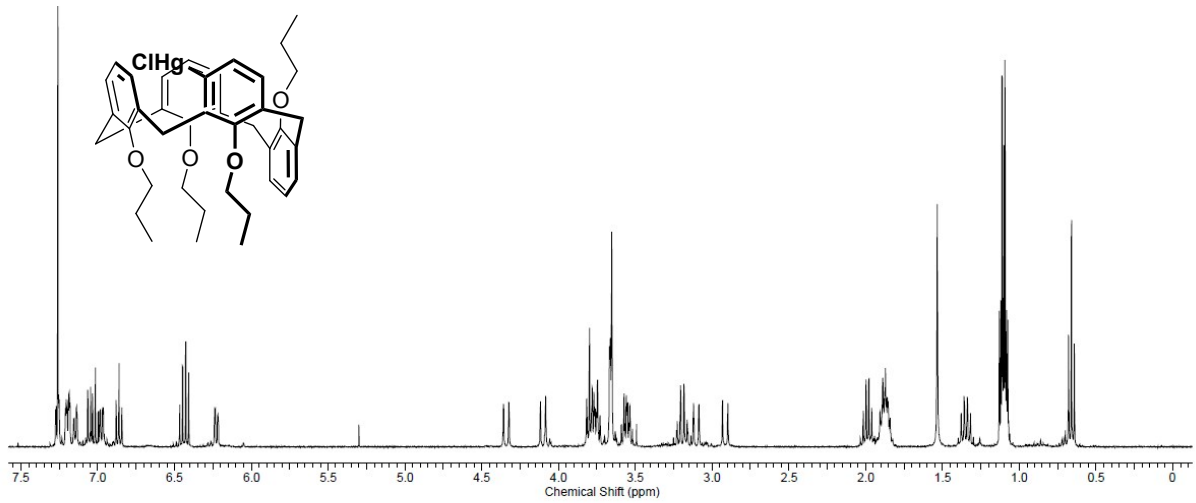

Figure 1. ^{1}H NMR of compound **2c** ($CDCl_3$, 400 MHz).

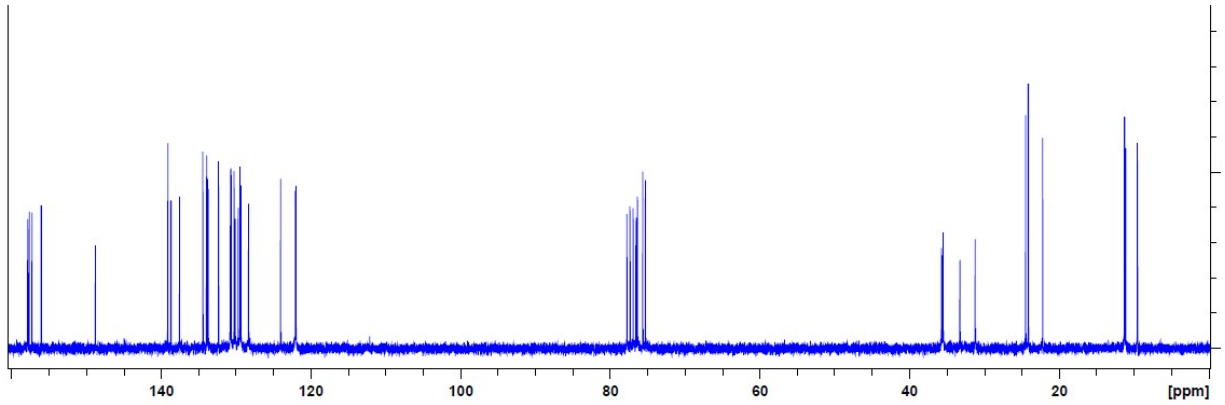

Figure 2. ^{13}C NMR of compound **2c** ($CDCl_3$, 75 MHz).

Compound 2c

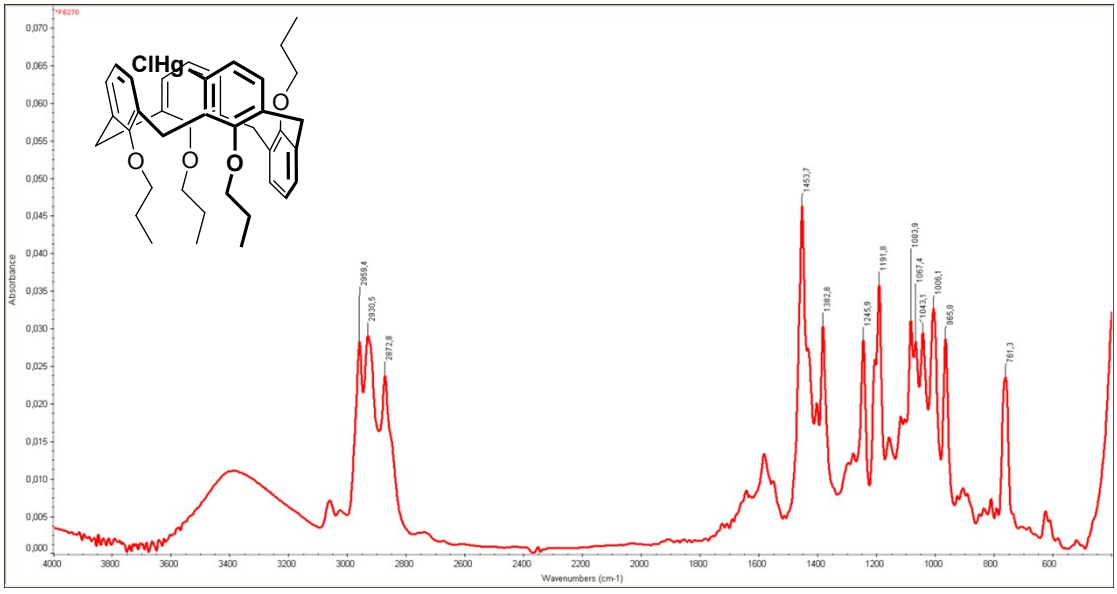

Figure 3. IR of compound **2c** (KBr).

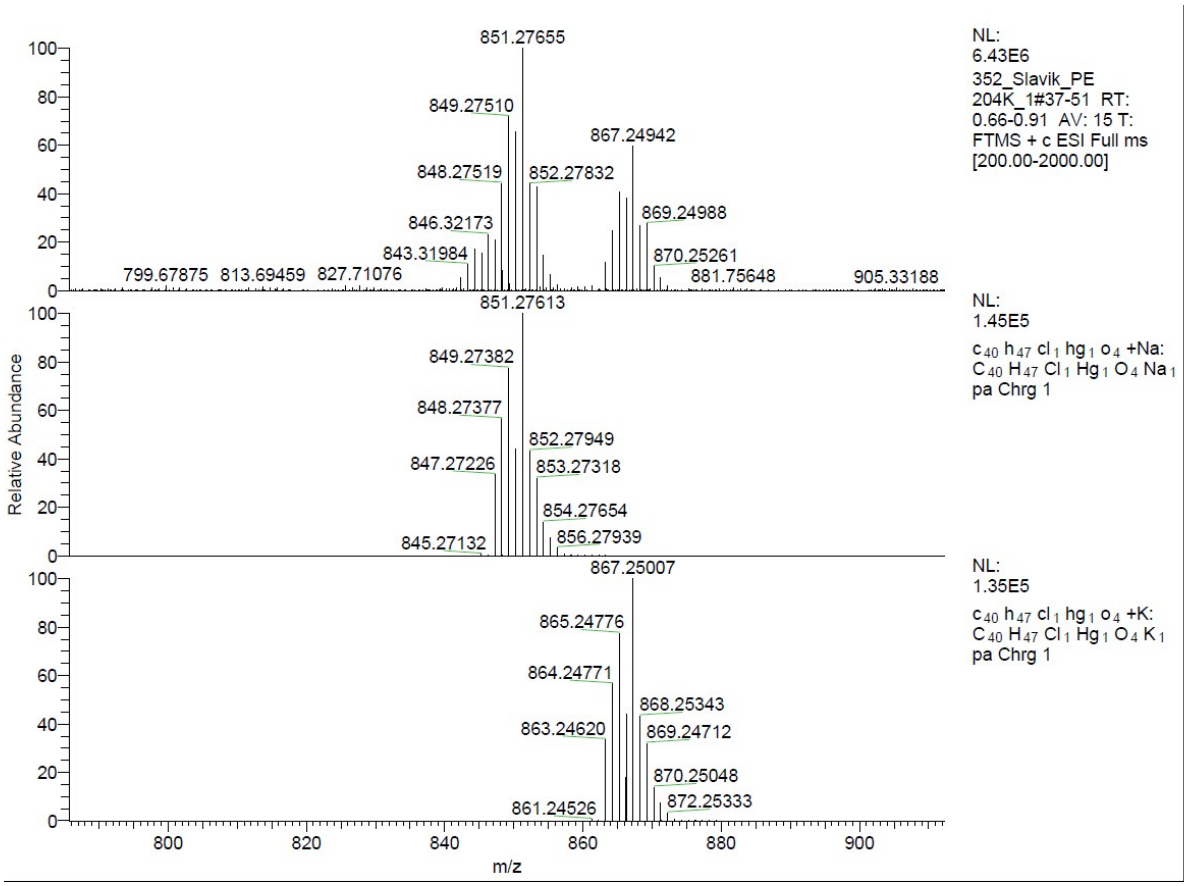

Figure 4. HRMS of compound **2c** (ESI^+).

Compound 2e

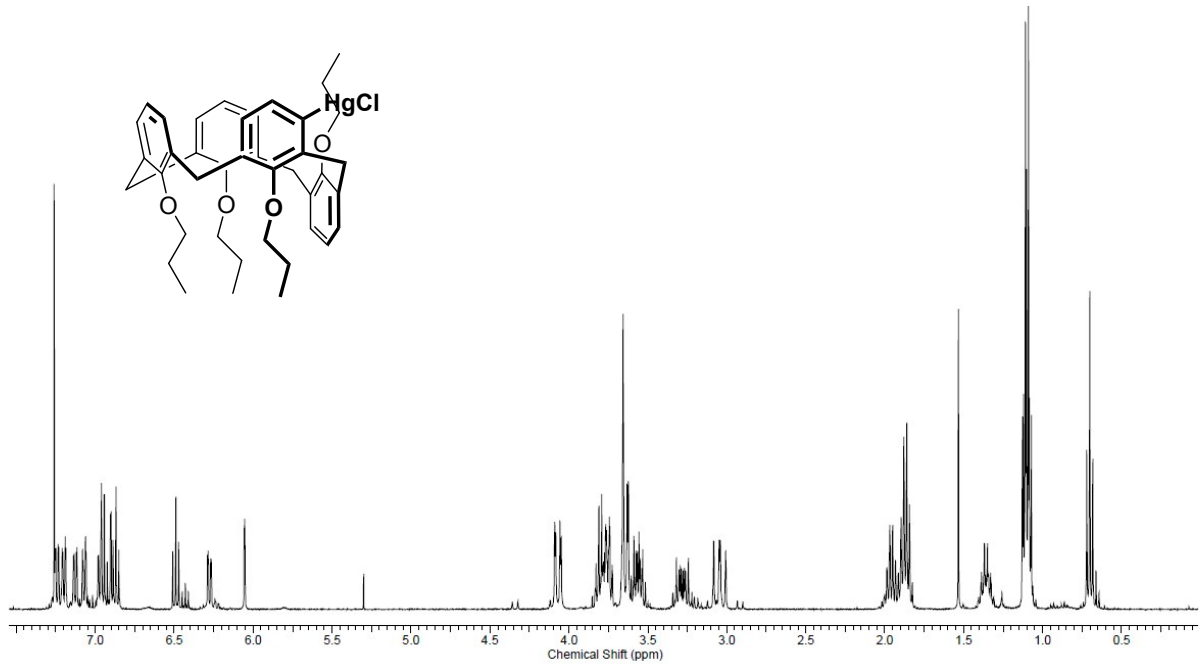

Figure 5. ^{1}H NMR of compound **2e** ($CDCl_3$, 400 MHz).

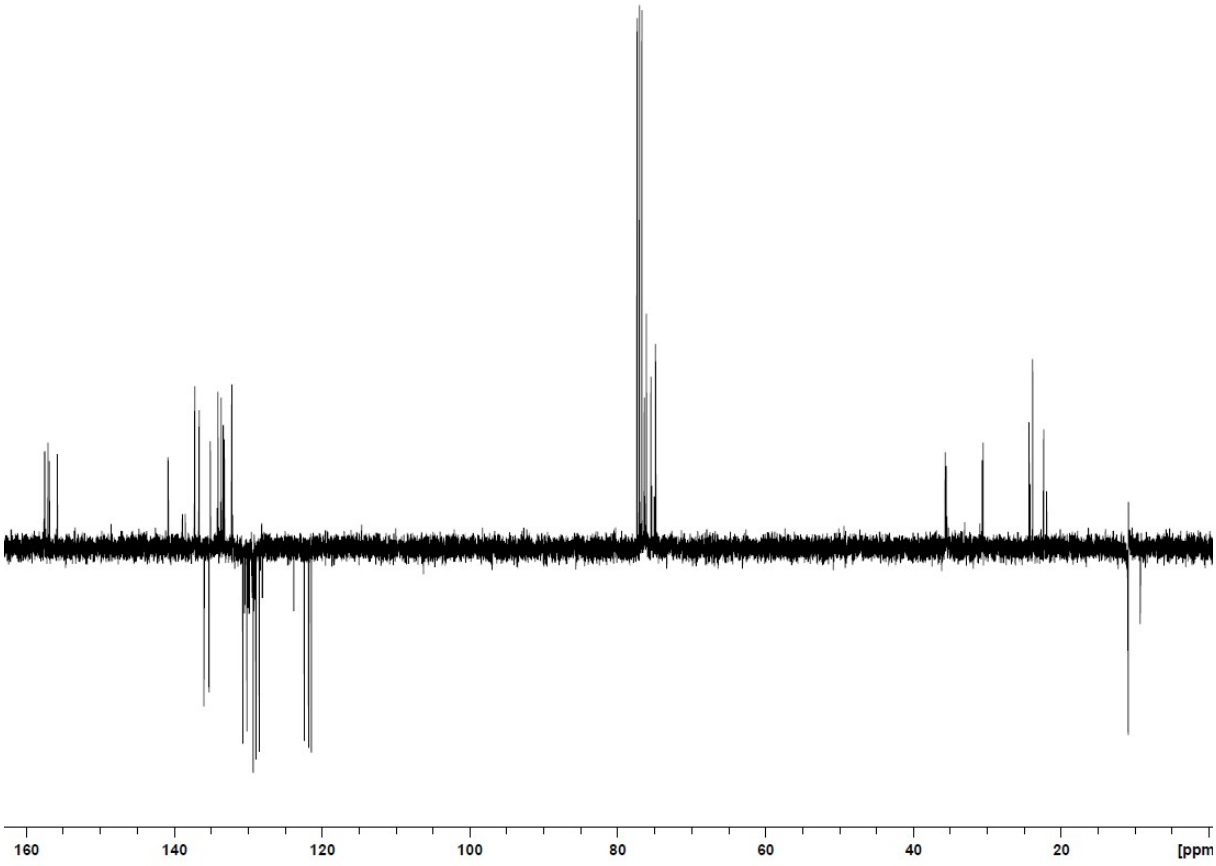

Figure 6. ^{13}C NMR of compound **2e** ($CDCl_3$, 100 MHz).

Compound 2c

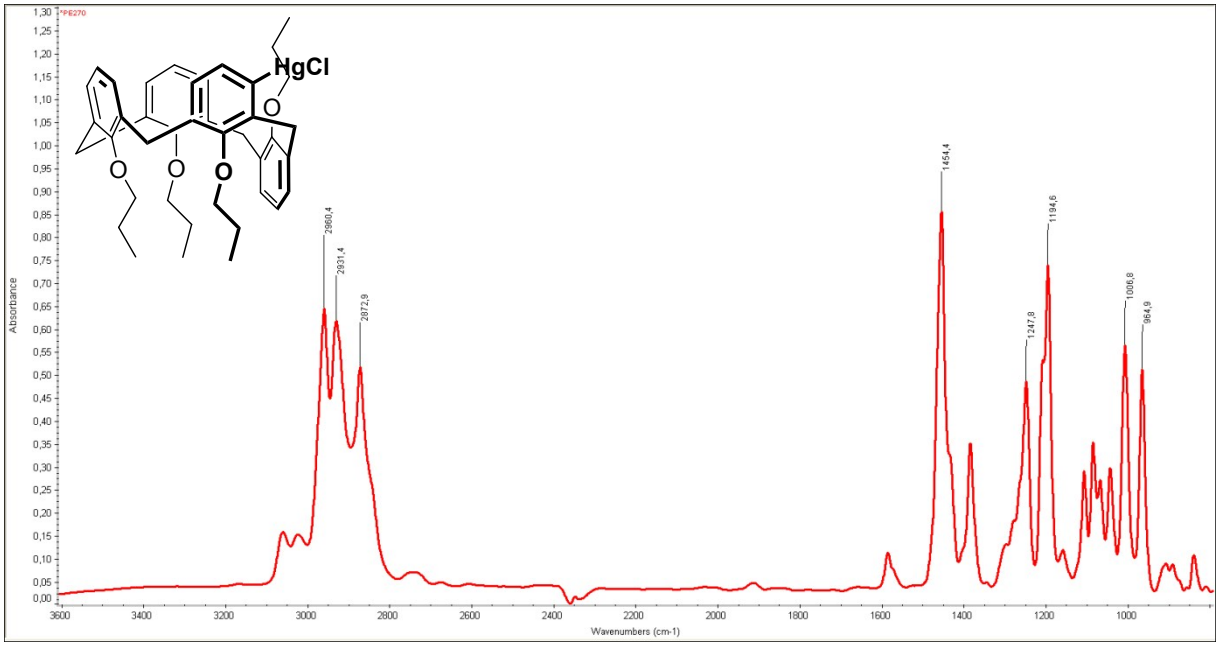

Figure 7. IR of compound **2e** (KBr).

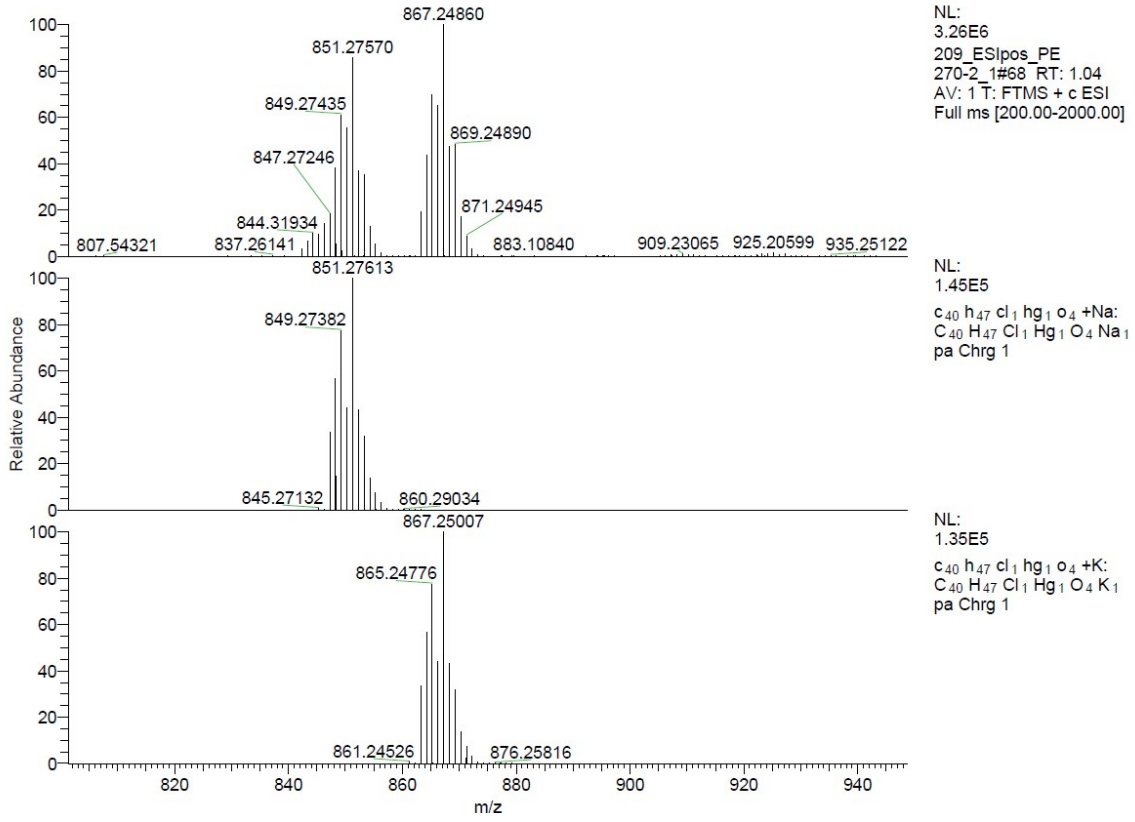

Figure 8. HRMS of compound **2e** (ESI^+).

Compound 3

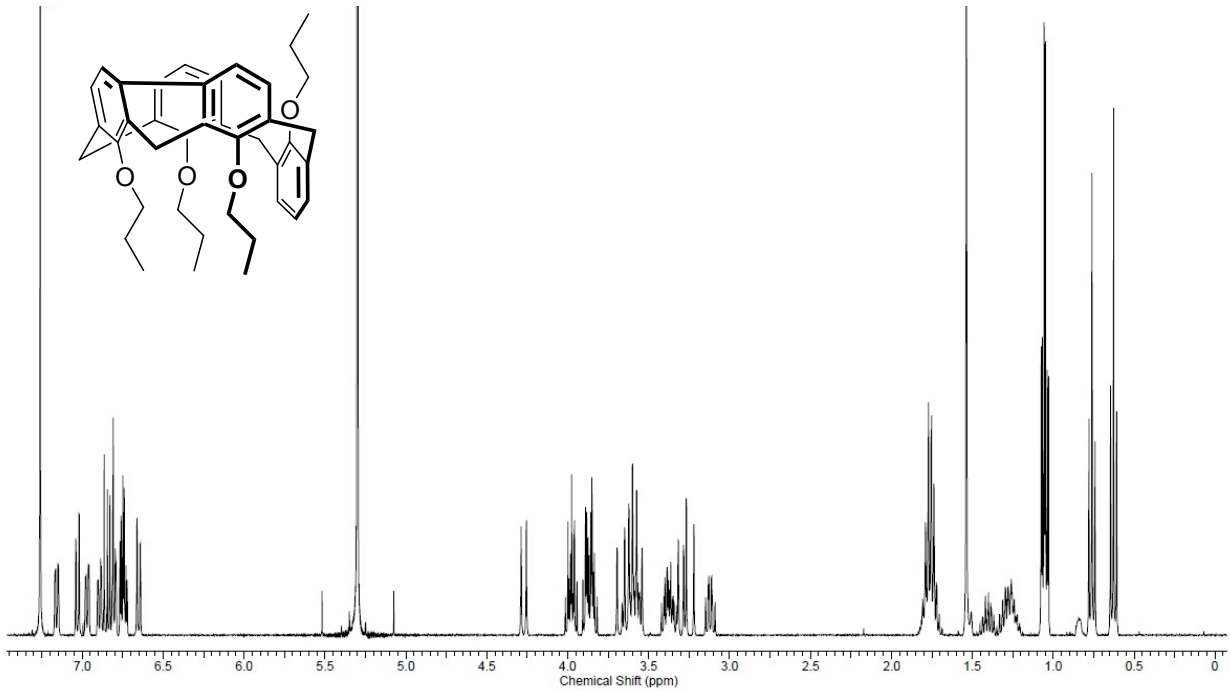

Figure 9. ^{1}H NMR of compound **3** ($CDCl_3$, 300 MHz).

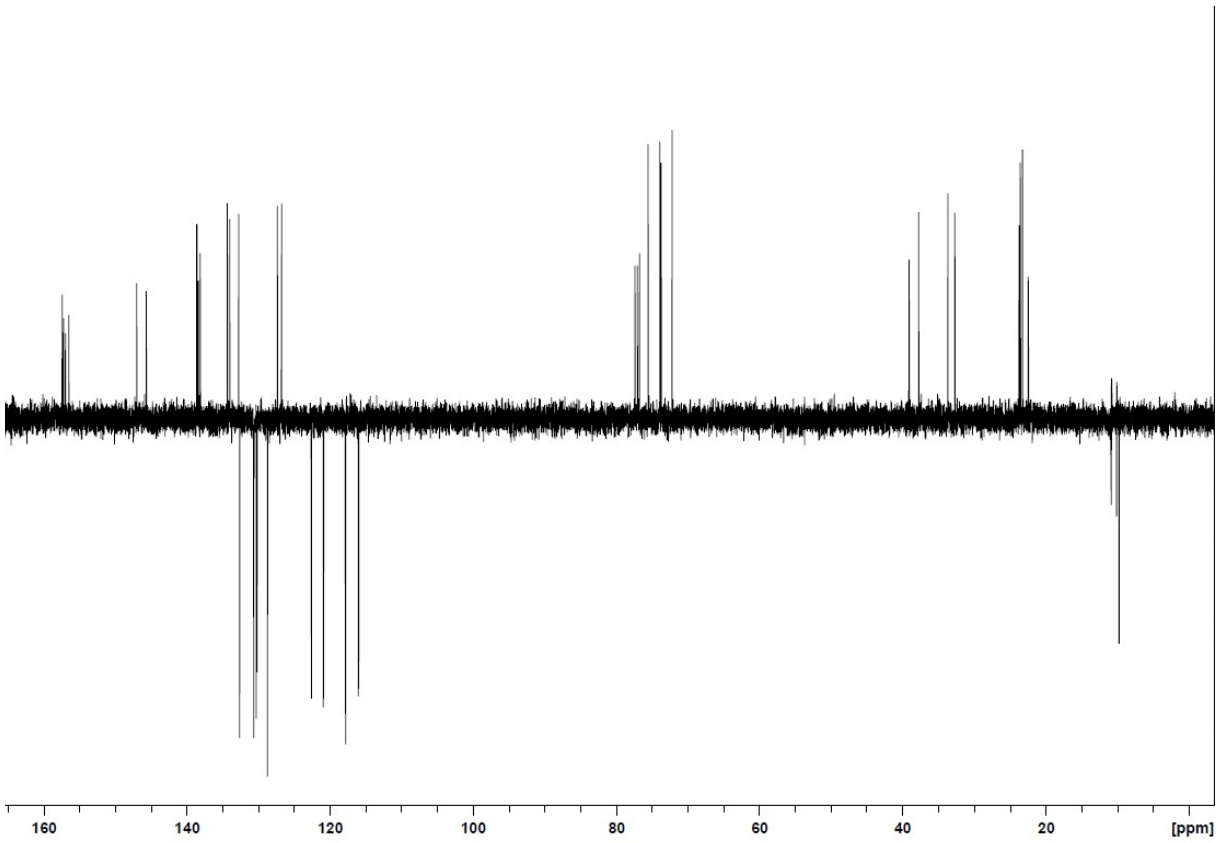

Figure 10. ^{13}C NMR of compound **3** ($CDCl_3$, 75 MHz).

Compound 3

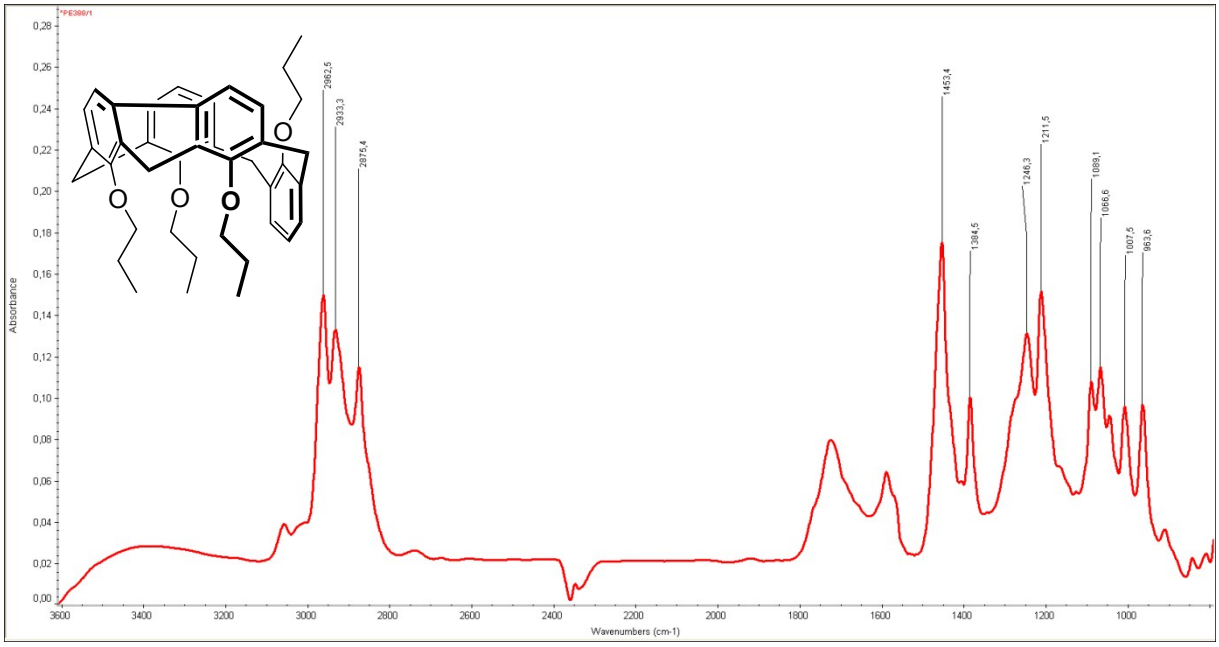

Figure 11. IR of compound **3** (KBr).

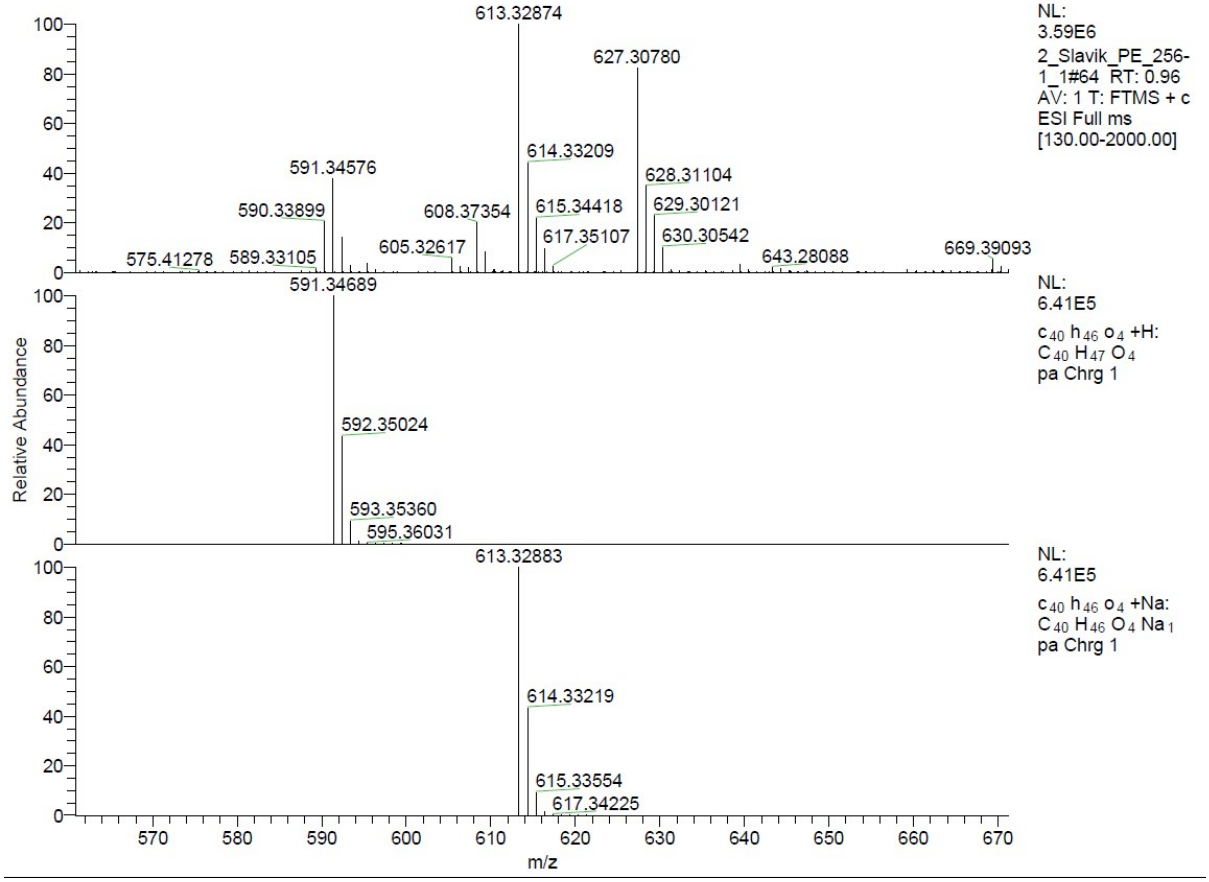

Figure 12. HRMS of compound **3** (ESI^+).

Compound 4

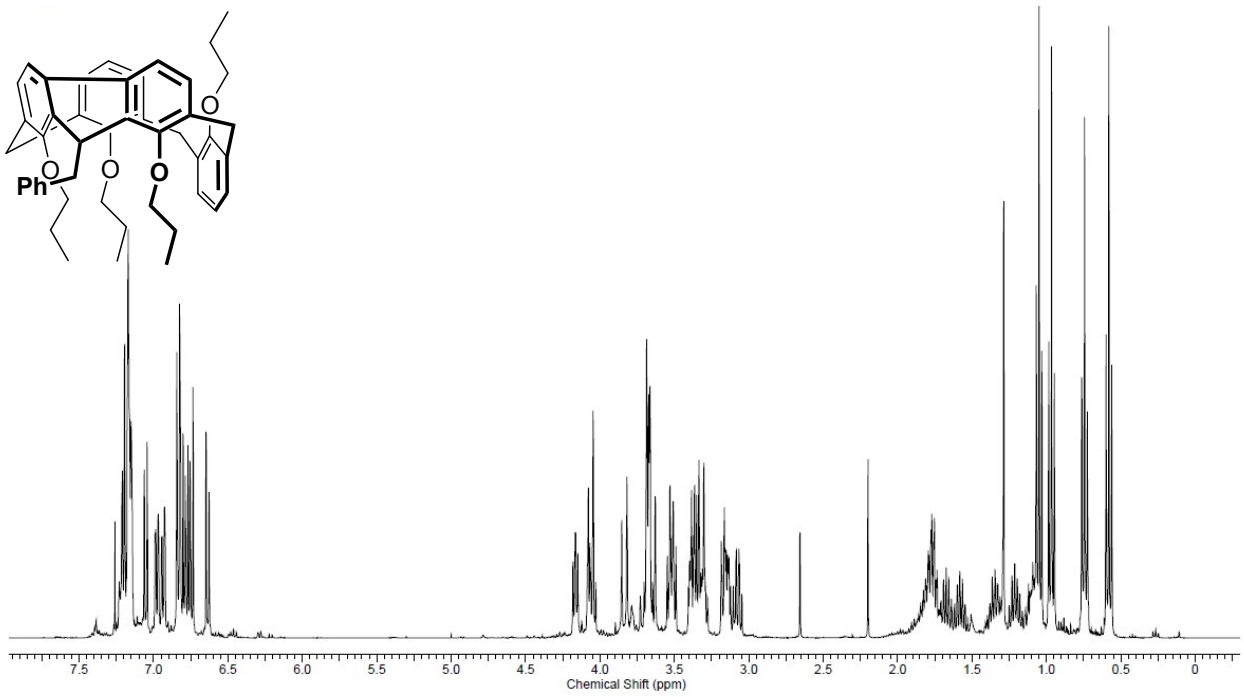

Figure 13. ^{1}H NMR of compound **4** ($CDCl_3$, 400 MHz).

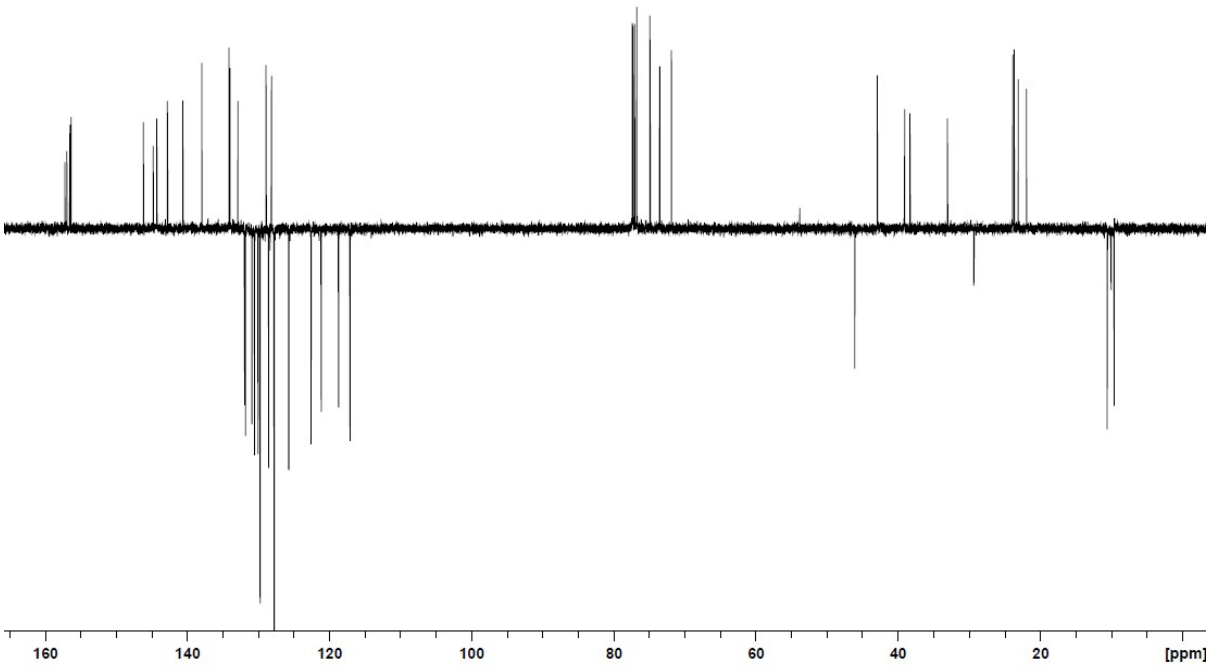

Figure 14. ^{13}C NMR of compound **4** ($CDCl_3$, 100 MHz).

Compound 4

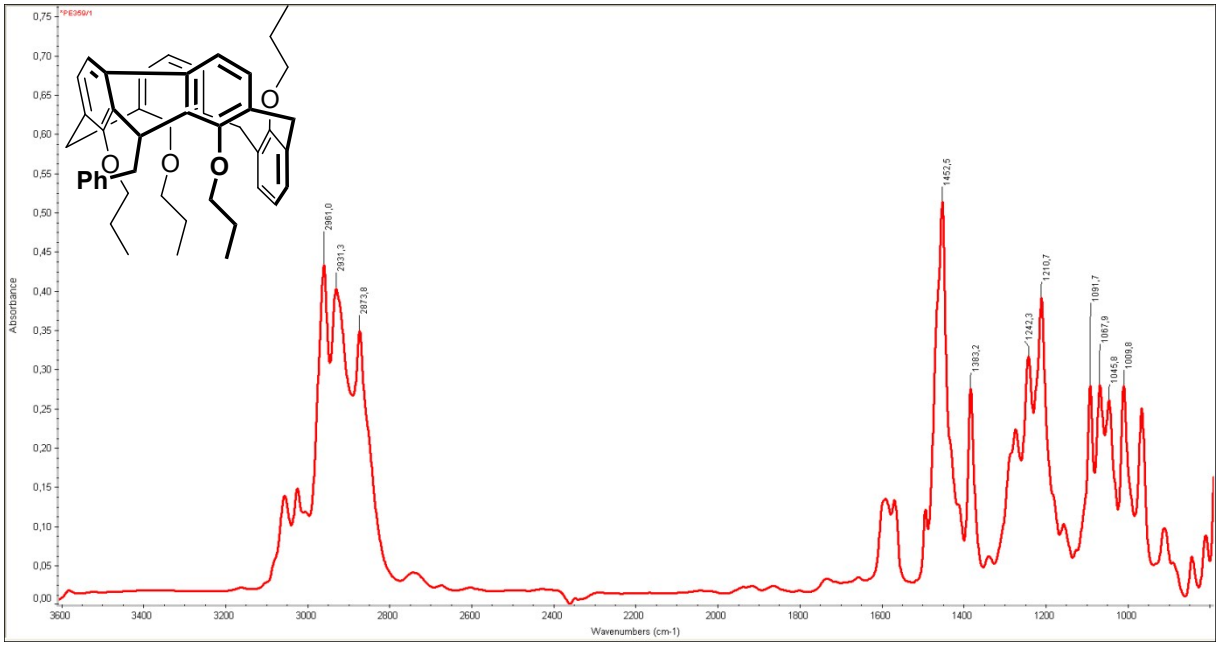

Figure 15. IR of compound **4** (KBr).

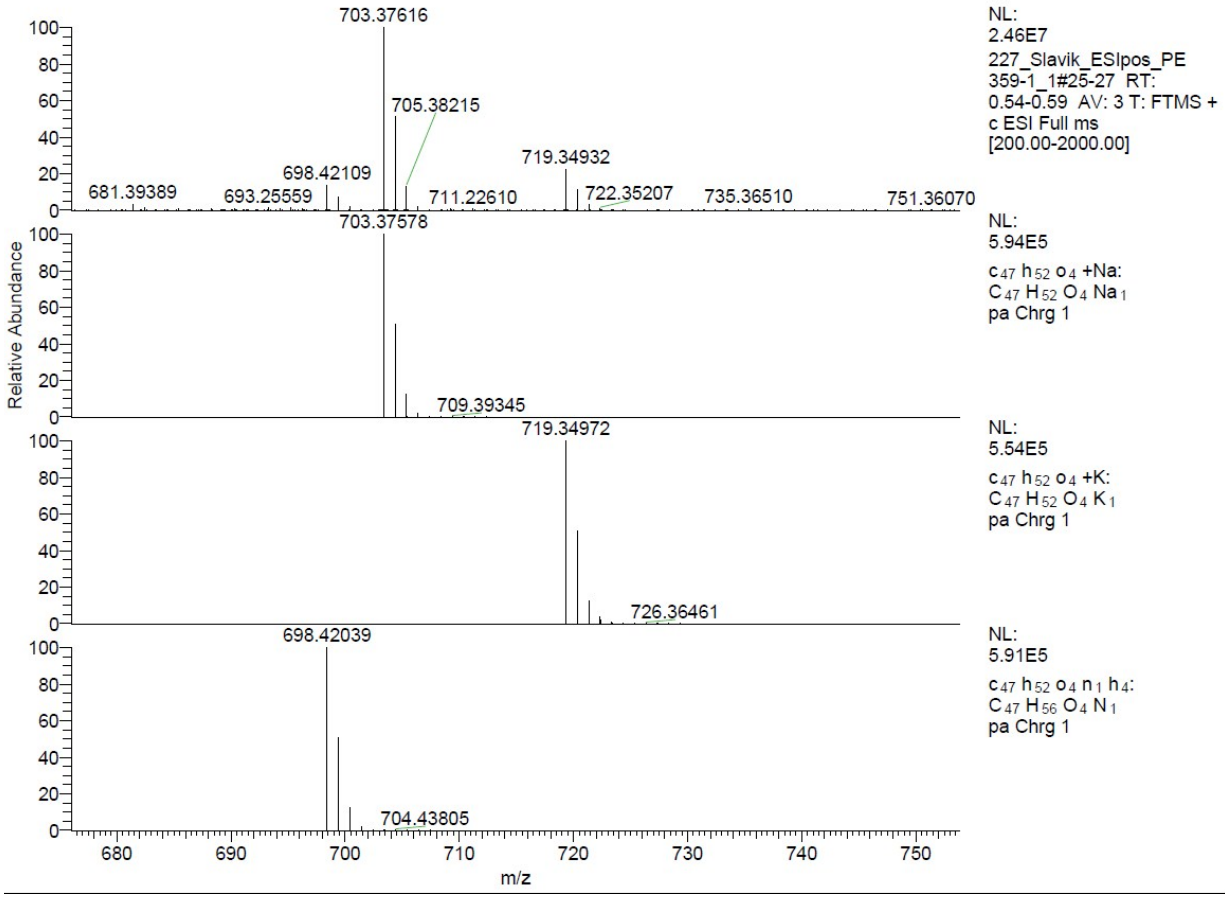

Figure 16. HRMS of compound **4** (ESI^+).

HPLC experiments, resolution of enantiomers

Chromatographic measurements were carried out on a 1100 HPLC system from Agilent Technologies, equipped with a degasser, quaternary pump, an auto sampler, a column oven and multiple wavelength detector. The flow rate was set to 1 mL/min and temperature to 20 °C for all measurements. The injection volume was 5 µL and the sample concentration was 1 mg/mL. Data analysis was carried out with Chemstation software (Agilent Technologies).

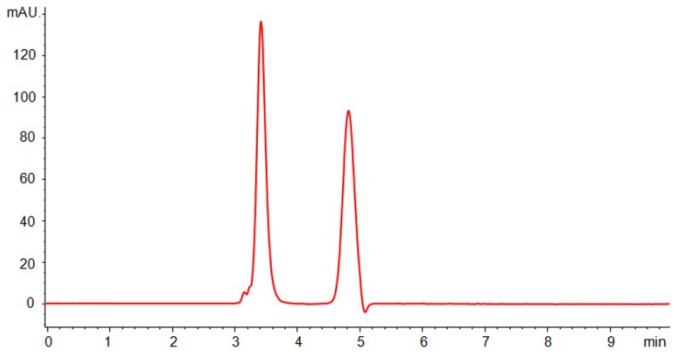

Figure. 17. Separation of **3** was performed on a polysaccharide chiral column Chiralpak AD-H, 250×4.6 id, 5 µm, using normal phase mode with 2.5% propan-2-ol in heptane as a bulk mobile phase containing 0.1% diethylamine as a basic additive, flow 1 mL/min, temperature 20 °C, detection wavelength 254 nm.

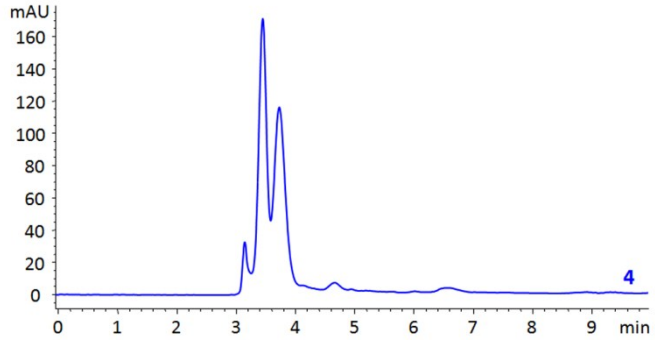

Figure 18. Separation of **4** was performed on a polysaccharide chiral column Chiralpak AD-H, 250×4.6 id, 5 µm, using normal phase mode with 2.5% propan-2-ol in heptane as a bulk mobile phase, flow 1 mL/min, temperature 20 °C, detection wavelength 254 nm.

Preparative HPLC:

The preparative separation was performed on the Chiralpak AD-H 250x4.6 ID, 5 um, column in the normal phase mode using 3% propan-2-ol in heptane. The sample concentration was 25 mg/ml, injection volume 25 μl, flow 1 ml/min, and temperature 20 °C.

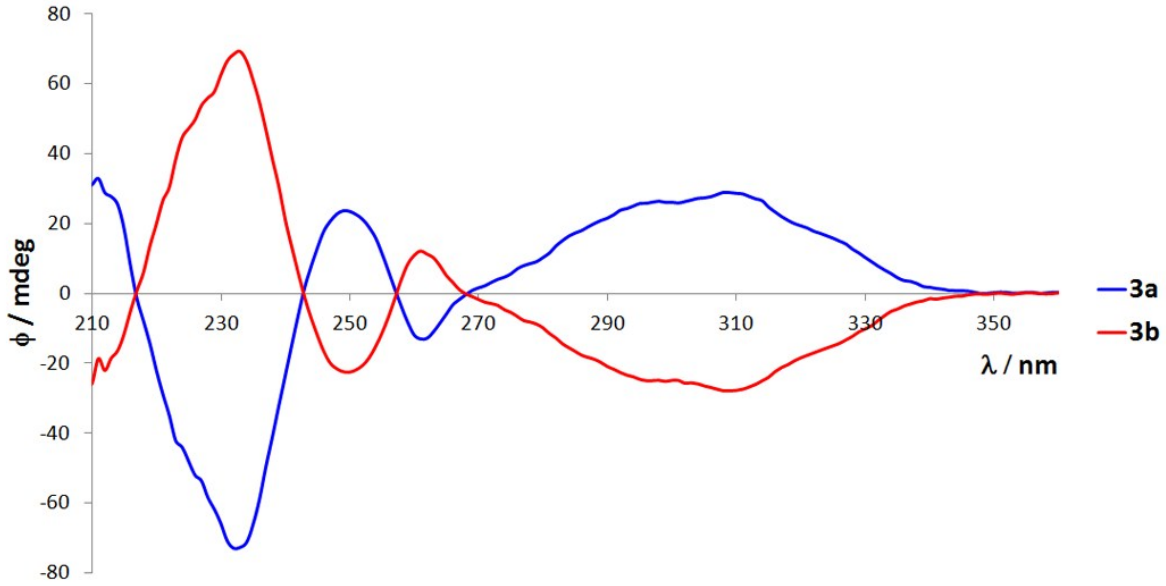

Figure 19. The measurements were carried out using spectrometer Ja-810 (Jasco, Japan) in the wavelength range of 400-200 nm. The sample concentration was 0.024 mg/ml and sample volume 2 ml.

Crystallographic data

The structure **2c** was measured using Xcalibur Onyx CCD diffractometer with graphite monochromated Cu-Kα radiation. Structures **2e** and **3** were measured using a Gemini Atlas CCD diffractometer with mirror-collimated Cu-Kα radiation. The data reduction and absorption correction were done with CrysAlis PRO software. The structures were solved using charge-flipping methods.[x1] The structures were refined by full matrix least squares on F squared value using Crystals software[x2] in case of structures **2c** and **3** and Jana2006 in case of structure **2e**.[x3] The MCE software[x4] was used for visualization of electron density maps. The positions of disordered functional groups and molecular fragments were found in difference Fourier maps; the bond lengths and angles were restrained. The overall occupancy of disordered functional groups and molecular fragment was constrained to 1. According to common practice the hydrogen atoms attached to carbon atoms were place geometrically with U_{iso}(H) in range 1.2-1.5 U_{eq} of parent atom (C). The structures were deposited to Cambridge Structural Database. For further information on data collection and structure refinement see Table 2.

Table 2. Crystallographic data for calix[4]arene derivatives **2c**, **2e** and **3**

Compound	**2c**	**2e**	**3**
Empirical formula	$C_{40}H_{47}ClHgO_4$	$C_{40}H_{47}ClHgO_4$	$C_{40}H_{46}O_4$
Formula wt.	827.85	827.9	590.80
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	*P*-1	*C*2/*c*	*P*-1
a (Å)	14.6684 (2)	36.8232 (11)	10.5111 (4)
b (Å)	16.1503 (3)	9.7905 (3)	17.7963 (5)
c (Å)	16.8665 (3)	26.7317 (9)	19.3271 (7)
α (°)	109.8701 (15)	90	110.342 (3)
β (°)	99.8419 (14)	131.016 (4)	96.592 (3)
γ (°)	95.2508 (14)	90	101.212 (2)
V (Å^3)	3653.92 (11)	7271.5 (6)	3259.1 (2)
Z	4	8	4
T (K)	180	120	120
ρ_{calc} (g cm^{-3})	1.505	1.512	1.204
μ (mm^{-1})	8.53	8.58	0.59
F(000)	1664	3328	1272
Reflns collected	39492	20101	22657
Indep. Reflns (R_{int})	14763 (0.055)	6388 (0.034)	11353 (0.031)
Ref. par. (Restrains)	856 (52)	429 (2)	849 (92)
GOF	0.99	1.37	0.94
R1, wR2 [I>3σ(I)]	0.046, 0.088	0.029, 0.081	0.043, 0.095
R1, wR2 (all data)	0.049, 0.091	0.032, 0.084	0.054, 0.107
Res. el. dens. (e Å^{-3})	1.59, -1.62	0.60, -0.49	0.46, -0.67
CCDC number	1435385	1435386	1435387

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[x2] P. W. Betteridge, J. R. Carruthers, R. I. Cooper, K. Prout, D. J. Watkin, *J. Appl. Crystallogr*. **2003**, *36*, 1487.

[x3] Petricek, V., Dusek, M. & Palatinus L. (2014). *Z. Kristallogr.* **229**(5), 345-352.

[x4] J. Rohlicek, M. Husak, *J. Appl. Crystallogr*. **2007**, *40*, 600-601.

Quantum chemical calculations

Table 1, compound 2a

scf done: -2419.321080

C	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.403506	1	0.000000	0	0.000000	0	1	0	0
C	1.408271	1	117.937996	1	0.000000	0	2	1	0
C	1.408578	1	122.009697	1	7.856799	1	3	2	1
C	1.403694	1	117.912346	1	-7.782125	1	4	3	2
C	1.400080	1	120.894081	1	1.814283	1	5	4	3
C	1.520816	1	121.113861	1	-169.442825	1	2	3	4
C	1.521328	1	112.234840	1	63.710403	1	7	2	3
C	1.409675	1	121.488518	1	68.788506	1	8	7	2
C	1.407424	1	121.845428	1	-171.732407	1	9	8	7
C	1.404749	1	118.258072	1	-5.092029	1	10	9	8
C	1.398240	1	120.815857	1	0.983028	1	11	10	9
C	1.399956	1	119.750435	1	2.634655	1	12	11	10
C	1.523261	1	120.184509	1	-175.710068	1	10	11	12
C	1.517945	1	110.582565	1	56.169605	1	14	10	11
C	1.408305	1	119.991623	1	69.223679	1	15	14	10
C	1.408282	1	122.106819	1	-170.417328	1	16	15	14
C	1.406132	1	118.283371	1	-5.555618	1	17	16	15
C	1.406435	1	120.488571	1	1.539613	1	18	17	16
C	1.406527	1	120.079391	1	2.237005	1	19	18	17
O	1.410246	1	119.331841	1	176.845764	1	9	10	11
C	1.462901	1	113.965378	1	-87.033005	1	21	9	10
C	1.520951	1	107.976143	1	178.339584	1	22	21	9
C	1.533846	1	111.783035	1	179.930222	1	23	22	21
O	1.410158	1	118.836082	1	9.607819	1	3	2	7
C	1.463789	1	113.030708	1	91.712486	1	25	3	2
C	1.521197	1	108.328316	1	-178.993927	1	26	25	3
C	1.533937	1	111.675484	1	-178.412247	1	27	26	25
C	1.521173	1	121.254555	1	169.351868	1	4	3	2
C	1.521213	1	112.082802	1	-63.598572	1	29	4	3
C	1.409896	1	121.544487	1	-69.925583	1	30	29	4
C	1.407399	1	121.737801	1	171.096771	1	31	30	29
C	1.404945	1	118.282875	1	5.364500	1	32	31	30
C	1.398019	1	120.858551	1	-0.988849	1	33	32	31
C	1.399778	1	119.687424	1	-2.831802	1	34	33	32
O	1.411238	1	118.852173	1	-7.612600	1	31	30	29
C	1.466251	1	113.014961	1	-92.000053	1	36	31	30
C	1.521335	1	108.489449	1	-179.611069	1	37	36	31
C	1.532423	1	113.163734	1	66.422050	1	38	37	36
C	1.523271	1	121.550179	1	-171.047623	1	32	31	30
O	1.393471	1	118.809151	1	-6.455258	1	16	17	40
C	1.469564	1	114.085495	1	-93.419037	1	41	16	17
C	1.515973	1	107.707458	1	-179.218155	1	42	41	16
C	1.533752	1	111.576820	1	178.414383	1	43	42	41
Hg	2.133046	1	120.254105	1	177.762955	1	19	20	15
O	2.151267	1	174.486145	1	-12.778458	1	45	19	20
C	1.315504	1	134.809357	1	-169.377579	1	46	45	19
C	1.560367	1	112.957039	1	13.110265	1	47	46	45
F	1.418616	1	110.824875	1	-42.365574	1	48	47	46
O	1.232946	1	128.301285	1	-168.491318	1	47	46	45

```
F    1.368139 1  114.362473 1 -163.191528 1      48   47   46
F    1.396128 1  111.149773 1   74.190369 1      48   47   46
H    1.086164 1  120.143799 1 -179.587936 1      12   11   10
H    1.101344 1  109.527122 1   57.433437 1      22   21    9
H    1.101263 1  109.557526 1  -60.555626 1      22   21    9
H    1.097612 1  108.786484 1  -58.010277 1      23   22   21
H    1.097358 1  108.860374 1   57.827156 1      23   22   21
H    1.095578 1  110.883286 1 -179.992645 1      24   23   22
H    1.097482 1  111.340721 1   60.129498 1      24   23   22
H    1.097463 1  111.328331 1  -60.120895 1      24   23   22
H    1.085670 1  118.858871 1 -179.733170 1      13    8    9
H    1.087448 1  119.221809 1  179.474548 1      11   10    9
H    1.097004 1  107.992828 1 -168.930161 1       7    8    9
H    1.096601 1  110.690910 1  -51.988632 1       7    8    9
H    1.101509 1  109.557396 1  -57.834179 1      26   25    3
H    1.101480 1  109.576462 1   59.974831 1      26   25    3
H    1.096939 1  109.011353 1   59.442398 1      27   26   25
H    1.096966 1  108.886353 1  -56.378059 1      27   26   25
H    1.095596 1  110.893585 1 -179.778442 1      28   27   26
H    1.097531 1  111.376808 1  -59.867779 1      28   27   26
H    1.097447 1  111.277031 1   60.364315 1      28   27   26
H    1.096991 1  110.786331 1   57.122162 1      29    4    3
H    1.096346 1  107.980721 1  174.080902 1      29    4    3
H    1.101330 1  109.240128 1  -58.570763 1      37   36   31
H    1.100344 1  109.086533 1   59.215916 1      37   36   31
H    1.099228 1  107.978493 1 -171.666901 1      38   37   36
H    1.097813 1  108.579391 1  -55.989262 1      38   37   36
H    1.096274 1  111.102844 1 -179.296814 1      39   38   37
H    1.097945 1  110.997826 1   60.768562 1      39   38   37
H    1.094401 1  110.430649 1  -59.276302 1      39   38   37
H    1.086137 1  120.173370 1  179.497009 1      34   33   32
H    1.087339 1  119.193680 1 -179.531189 1      33   32   31
H    1.085654 1  118.830986 1    2.936196 1      35   30   29
H    1.097938 1  110.601807 1 -117.842873 1      40   32   31
H    1.093830 1  108.367638 1    0.255724 1      40   32   31
H    1.097983 1  110.490494 1  -64.473495 1      14   10   11
H    1.093883 1  108.356644 1  177.552155 1      14   10   11
H    1.087846 1  118.312012 1  178.767120 1      20   15   16
H    1.087711 1  118.359177 1    5.363070 1      18   17   40
H    1.086783 1  118.982101 1 -179.574326 1       5    4    3
H    1.086796 1  118.982422 1   -3.214806 1       1    2    7
H    1.086428 1  120.064560 1 -179.094666 1       6    5    4
H    1.101578 1  109.234337 1  -58.273659 1      42   41   16
H    1.102022 1  109.020660 1   59.454636 1      42   41   16
H    1.094290 1  107.966667 1   56.468834 1      43   42   41
H    1.095052 1  108.397354 1  -58.996201 1      43   42   41
H    1.096359 1  110.565140 1  179.628113 1      44   43   42
H    1.098614 1  111.526100 1  -60.763565 1      44   43   42
H    1.098522 1  111.811996 1   59.846058 1      44   43   42
```

Table 1, compound 2b

scf done: -2419.319321

C	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.404244	1	0.000000	0	0.000000	0	1	0	0
C	1.408072	1	117.983109	1	0.000000	0	2	1	0
C	1.407922	1	122.080536	1	7.647026	1	3	2	1
C	1.404059	1	117.949493	1	-7.488802	1	4	3	2
C	1.400676	1	120.774376	1	1.670493	1	5	4	3
C	1.522182	1	120.586533	1	-165.956131	1	2	3	4
C	1.521817	1	108.943596	1	70.158707	1	7	2	3
C	1.409301	1	120.750122	1	72.395149	1	8	7	2
C	1.406282	1	121.961426	1	-167.201431	1	9	8	7
C	1.404782	1	118.175156	1	-6.059016	1	10	9	8
C	1.397886	1	120.713043	1	0.897913	1	11	10	9
C	1.400750	1	119.928993	1	3.447344	1	12	11	10
C	1.523401	1	120.747795	1	-175.734848	1	10	11	12
C	1.521201	1	111.126129	1	49.306015	1	14	10	11
C	1.418653	1	119.883438	1	64.204498	1	15	14	10
C	1.413544	1	121.805511	1	-164.007553	1	16	15	14
C	1.401054	1	118.358086	1	-8.110353	1	17	16	15
C	1.403497	1	121.088799	1	1.346048	1	18	17	16
C	1.405103	1	119.299690	1	4.049060	1	19	18	17
O	1.411426	1	119.275307	1	176.934006	1	9	10	11
C	1.465770	1	113.753441	1	-87.226707	1	21	9	10
C	1.520512	1	108.120918	1	179.467651	1	22	21	9
C	1.534198	1	111.619278	1	-179.864258	1	23	22	21
O	1.410924	1	118.881233	1	11.388728	1	3	2	7
C	1.463851	1	113.301811	1	91.313187	1	25	3	2
C	1.521056	1	108.112183	1	-179.962784	1	26	25	3
C	1.534019	1	111.750984	1	-179.784958	1	27	26	25
C	1.521753	1	120.672844	1	166.437469	1	4	3	2
C	1.522499	1	109.330414	1	-70.582138	1	29	4	3
C	1.410295	1	120.867523	1	-73.145050	1	30	29	4
C	1.406128	1	121.815750	1	167.644485	1	31	30	29
C	1.405464	1	118.084969	1	6.518900	1	32	31	30
C	1.398321	1	120.911819	1	-1.328329	1	33	32	31
C	1.400429	1	119.811279	1	-3.440121	1	34	33	32
O	1.412897	1	118.486214	1	-11.120617	1	31	30	29
C	1.467928	1	112.088516	1	-90.592598	1	36	31	30
C	1.521259	1	109.023941	1	172.084885	1	37	36	31
C	1.531696	1	113.372574	1	65.812469	1	38	37	36
C	1.523472	1	121.383904	1	-169.294983	1	32	31	30
O	1.383636	1	116.033134	1	-6.259892	1	16	17	40
C	1.475262	1	120.187111	1	-126.422279	1	41	16	17
C	1.524409	1	109.660561	1	114.131348	1	42	41	16
C	1.533511	1	113.186340	1	-79.784279	1	43	42	41
Hg	2.142250	1	119.451508	1	176.756668	1	20	15	16
O	2.155465	1	176.029770	1	156.690552	1	45	20	15
C	1.315786	1	133.851303	1	178.820679	1	46	45	20
C	1.559716	1	112.369370	1	0.785876	1	47	46	45
F	1.408821	1	110.731857	1	-55.662895	1	48	47	46
O	1.232616	1	128.421814	1	-179.337082	1	47	46	45
F	1.366411	1	114.808861	1	-177.662399	1	48	47	46
F	1.407929	1	110.785622	1	60.240459	1	48	47	46

```
H    1.086070 1  120.053711 1 -179.474335 1      12   11   10
H    1.100764 1  109.429909 1   58.438282 1      22   21    9
H    1.100661 1  109.197517 1  -59.432617 1      22   21    9
H    1.097513 1  108.844597 1  -57.975243 1      23   22   21
H    1.097546 1  108.928123 1   58.167229 1      23   22   21
H    1.095457 1  110.875763 1  179.740005 1      24   23   22
H    1.097162 1  111.308350 1   59.854607 1      24   23   22
H    1.097325 1  111.313721 1  -60.382702 1      24   23   22
H    1.084848 1  118.933037 1 -179.137329 1      13    8    9
H    1.087381 1  119.352539 1  178.922684 1      11   10    9
H    1.095438 1  108.771568 1 -166.111115 1       7    8    9
H    1.095345 1  111.113350 1  -47.485699 1       7    8    9
H    1.101272 1  109.494598 1  -58.885315 1      26   25    3
H    1.101197 1  109.509285 1   58.994114 1      26   25    3
H    1.097427 1  108.916588 1   58.198807 1      27   26   25
H    1.097415 1  108.875870 1  -57.807590 1      27   26   25
H    1.095562 1  110.891533 1  179.976563 1      28   27   26
H    1.097417 1  111.328773 1  -60.134251 1      28   27   26
H    1.097410 1  111.294235 1   60.101715 1      28   27   26
H    1.095559 1  111.145287 1   49.369789 1      29    4    3
H    1.095464 1  108.690353 1  167.831223 1      29    4    3
H    1.101297 1  109.053276 1  -66.613731 1      37   36   31
H    1.100268 1  108.860779 1   51.011639 1      37   36   31
H    1.099446 1  107.780350 1 -172.334915 1      38   37   36
H    1.098118 1  108.659874 1  -56.901058 1      38   37   36
H    1.096356 1  111.107948 1 -179.713394 1      39   38   37
H    1.097827 1  110.974709 1   60.325096 1      39   38   37
H    1.093389 1  110.505424 1  -59.441174 1      39   38   37
H    1.086323 1  120.104134 1  179.398529 1      34   33   32
H    1.087297 1  119.160416 1 -179.676041 1      33   32   31
H    1.085131 1  118.933762 1    4.679458 1      35   30   29
H    1.098104 1  110.805717 1 -113.499573 1      40   32   31
H    1.093961 1  107.867500 1    4.707249 1      40   32   31
H    1.100955 1  109.948448 1  -71.614304 1      14   10   11
H    1.092375 1  108.264664 1  172.893341 1      14   10   11
H    1.087514 1  119.280708 1    5.501292 1      18   17   40
H    1.086105 1  121.441490 1  178.940063 1      19   20   15
H    1.085671 1  118.935555 1  179.333389 1       5    4    3
H    1.085838 1  118.953362 1   -6.119593 1       1    2    7
H    1.086551 1  119.961311 1 -179.077896 1       6    5    4
H    1.091915 1  105.981415 1 -124.801285 1      42   41   16
H    1.099420 1  109.555367 1   -6.775812 1      42   41   16
H    1.100296 1  107.945206 1  158.756424 1      43   42   41
H    1.096595 1  107.591743 1   43.450520 1      43   42   41
H    1.096400 1  111.470421 1  177.995193 1      44   43   42
H    1.098076 1  110.931419 1  -62.068420 1      44   43   42
H    1.096156 1  111.258247 1   57.668358 1      44   43   42
```

Table 1, compound 2c

scf done: -2419.334580

C	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.404023	1	0.000000	0	0.000000	0	1	0	0
C	1.408425	1	117.994667	1	0.000000	0	2	1	0
C	1.407816	1	122.085075	1	7.671199	1	3	2	1
C	1.404189	1	117.918777	1	-7.493996	1	4	3	2
C	1.400713	1	120.801933	1	1.648151	1	5	4	3
C	1.522159	1	120.599358	1	-166.230988	1	2	3	4
C	1.521400	1	109.044785	1	68.217979	1	7	2	3
C	1.409487	1	121.081551	1	72.435471	1	8	7	2
C	1.410921	1	122.443619	1	-166.586594	1	9	8	7
C	1.409783	1	117.657471	1	-6.072530	1	10	9	8
C	1.403950	1	120.576233	1	0.390825	1	11	10	9
C	1.400775	1	120.139404	1	3.950879	1	12	11	10
Hg	2.155321	1	120.943878	1	174.866058	1	11	10	9
O	2.224354	1	169.623505	1	-166.403030	1	14	11	10
C	1.306525	1	106.973450	1	-146.628372	1	15	14	11
C	1.542291	1	113.423424	1	-175.196442	1	16	15	14
F	1.382014	1	112.532616	1	-170.284912	1	17	16	15
C	1.530190	1	122.501045	1	-2.774203	1	10	11	14
C	1.520703	1	111.970680	1	53.061058	1	19	10	11
C	1.414248	1	121.718620	1	60.084064	1	20	19	10
C	1.414391	1	121.377678	1	-164.105042	1	21	20	19
C	1.403763	1	118.536064	1	-7.991577	1	22	21	20
C	1.402495	1	120.901649	1	1.062219	1	23	22	21
C	1.404886	1	119.558739	1	4.084469	1	24	23	22
O	1.410510	1	119.346535	1	176.974213	1	9	10	11
C	1.465070	1	114.018059	1	-89.588608	1	26	9	10
C	1.520570	1	108.021065	1	-177.805054	1	27	26	9
C	1.534101	1	111.697853	1	-179.268555	1	28	27	26
O	1.410796	1	118.877823	1	11.439499	1	3	2	7
C	1.464406	1	113.203712	1	91.708267	1	30	3	2
C	1.521050	1	108.184113	1	179.475098	1	31	30	3
C	1.534081	1	111.715561	1	-179.478897	1	32	31	30
C	1.521710	1	120.736214	1	166.873550	1	4	3	2
C	1.522447	1	109.646904	1	-71.003334	1	34	4	3
C	1.410131	1	120.809494	1	-73.237152	1	35	34	4
C	1.405787	1	121.846565	1	168.172165	1	36	35	34
C	1.405705	1	118.077057	1	6.911702	1	37	36	35
C	1.398710	1	120.887688	1	-1.835832	1	38	37	36
C	1.400932	1	119.810539	1	-3.221539	1	39	38	37
O	1.412677	1	118.479309	1	-10.788947	1	36	35	34
C	1.468480	1	111.994453	1	-91.260651	1	41	36	35
C	1.521052	1	109.034927	1	173.594757	1	42	41	36
C	1.531802	1	113.402008	1	66.318138	1	43	42	41
C	1.522582	1	121.355759	1	-168.852982	1	37	36	35
O	1.385387	1	116.600357	1	-6.188932	1	21	22	45
C	1.475752	1	119.320824	1	-124.395935	1	46	21	22
C	1.524526	1	110.201309	1	109.226921	1	47	46	21
C	1.533683	1	113.425995	1	-79.782394	1	48	47	46
O	1.253614	1	120.352547	1	11.286208	1	16	17	18
F	1.396204	1	110.170830	1	-108.155571	1	17	16	50
F	1.387033	1	112.157349	1	132.419952	1	17	16	50

```
H    1.100852 1  109.350128 1   61.259899 1      27   26    9
H    1.100767 1  109.289780 1  -56.646954 1      27   26    9
H    1.097379 1  108.826141 1  -57.304562 1      28   27   26
H    1.097468 1  108.913002 1   58.774921 1      28   27   26
H    1.095432 1  110.843948 1 -179.959122 1      29   28   27
H    1.097260 1  111.328041 1   60.201347 1      29   28   27
H    1.097347 1  111.336395 1  -60.098656 1      29   28   27
H    1.084792 1  119.169182 1 -179.399246 1      13    8    9
H    1.086341 1  121.103920 1    6.557859 1      12   11   14
H    1.095761 1  108.658966 1 -166.098984 1       7    8    9
H    1.095300 1  111.250633 1  -47.587868 1       7    8    9
H    1.101305 1  109.449997 1  -59.404282 1      31   30    3
H    1.101065 1  109.499664 1   58.439217 1      31   30    3
H    1.097488 1  109.004662 1   58.515198 1      32   31   30
H    1.097378 1  108.873085 1  -57.522266 1      32   31   30
H    1.095508 1  110.884613 1  179.942520 1      33   32   31
H    1.097441 1  111.349976 1  -60.156647 1      33   32   31
H    1.097353 1  111.295891 1   60.086239 1      33   32   31
H    1.095618 1  111.121162 1   49.068745 1      34    4    3
H    1.095354 1  108.627274 1  167.494934 1      34    4    3
H    1.101077 1  109.048958 1  -65.085938 1      42   41   36
H    1.100290 1  108.814522 1   52.513744 1      42   41   36
H    1.099405 1  107.755348 1 -171.865219 1      43   42   41
H    1.098180 1  108.664978 1  -56.467007 1      43   42   41
H    1.096358 1  111.080711 1 -179.587463 1      44   43   42
H    1.097805 1  110.993202 1   60.503021 1      44   43   42
H    1.093506 1  110.593430 1  -59.328651 1      44   43   42
H    1.088096 1  119.051483 1  178.955307 1      38   37   36
H    1.086603 1  120.142700 1  178.956436 1      39   38   37
H    1.085206 1  118.924484 1    4.346470 1      40   35   34
H    1.098024 1  110.875511 1 -114.994019 1      45   37   36
H    1.094336 1  107.947823 1    3.205462 1      45   37   36
H    1.098556 1  109.796715 1  -67.075867 1      19   10   11
H    1.092851 1  107.780617 1  176.652817 1      19   10   11
H    1.088867 1  119.478096 1  175.957840 1      25   20   21
H    1.085668 1  120.008644 1  179.496994 1      24   25   20
H    1.087193 1  119.240204 1    4.787031 1      23   22   45
H    1.085657 1  118.922874 1  179.385132 1       5    4    3
H    1.086476 1  119.953407 1 -179.037323 1       6    5    4
H    1.086088 1  119.011360 1   -6.092678 1       1    2    7
H    1.090867 1  105.672150 1 -129.680313 1      47   46   21
H    1.098914 1  109.537148 1  -12.221785 1      47   46   21
H    1.100605 1  107.824120 1  158.817200 1      48   47   46
H    1.096630 1  107.559998 1   43.630707 1      48   47   46
H    1.096608 1  111.430267 1  178.446030 1      49   48   47
H    1.098052 1  110.937950 1  -61.618759 1      49   48   47
H    1.096041 1  111.389175 1   58.086391 1      49   48   47
```

Table 1, compound 2d

scf done: -2419.322614

C	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.404260	1	0.000000	0	0.000000	0	1	0	0
C	1.409467	1	117.979301	1	0.000000	0	2	1	0
C	1.407520	1	122.070900	1	7.609000	1	3	2	1
C	1.404071	1	117.907990	1	-7.854504	1	4	3	2
C	1.400336	1	120.825096	1	2.121512	1	5	4	3
C	1.523502	1	120.877434	1	-165.372269	1	2	3	4
C	1.521616	1	108.016472	1	69.562500	1	7	2	3
C	1.409873	1	121.410286	1	77.219688	1	8	7	2
C	1.407083	1	121.813530	1	-165.597214	1	9	8	7
C	1.406152	1	118.318283	1	-4.242610	1	10	9	8
C	1.399449	1	120.636940	1	0.977927	1	11	10	9
C	1.402316	1	120.120499	1	1.119330	1	12	11	10
C	1.524667	1	119.233475	1	-172.719254	1	10	11	12
C	1.522694	1	109.827850	1	45.208443	1	14	10	11
C	1.414462	1	121.503151	1	60.360855	1	15	14	10
C	1.412866	1	121.471603	1	-163.054382	1	16	15	14
C	1.403292	1	118.393356	1	-7.564023	1	17	16	15
C	1.402623	1	120.905739	1	1.467896	1	18	17	16
C	1.401207	1	119.541016	1	3.622773	1	19	18	17
O	1.408923	1	119.593956	1	-179.331558	1	9	10	11
C	1.464814	1	114.352119	1	-85.538795	1	21	9	10
C	1.520471	1	107.928131	1	179.981567	1	22	21	9
C	1.534048	1	111.709602	1	-179.717529	1	23	22	21
Hg	2.130448	1	119.829559	1	165.426849	1	12	11	10
O	2.163091	1	170.710297	1	-102.551231	1	25	12	11
C	1.314989	1	135.359314	1	-179.985825	1	26	25	12
O	1.233703	1	128.321304	1	-173.865799	1	27	26	25
O	1.412085	1	119.095520	1	11.894572	1	3	2	7
C	1.465083	1	113.349365	1	93.174316	1	29	3	2
C	1.521212	1	108.165970	1	178.857162	1	30	29	3
C	1.534046	1	111.720901	1	-179.110031	1	31	30	29
C	1.521974	1	120.703705	1	166.527695	1	4	3	2
C	1.523197	1	110.056679	1	-71.584221	1	33	4	3
C	1.411116	1	120.604469	1	-69.954788	1	34	33	4
C	1.406729	1	121.971657	1	168.645233	1	35	34	33
C	1.406390	1	117.873985	1	8.072281	1	36	35	34
C	1.401645	1	121.010414	1	-1.406777	1	37	36	35
C	1.403931	1	119.600143	1	-4.768051	1	38	37	36
O	1.411699	1	118.205582	1	-11.756392	1	35	34	33
C	1.469966	1	111.610588	1	-91.375229	1	40	35	34
C	1.520965	1	109.268288	1	170.617279	1	41	40	35
C	1.531364	1	113.493309	1	65.341789	1	42	41	40
C	1.523855	1	121.199089	1	-169.749634	1	36	35	34
O	1.388433	1	116.117081	1	-5.346528	1	16	17	44
C	1.472488	1	119.576820	1	-129.386017	1	45	16	17
C	1.524023	1	109.572021	1	116.185982	1	46	45	16
C	1.533314	1	113.076149	1	-78.569191	1	47	46	45
C	1.559104	1	112.594421	1	7.023977	1	27	26	25
F	1.368449	1	114.511055	1	-169.738144	1	49	27	26
F	1.400603	1	110.894592	1	68.023651	1	49	27	26
F	1.412319	1	110.724655	1	-48.426403	1	49	27	26

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H    1.086436 1  118.019928 1  177.274811 1      11   10    9
H    1.100666 1  109.420807 1   59.016373 1      22   21    9
H    1.100727 1  109.194466 1  -58.976120 1      22   21    9
H    1.097319 1  108.790863 1  -57.703602 1      23   22   21
H    1.097439 1  108.852768 1   58.338280 1      23   22   21
H    1.095421 1  110.850739 1 -179.877914 1      24   23   22
H    1.097355 1  111.343353 1   60.273193 1      24   23   22
H    1.097324 1  111.320213 1  -60.030327 1      24   23   22
H    1.083505 1  117.803963 1 -177.878723 1      13    8    9
H    1.095605 1  109.065300 1 -161.567551 1       7    8    9
H    1.094524 1  111.239532 1  -42.377697 1       7    8    9
H    1.101077 1  109.369408 1  -60.012760 1      30   29    3
H    1.100735 1  109.465630 1   57.859230 1      30   29    3
H    1.098087 1  109.035599 1   59.067875 1      31   30   29
H    1.097487 1  108.902878 1  -57.199486 1      31   30   29
H    1.095314 1  110.840866 1  179.963638 1      32   31   30
H    1.097356 1  111.356354 1  -60.119858 1      32   31   30
H    1.097253 1  111.259132 1   60.163925 1      32   31   30
H    1.095448 1  111.164421 1   48.627892 1      33    4    3
H    1.095894 1  108.600128 1  166.926422 1      33    4    3
H    1.100960 1  108.957741 1  -68.009407 1      41   40   35
H    1.100227 1  108.779213 1   49.569218 1      41   40   35
H    1.099490 1  107.579803 1 -172.890869 1      42   41   40
H    1.098170 1  108.774246 1  -57.587353 1      42   41   40
H    1.096364 1  111.078514 1  179.439774 1      43   42   41
H    1.097825 1  110.971596 1   59.488239 1      43   42   41
H    1.093169 1  110.555443 1  -60.239613 1      43   42   41
H    1.087843 1  118.961205 1  178.030731 1      37   36   35
H    1.089262 1  120.421982 1  173.980133 1      38   37   36
H    1.086257 1  119.018272 1    4.813723 1      39   34   33
H    1.098126 1  110.466812 1 -115.827637 1      44   36   35
H    1.094025 1  107.841026 1    2.264297 1      44   36   35
H    1.098006 1  110.381630 1  -74.080444 1      14   10   11
H    1.093093 1  108.471390 1  169.009247 1      14   10   11
H    1.088097 1  118.927055 1  178.979095 1      20   15   16
H    1.085952 1  120.164780 1  179.487732 1      19   20   15
H    1.087750 1  119.121185 1    4.765546 1      18   17   44
H    1.085218 1  118.928032 1  179.600571 1       5    4    3
H    1.086406 1  119.944466 1 -179.325073 1       6    5    4
H    1.086175 1  118.943405 1   -6.457591 1       1    2    7
H    1.092485 1  106.462280 1 -122.720070 1      46   45   16
H    1.098947 1  109.523972 1   -4.609337 1      46   45   16
H    1.100505 1  108.059242 1  159.865646 1      47   46   45
H    1.096521 1  107.508797 1   44.446690 1      47   46   45
H    1.096432 1  111.501175 1  177.959534 1      48   47   46
H    1.098030 1  110.945671 1  -62.033997 1      48   47   46
H    1.096073 1  111.145988 1   57.649197 1      48   47   46
```

Table 1, compound 2e

scf done: -2419.336498

C	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.406337	1	0.000000	0	0.000000	0	1	0	0
C	1.407213	1	117.742126	1	0.000000	0	2	1	0
C	1.410923	1	121.651833	1	10.580659	1	3	2	1
C	1.402862	1	118.039673	1	-10.600824	1	4	3	2
C	1.399743	1	120.820480	1	2.610060	1	5	4	3
C	1.520959	1	122.195229	1	-162.831329	1	2	3	4
C	1.526706	1	109.323952	1	74.987015	1	7	2	3
C	1.414598	1	119.763092	1	74.454086	1	8	7	2
C	1.406633	1	122.255455	1	-168.403870	1	9	8	7
C	1.403646	1	118.030525	1	-7.350856	1	10	9	8
C	1.397244	1	120.912666	1	2.547284	1	11	10	9
C	1.405657	1	119.922668	1	3.078296	1	12	11	10
C	1.524398	1	119.752846	1	-172.395386	1	10	11	12
C	1.522143	1	109.413605	1	49.647785	1	14	10	11
C	1.413157	1	121.270256	1	63.318855	1	15	14	10
C	1.412076	1	121.535873	1	-163.894882	1	16	15	14
C	1.403148	1	118.386757	1	-7.035002	1	17	16	15
C	1.402632	1	120.879166	1	1.222920	1	18	17	16
C	1.401117	1	119.593918	1	3.474473	1	19	18	17
O	1.409925	1	119.266335	1	175.947342	1	9	10	11
C	1.465222	1	114.068275	1	-81.988960	1	21	9	10
C	1.520777	1	107.987526	1	179.933899	1	22	21	9
C	1.534096	1	111.678375	1	-179.175629	1	23	22	21
Hg	2.145231	1	119.059128	1	-173.679520	1	13	8	9
O	2.231743	1	166.963394	1	-149.641037	1	25	13	8
C	1.306177	1	107.473961	1	126.565392	1	26	25	13
O	1.253962	1	126.113075	1	3.346800	1	27	26	25
O	1.424662	1	119.907089	1	17.434053	1	3	2	7
C	1.487587	1	112.384811	1	103.703735	1	29	3	2
C	1.522747	1	110.187813	1	145.405060	1	30	29	3
C	1.535547	1	110.755577	1	172.525314	1	31	30	29
C	1.522270	1	121.391258	1	162.156525	1	4	3	2
C	1.523075	1	108.638405	1	-71.430725	1	33	4	3
C	1.410299	1	120.644394	1	-72.836502	1	34	33	4
C	1.407220	1	121.975029	1	168.397949	1	35	34	33
C	1.405088	1	118.010376	1	5.738557	1	36	35	34
C	1.399262	1	120.908951	1	-0.914141	1	37	36	35
C	1.401340	1	119.916573	1	-3.162281	1	38	37	36
O	1.410276	1	118.277901	1	-9.279776	1	35	34	33
C	1.463750	1	113.782417	1	-98.624756	1	40	35	34
C	1.520887	1	108.032806	1	-178.908752	1	41	40	35
C	1.534038	1	111.707420	1	179.559464	1	42	41	40
C	1.523215	1	121.314377	1	-171.013290	1	36	35	34
O	1.388916	1	116.325958	1	-4.554955	1	16	17	44
C	1.473144	1	119.516357	1	-126.005409	1	45	16	17
C	1.525646	1	109.602150	1	116.353271	1	46	45	16
C	1.533325	1	113.401268	1	-80.680557	1	47	46	45
C	1.542728	1	113.468063	1	-176.480072	1	27	26	25
F	1.390577	1	111.645042	1	-49.260220	1	49	27	26
F	1.383277	1	112.362282	1	-169.567505	1	49	27	26
F	1.390743	1	110.848946	1	70.310120	1	49	27	26

```
H    1.086773 1  119.247849 1  179.844650 1      11   10    9
H    1.100521 1  109.463654 1   58.978737 1      22   21    9
H    1.100676 1  109.169998 1  -59.001797 1      22   21    9
H    1.097407 1  108.796898 1  -57.204079 1      23   22   21
H    1.097515 1  108.963722 1   58.950153 1      23   22   21
H    1.095419 1  110.856720 1 -179.889893 1      24   23   22
H    1.097324 1  111.318100 1   60.239944 1      24   23   22
H    1.097308 1  111.321251 1  -60.051247 1      24   23   22
H    1.086353 1  119.026169 1 -179.638916 1      12   11   10
H    1.097030 1  109.724342 1 -162.934006 1       7    8    9
H    1.094765 1  110.262993 1  -45.155388 1       7    8    9
H    1.097315 1  107.676628 1  -93.608345 1      30   29    3
H    1.096597 1  108.334778 1   23.933979 1      30   29    3
H    1.096064 1  110.073395 1   51.251080 1      31   30   29
H    1.097315 1  109.812157 1  -65.821861 1      31   30   29
H    1.094844 1  110.732468 1 -179.065109 1      32   31   30
H    1.096846 1  111.227806 1  -59.270145 1      32   31   30
H    1.097357 1  111.324013 1   60.894173 1      32   31   30
H    1.093986 1  111.949432 1   48.944183 1      33    4    3
H    1.094977 1  108.640617 1  167.902115 1      33    4    3
H    1.100677 1  109.564949 1  -58.005726 1      41   40   35
H    1.101360 1  109.374931 1   60.014923 1      41   40   35
H    1.097661 1  108.932930 1  -58.497948 1      42   41   40
H    1.097075 1  108.704163 1   57.576870 1      42   41   40
H    1.095567 1  110.908150 1  179.848679 1      43   42   41
H    1.097446 1  111.327400 1   59.948524 1      43   42   41
H    1.097386 1  111.272179 1  -60.283508 1      43   42   41
H    1.087222 1  119.030876 1 -179.478683 1      37   36   35
H    1.086727 1  120.027397 1  178.653000 1      38   37   36
H    1.086100 1  119.029106 1    6.053889 1      39   34   33
H    1.098401 1  110.393471 1 -114.834953 1      44   36   35
H    1.093863 1  107.870605 1    3.119662 1      44   36   35
H    1.097915 1  110.528999 1  -69.614769 1      14   10   11
H    1.092904 1  108.743919 1  172.987335 1      14   10   11
H    1.088089 1  118.942986 1  178.870972 1      20   15   16
H    1.086052 1  120.155502 1  179.575775 1      19   20   15
H    1.087830 1  119.159546 1    4.099474 1      18   17   44
H    1.085082 1  118.771980 1  179.872208 1       5    4    3
H    1.086153 1  120.113899 1 -178.479599 1       6    5    4
H    1.084848 1  118.559479 1   -7.063306 1       1    2    7
H    1.092774 1  106.188286 1 -122.893280 1      46   45   16
H    1.099599 1  109.508049 1   -4.841047 1      46   45   16
H    1.100610 1  108.145523 1  157.651245 1      47   46   45
H    1.096045 1  107.486732 1   42.027088 1      47   46   45
H    1.097149 1  111.298576 1  176.104156 1      48   47   46
H    1.098123 1  111.182678 1  -63.883255 1      48   47   46
H    1.095969 1  111.178268 1   55.845535 1      48   47   46
```

Table 1, compound 2f

scf done: -2419.335288

C	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.408823	1	0.000000	0	0.000000	0	1	0	0
C	1.411959	1	117.602325	1	0.000000	0	2	1	0
C	1.408300	1	122.226318	1	7.830110	1	3	2	1
C	1.402600	1	117.957703	1	-8.583925	1	4	3	2
C	1.400867	1	120.909058	1	2.643931	1	5	4	3
C	1.525162	1	119.437187	1	-166.552338	1	2	3	4
C	1.521430	1	109.971252	1	72.752419	1	7	2	3
C	1.410303	1	122.508385	1	74.886047	1	8	7	2
C	1.409316	1	121.432220	1	-165.363464	1	9	8	7
C	1.404477	1	118.125435	1	-8.926517	1	10	9	8
C	1.397175	1	121.079048	1	2.389637	1	11	10	9
C	1.398182	1	119.476509	1	4.047908	1	12	11	10
C	1.524966	1	119.426483	1	-172.372650	1	10	11	12
C	1.517068	1	110.241714	1	47.924950	1	14	10	11
C	1.412540	1	119.281998	1	66.854477	1	15	14	10
C	1.412731	1	121.476578	1	-168.964111	1	16	15	14
C	1.406742	1	117.789703	1	-7.894813	1	17	16	15
C	1.400890	1	121.350960	1	2.862344	1	18	17	16
C	1.402639	1	119.565063	1	2.686090	1	19	18	17
O	1.421973	1	119.393600	1	172.634995	1	9	10	11
Hg	2.749108	1	128.936813	1	151.058075	1	21	9	10
O	2.237056	1	98.027626	1	143.352463	1	22	21	9
C	1.306779	1	105.980484	1	115.617584	1	23	22	21
C	1.541653	1	113.525787	1	175.231705	1	24	23	22
F	1.391038	1	110.974281	1	-62.992584	1	25	24	23
O	1.409133	1	118.916580	1	10.658607	1	3	2	7
C	1.465553	1	113.349724	1	94.123177	1	27	3	2
C	1.520809	1	108.075050	1	178.336075	1	28	27	3
C	1.534022	1	111.707588	1	179.860672	1	29	28	27
C	1.520869	1	120.817802	1	165.048370	1	4	3	2
C	1.522231	1	109.207390	1	-70.550972	1	31	4	3
C	1.409911	1	120.871696	1	-70.649391	1	32	31	4
C	1.406464	1	122.049812	1	168.291275	1	33	32	31
C	1.405531	1	117.987129	1	5.922023	1	34	33	32
C	1.398231	1	120.849281	1	-1.132698	1	35	34	33
C	1.401027	1	119.937004	1	-3.183250	1	36	35	34
O	1.412453	1	118.429459	1	-8.884267	1	33	32	31
C	1.463995	1	113.865616	1	-98.084724	1	38	33	32
C	1.520984	1	108.174210	1	-179.207184	1	39	38	33
C	1.534308	1	111.648430	1	179.146011	1	40	39	38
C	1.524588	1	121.532578	1	-170.468796	1	34	33	32
O	1.390069	1	122.231628	1	-9.191782	1	16	17	42
C	1.472978	1	119.772415	1	-59.288662	1	43	16	17
C	1.526165	1	109.489594	1	-115.706093	1	44	43	16
C	1.533066	1	113.585388	1	81.072807	1	45	44	43
C	1.482390	1	114.792274	1	-67.204384	1	21	9	10
C	1.522564	1	110.305977	1	141.388367	1	47	21	9
C	1.534506	1	110.909203	1	171.805527	1	48	47	21
O	1.254042	1	125.797539	1	-4.455612	1	24	23	22
F	1.392893	1	111.264450	1	56.265621	1	25	24	23
F	1.381165	1	112.646591	1	176.611008	1	25	24	23

```
H    1.085932 1  120.269669 1 -179.459747 1      12   11   10
H    1.096223 1  108.754295 1   19.423256 1      47   21    9
H    1.098717 1  107.634384 1  -97.883888 1      47   21    9
H    1.095887 1  109.767799 1  -65.967834 1      48   47   21
H    1.096806 1  109.684013 1   50.848991 1      48   47   21
H    1.095088 1  110.726799 1  178.107834 1      49   48   47
H    1.097731 1  111.324249 1   58.286236 1      49   48   47
H    1.095923 1  111.076141 1  -62.454456 1      49   48   47
H    1.084539 1  118.611183 1 -179.512680 1      13    8    9
H    1.086749 1  118.874619 1  179.867706 1      11   10    9
H    1.094942 1  108.553078 1 -164.138992 1       7    8    9
H    1.097989 1  111.268761 1  -46.783764 1       7    8    9
H    1.101293 1  109.379219 1  -60.619644 1      28   27    3
H    1.100912 1  109.496758 1   57.242210 1      28   27    3
H    1.097395 1  108.937630 1   57.868397 1      29   28   27
H    1.097361 1  108.878578 1  -58.159126 1      29   28   27
H    1.095472 1  110.854431 1  179.881989 1      30   29   28
H    1.097318 1  111.333427 1  -60.268417 1      30   29   28
H    1.097394 1  111.333443 1   60.015808 1      30   29   28
H    1.095241 1  111.331337 1   49.400444 1      31    4    3
H    1.095613 1  108.781380 1  168.062912 1      31    4    3
H    1.100705 1  109.455688 1  -58.266445 1      39   38   33
H    1.100995 1  109.275810 1   59.646057 1      39   38   33
H    1.097483 1  109.014153 1  -58.928741 1      40   39   38
H    1.097372 1  108.855133 1   57.235695 1      40   39   38
H    1.095450 1  110.872581 1  179.938950 1      41   40   39
H    1.097337 1  111.324844 1   60.051495 1      41   40   39
H    1.097323 1  111.270943 1  -60.215111 1      41   40   39
H    1.086276 1  120.034531 1  179.556870 1      36   35   34
H    1.087003 1  119.056290 1 -179.217285 1      35   34   33
H    1.085449 1  118.975578 1    4.690956 1      37   32   31
H    1.098050 1  110.163658 1 -115.461525 1      42   34   33
H    1.092849 1  108.477936 1    1.450947 1      42   34   33
H    1.098475 1  111.182693 1  -73.095863 1      14   10   11
H    1.092379 1  108.328705 1  168.171295 1      14   10   11
H    1.087799 1  119.214287 1  178.695114 1      20   15   16
H    1.088040 1  118.850441 1    7.915249 1      18   17   42
H    1.086045 1  120.226379 1  178.706146 1      19   20   15
H    1.085498 1  119.080231 1 -179.858658 1       5    4    3
H    1.086438 1  119.218750 1 -178.998367 1       6    5    4
H    1.099101 1  109.598366 1    5.221211 1      44   43   16
H    1.092766 1  106.194656 1  123.234673 1      44   43   16
H    1.097270 1  107.295670 1  -41.436264 1      45   44   43
H    1.099886 1  108.507446 1 -156.853333 1      45   44   43
H    1.096335 1  111.222343 1 -175.228119 1      46   45   44
H    1.096434 1  111.272453 1  -54.654785 1      46   45   44
H    1.097772 1  110.926216 1   64.882774 1      46   45   44
```

Table 1, compound 2g

scf done: -2419.323975

C	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.404773	1	0.000000	0	0.000000	0	1	0	0
C	1.408851	1	118.178619	1	0.000000	0	2	1	0
C	1.408364	1	121.931427	1	7.693179	1	3	2	1
C	1.404117	1	118.159790	1	-7.716576	1	4	3	2
C	1.402705	1	120.555588	1	2.166643	1	5	4	3
C	1.520862	1	121.235939	1	-168.364151	1	2	3	4
C	1.521079	1	111.351128	1	65.941956	1	7	2	3
C	1.410060	1	121.221642	1	69.947426	1	8	7	2
C	1.407297	1	121.787148	1	-171.098068	1	9	8	7
C	1.405233	1	118.090103	1	-5.297719	1	10	9	8
C	1.397955	1	120.998436	1	1.001366	1	11	10	9
C	1.400024	1	119.739891	1	2.844593	1	12	11	10
C	1.524102	1	119.936348	1	-175.254333	1	10	11	12
C	1.518475	1	110.168869	1	54.318741	1	14	10	11
C	1.407399	1	119.715431	1	70.694969	1	15	14	10
C	1.406779	1	122.327965	1	-169.574692	1	16	15	14
C	1.405215	1	117.960640	1	-5.488889	1	17	16	15
C	1.402322	1	120.731995	1	1.420790	1	18	17	16
C	1.402526	1	120.020241	1	2.427510	1	19	18	17
O	1.411959	1	119.832436	1	176.492645	1	9	10	11
C	1.463632	1	113.745422	1	-83.254379	1	21	9	10
C	1.520998	1	108.075874	1	-179.816803	1	22	21	9
C	1.533859	1	111.838531	1	-179.213226	1	23	22	21
O	1.405831	1	119.060722	1	9.450618	1	3	2	7
C	1.465410	1	113.520729	1	90.946762	1	25	3	2
C	1.520774	1	108.132332	1	179.221069	1	26	25	3
C	1.534017	1	111.670357	1	179.818207	1	27	26	25
C	1.519890	1	121.357056	1	168.297470	1	4	3	2
C	1.521096	1	111.238350	1	-66.741440	1	29	4	3
C	1.410855	1	121.319855	1	-68.954765	1	30	29	4
C	1.407340	1	121.665985	1	170.952637	1	31	30	29
C	1.405634	1	118.135338	1	5.439965	1	32	31	30
C	1.397828	1	121.022430	1	-1.158883	1	33	32	31
C	1.399959	1	119.708977	1	-2.834117	1	34	33	32
O	1.411409	1	118.572792	1	-7.626700	1	31	30	29
C	1.467247	1	113.127480	1	-95.238914	1	36	31	30
C	1.521577	1	108.554932	1	-179.918060	1	37	36	31
C	1.532208	1	113.272049	1	65.563721	1	38	37	36
C	1.524328	1	121.764763	1	-170.653275	1	32	31	30
O	1.401702	1	118.935013	1	-8.116205	1	16	17	40
C	1.464938	1	112.835442	1	-92.888672	1	41	16	17
C	1.517262	1	108.267265	1	-174.864426	1	42	41	16
C	1.534817	1	110.945633	1	178.121231	1	43	42	41
Hg	2.129994	1	118.644020	1	176.631958	1	6	5	4
O	2.160430	1	176.493408	1	-148.072968	1	45	6	5
C	1.315376	1	133.192032	1	146.476807	1	46	45	6
C	1.560368	1	112.354767	1	2.368025	1	47	46	45
F	1.406933	1	110.802719	1	58.089111	1	48	47	46
O	1.232982	1	128.489731	1	-177.684021	1	47	46	45
F	1.366368	1	114.827003	1	-179.698608	1	48	47	46
F	1.410568	1	110.699516	1	-57.788227	1	48	47	46

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H    1.086113 1  120.115784 1 -179.652481 1      12   11   10
H    1.100718 1  109.587776 1   59.312489 1      22   21    9
H    1.101343 1  109.423248 1  -58.684933 1      22   21    9
H    1.097593 1  108.807976 1  -57.188183 1      23   22   21
H    1.098054 1  108.908936 1   58.872192 1      23   22   21
H    1.095446 1  110.878304 1  179.909531 1      24   23   22
H    1.097312 1  111.258942 1   60.086155 1      24   23   22
H    1.097432 1  111.375664 1  -60.174950 1      24   23   22
H    1.085645 1  118.936615 1 -179.621170 1      13    8    9
H    1.086992 1  119.034187 1  179.202744 1      11   10    9
H    1.096403 1  108.269928 1 -168.012390 1       7    8    9
H    1.096264 1  110.721558 1  -50.584564 1       7    8    9
H    1.101297 1  109.511627 1  -59.745560 1      26   25    3
H    1.101254 1  109.528191 1   58.185390 1      26   25    3
H    1.096928 1  108.931145 1   57.738846 1      27   26   25
H    1.096961 1  108.910812 1  -58.115395 1      27   26   25
H    1.095487 1  110.833374 1  179.834503 1      28   27   26
H    1.097436 1  111.363266 1  -60.313828 1      28   27   26
H    1.097425 1  111.346527 1   59.993282 1      28   27   26
H    1.096256 1  110.800644 1   53.710243 1      29    4    3
H    1.096216 1  108.292465 1  171.208466 1      29    4    3
H    1.100967 1  109.222168 1  -58.881535 1      37   36   31
H    1.100689 1  108.991531 1   58.900295 1      37   36   31
H    1.099172 1  107.960953 1 -172.470398 1      38   37   36
H    1.098102 1  108.847206 1  -56.996777 1      38   37   36
H    1.095653 1  110.967339 1 -178.096954 1      39   38   37
H    1.097903 1  110.996025 1   61.773937 1      39   38   37
H    1.094579 1  110.388535 1  -58.145626 1      39   38   37
H    1.086164 1  120.127991 1  179.656616 1      34   33   32
H    1.086977 1  119.068428 1 -179.286514 1      33   32   31
H    1.085793 1  118.936531 1    2.940937 1      35   30   29
H    1.097989 1  110.535782 1 -117.012375 1      40   32   31
H    1.093613 1  108.418121 1    1.149545 1      40   32   31
H    1.098006 1  110.485840 1  -66.106422 1      14   10   11
H    1.093858 1  108.497406 1  175.794403 1      14   10   11
H    1.087899 1  119.357414 1  178.972504 1      20   15   16
H    1.087826 1  119.280609 1    6.255073 1      18   17   40
H    1.086353 1  119.979111 1  179.115295 1      19   20   15
H    1.085888 1  118.012352 1  179.910995 1       5    4    3
H    1.086039 1  118.032898 1   -3.772216 1       1    2    7
H    1.101752 1  109.305069 1  -53.962406 1      42   41   16
H    1.101826 1  109.248993 1   63.658287 1      42   41   16
H    1.096113 1  107.814407 1   55.775448 1      43   42   41
H    1.096596 1  108.192116 1  -59.511925 1      43   42   41
H    1.098420 1  112.109329 1 -178.367233 1      44   43   42
H    1.098008 1  111.301247 1  -58.831200 1      44   43   42
H    1.097577 1  111.612709 1   61.588413 1      44   43   42
```

Table 2, 1,2-alternate

```
scf done: -1853.268005

 C    0.000000 0    0.000000 0    0.000000 0       0    0    0
 C    1.410741 1    0.000000 0    0.000000 0       1    0    0
 C    1.396021 1  117.714569 1    0.000000 0       2    1    0
 C    1.390651 1  121.358971 1    0.144330 1       3    2    1
 C    1.389670 1  119.812561 1   -2.782833 1       4    3    2
 C    1.398990 1  121.191154 1    1.245381 1       5    4    3
 C    1.535267 1  119.263306 1  177.297897 1       2    3    4
 C    1.520963 1  111.692078 1 -125.504410 1       7    2    3
 C    1.398826 1  120.112457 1 -110.000504 1       8    7    2
 C    1.392469 1  122.048195 1  151.835068 1       9    8    7
 C    1.393189 1  117.866669 1   -1.900984 1      10    9    8
 C    1.406960 1  119.778984 1   13.870002 1      11   10    9
 C    1.387197 1  120.462234 1  -11.334723 1      12   11   10
 C    1.512939 1  110.419312 1 -175.503754 1      12   11   10
 C    1.515150 1  100.749153 1   16.603409 1      14   12   11
 C    1.406545 1  110.462418 1  -14.960935 1      15   14   12
 C    1.395095 1  120.060997 1  168.684937 1      16   15   14
 C    1.391746 1  117.888847 1  -12.413643 1      17   16   15
 C    1.399136 1  122.212410 1    3.981395 1      18   17   16
 C    1.407974 1  118.078911 1    9.670609 1      19   18   17
 C    1.521070 1  120.947800 1 -155.822128 1      19   18   17
 C    1.535282 1  108.773735 1  106.974739 1      21   19   18
 C    1.394191 1  119.094406 1  110.408867 1      22   21   19
 C    1.390950 1  121.203674 1 -169.036133 1      23   22   21
 C    1.387637 1  119.713310 1    2.836936 1      24   23   22
 C    1.399567 1  121.429977 1   -3.865048 1      25   24   23
 C    1.407282 1  117.695251 1   -0.964569 1      26   25   24
 C    1.532225 1  120.499496 1  179.702362 1      26   25   24
 O    1.378313 1  120.958260 1   18.755945 1      13    8    7
 C    1.438553 1  116.206192 1   72.598022 1      29   13    8
 C    1.526761 1  112.380096 1   88.456924 1      30   29   13
 C    1.530685 1  113.516411 1   63.253262 1      31   30   29
 O    1.377163 1  121.069336 1   16.376392 1      20   15   14
 C    1.435311 1  116.852310 1   64.539505 1      33   20   15
 C    1.526325 1  112.433502 1   79.532410 1      34   33   20
 C    1.531850 1  112.065193 1  178.543488 1      35   34   33
 O    1.383891 1  119.300858 1  -13.122023 1      27   22   21
 C    1.436074 1  115.873497 1  -74.594261 1      37   27   22
 C    1.527085 1  113.260643 1  -85.308830 1      38   37   27
 C    1.531978 1  111.833961 1 -178.044693 1      39   38   37
 O    1.380837 1  119.816696 1    5.443407 1       1    2    7
 C    1.433202 1  114.829292 1   90.994385 1      41    1    2
 C    1.520576 1  108.387909 1  170.145615 1      42   41    1
 C    1.531230 1  112.334473 1 -178.774994 1      43   42   41
 H    1.085387 1  107.882584 1  176.963196 1      28   26   25
 H    1.095885 1  108.400604 1   60.778500 1      28   26   25
 H    1.093828 1  105.389519 1  154.193604 1      38   37   27
 H    1.096058 1  110.090157 1   37.942169 1      38   37   27
 H    1.094563 1  108.890678 1  -56.250565 1      39   38   37
 H    1.094425 1  109.147629 1   60.183151 1      39   38   37
 H    1.083774 1  118.868088 1    8.126792 1      23   22   21
 H    1.084262 1  120.132614 1 -179.936905 1      24   23   22
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H    1.083044 1  119.279625 1  176.294815 1      25   24   23
H    1.092482 1  108.890099 1  -15.724720 1      21   19   18
H    1.092362 1  111.806618 1 -134.023407 1      21   19   18
H    1.095135 1  110.382713 1  -44.106308 1      34   33   20
H    1.092847 1  105.025917 1 -160.134781 1      34   33   20
H    1.094695 1  108.987465 1  -59.516113 1      35   34   33
H    1.094764 1  108.655281 1   56.577305 1      35   34   33
H    1.097755 1  111.425011 1 -103.498199 1      14   12   11
H    1.091808 1  112.510162 1  136.027847 1      14   12   11
H    1.094681 1  109.769020 1  -34.534458 1      30   29   13
H    1.093817 1  105.437164 1 -151.169754 1      30   29   13
H    1.096971 1  107.630577 1 -174.825684 1      31   30   29
H    1.095412 1  108.737450 1  -59.993855 1      31   30   29
H    1.094528 1  110.508514 1  113.923462 1       7    2    3
H    1.093625 1  107.320999 1   -1.409977 1       7    2    3
H    1.085084 1  118.917374 1   -2.661772 1      3    2    7
H    1.084267 1  120.092331 1  179.940460 1       4    5    6
H    1.084376 1  119.395973 1    2.982373 1       5    6   28
H    1.085639 1  118.399498 1  -18.907654 1       9    8    7
H    1.084032 1  119.986038 1 -171.648224 1      10    9    8
H    1.083775 1  121.249054 1  -25.616478 1      17   16   11
H    1.084840 1  119.062317 1 -169.216278 1      18   17   16
H    1.099109 1  109.961235 1  -68.531502 1      42   41    1
H    1.098475 1  109.758369 1   49.245743 1      42   41    1
H    1.093243 1  108.574722 1   58.849171 1      43   42   41
H    1.093745 1  108.191330 1  -56.164486 1      43   42   41
H    1.092557 1  111.061043 1 -179.238815 1      36   35   34
H    1.094324 1  111.384903 1   60.918560 1      36   35   34
H    1.094541 1  111.428467 1  -59.322178 1      36   35   34
H    1.093179 1  111.236107 1 -177.959976 1      32   31   30
H    1.094693 1  111.032898 1   62.072865 1      32   31   30
H    1.091671 1  110.889557 1  -57.532196 1      32   31   30
H    1.092565 1  111.081581 1  179.296844 1      40   39   38
H    1.094582 1  111.405701 1   59.386490 1      40   39   38
H    1.094379 1  111.409676 1  -60.828663 1      40   39   38
H    1.092751 1  111.000580 1 -179.975311 1      44   43   42
H    1.094617 1  111.539543 1   60.128460 1      44   43   42
H    1.094601 1  111.539497 1  -60.142548 1      44   43   42
```

Table 2, cone

```
scf done: -1853.266861

 C    0.000000 0    0.000000 0    0.000000 0       0    0    0
 C    1.416151 1    0.000000 0    0.000000 0       1    0    0
 C    1.396420 1  117.888985 1    0.000000 0       2    1    0
 C    1.390682 1  121.324852 1    3.296457 1       3    2    1
 C    1.389081 1  119.533508 1    2.692884 1       4    3    2
 C    1.399154 1  121.642044 1   -3.417043 1       5    4    3
 C    1.535288 1  118.621750 1 -167.143723 1       2    3    4
 C    1.524531 1  106.778664 1  100.681404 1       7    2    3
 C    1.403706 1  119.413719 1  -62.970669 1       8    7    2
 C    1.388634 1  122.126518 1  153.103760 1       9    8    7
 C    1.396666 1  117.954651 1   -2.751911 1      10    9    8
 C    1.403772 1  119.951012 1   12.604387 1      11   10    9
 C    1.390916 1  120.351128 1   -8.859311 1      12   11   10
 C    1.514426 1  110.532410 1 -171.416977 1      12   11   10
 C    1.514421 1  100.758949 1   14.711074 1      14   12   11
 C    1.403781 1  110.532364 1  -14.711846 1      15   14   12
 C    1.396657 1  119.950768 1  171.420624 1      16   15   14
 C    1.388642 1  117.955078 1  -12.603524 1      17   16   15
 C    1.403698 1  122.126312 1    2.750731 1      18   17   16
 C    1.403836 1  117.949753 1   10.804379 1      19   18   17
 C    1.524538 1  119.414474 1 -153.099426 1      19   18   17
 C    1.535287 1  106.777725 1   62.970238 1      21   19   18
 C    1.396417 1  118.620949 1 -100.674530 1      22   21   19
 C    1.390684 1  121.325401 1  167.138672 1      23   22   21
 C    1.389078 1  119.533607 1   -2.690626 1      24   23   22
 C    1.399157 1  121.641769 1    3.417906 1      25   24   23
 C    1.410552 1  117.644409 1    1.916773 1      26   25   24
 C    1.531416 1  121.008987 1  179.357559 1      26   25   24
 O    1.384079 1  120.449654 1   21.839058 1      13    8    7
 C    1.436006 1  113.853928 1  105.983246 1      29   13    8
 C    1.520201 1  108.723228 1  177.577560 1      30   29   13
 C    1.531332 1  112.223877 1 -179.406906 1      31   30   29
 O    1.384085 1  119.569092 1   16.530920 1      20   15   14
 C    1.436011 1  113.851311 1   83.065987 1      33   20   15
 C    1.520201 1  108.722847 1 -177.586563 1      34   33   20
 C    1.531329 1  112.224579 1  179.405167 1      35   34   33
 O    1.374494 1  120.977386 1   15.944660 1      27   22   21
 C    1.445618 1  118.229309 1   58.476635 1      37   27   22
 C    1.525081 1  111.080818 1  121.680489 1      38   37   27
 C    1.530802 1  114.888527 1  -75.151558 1      39   38   37
 O    1.374489 1  120.976097 1  -15.941829 1       1    2    7
 C    1.445628 1  118.227577 1  -58.485600 1      41    1    2
 C    1.525083 1  111.080856 1 -121.668434 1      42   41    1
 C    1.530802 1  114.888023 1   75.160454 1      43   42   41
 H    1.093420 1  108.398132 1  -19.247431 1       7    2    3
 H    1.087754 1  113.027306 1 -138.404190 1       7    2    3
 H    1.084852 1  118.519897 1  -18.802483 1       9    8    7
 H    1.083966 1  119.980370 1 -172.952362 1      10    9    8
 H    1.091730 1  111.869873 1  133.712646 1      14   12   11
 H    1.097948 1  112.466141 1 -105.254890 1      14   12   11
 H    1.083966 1  121.313690 1  -25.367739 1      17   16   11
 H    1.084852 1  118.866661 1 -169.125610 1      18   17   16
```

```
H    1.093421 1  111.233086 1  -55.116592 1      21   19   18
H    1.087752 1  109.862770 1 -174.119370 1      21   19   18
H    1.085490 1  118.904930 1  -11.193686 1      23   22   21
H    1.084138 1  120.257095 1  179.006119 1      24   23   22
H    1.083102 1  119.058830 1 -178.258667 1      25   24   23
H    1.096509 1  107.806229 1  -53.114658 1      28   26   25
H    1.085046 1  108.035713 1 -169.410645 1      28   26   25
H    1.083103 1  119.278313 1   -1.043073 1       5    6   28
H    1.084137 1  120.187126 1  178.278732 1       4    5    6
H    1.085491 1  118.904663 1   11.190740 1       3    2    7
H    1.097628 1  109.686775 1   56.588718 1      30   29   13
H    1.098242 1  109.347389 1  -61.239056 1      30   29   13
H    1.094603 1  108.569710 1  -57.273415 1      31   30   29
H    1.094734 1  108.788971 1   58.568851 1      31   30   29
H    1.092434 1  110.950089 1 -179.853775 1      32   31   30
H    1.094215 1  111.434532 1  -59.981270 1      32   31   30
H    1.094236 1  111.422028 1   60.292694 1      32   31   30
H    1.098239 1  109.348206 1   61.229134 1      34   33   20
H    1.097631 1  109.685684 1  -56.598545 1      34   33   20
H    1.094733 1  108.788788 1  -58.570164 1      35   34   33
H    1.094603 1  108.569511 1   57.271828 1      35   34   33
H    1.092435 1  110.949585 1  179.862930 1      36   35   34
H    1.094237 1  111.422302 1  -60.284164 1      36   35   34
H    1.094215 1  111.435493 1   59.990402 1      36   35   34
H    1.095279 1  109.475517 1   -0.373570 1      38   37   27
H    1.089915 1  106.675362 1 -118.230125 1      38   37   27
H    1.097341 1  107.058632 1  163.221405 1      39   38   37
H    1.094631 1  108.225555 1   48.969078 1      39   38   37
H    1.093405 1  111.064850 1 -179.432373 1      40   39   38
H    1.094556 1  110.954094 1  -59.704044 1      40   39   38
H    1.090965 1  111.604362 1   60.423859 1      40   39   38
H    1.089916 1  106.673592 1  118.241684 1      42   41    1
H    1.095276 1  109.475143 1    0.386610 1      42   41    1
H    1.094632 1  108.224373 1  -48.959877 1      43   42   41
H    1.097340 1  107.059784 1 -163.212479 1      43   42   41
H    1.093405 1  111.065300 1  179.438568 1      44   43   42
H    1.090966 1  111.604729 1  -60.416950 1      44   43   42
H    1.094558 1  110.953796 1   59.710266 1      44   43   42
```

Table 2, partial cone

scf done: -1853.267478

C	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.412264	1	0.000000	0	0.000000	0	1	0	0
C	1.396310	1	117.979225	1	0.000000	0	2	1	0
C	1.389895	1	121.271629	1	-1.546826	1	3	2	1
C	1.388370	1	119.589340	1	-2.058842	1	4	3	2
C	1.398697	1	121.538284	1	2.319911	1	5	4	3
C	1.534508	1	118.864410	1	172.854492	1	2	3	4
C	1.519192	1	109.038162	1	-108.169724	1	7	2	3
C	1.395821	1	120.694664	1	-105.848923	1	8	7	2
C	1.391659	1	122.167465	1	154.925491	1	9	8	7
C	1.393498	1	117.497154	1	-4.573750	1	10	9	8
C	1.409350	1	120.565483	1	13.928326	1	11	10	9
C	1.392842	1	119.787277	1	-7.787164	1	12	11	10
C	1.520801	1	110.011894	1	-168.498123	1	12	11	10
C	1.512825	1	100.776840	1	15.538577	1	14	12	11
C	1.402981	1	110.501839	1	-16.515511	1	15	14	12
C	1.396679	1	119.846886	1	172.179001	1	16	15	14
C	1.388939	1	117.906189	1	-13.779891	1	17	16	15
C	1.403334	1	121.948311	1	2.440369	1	18	17	16
C	1.403259	1	118.011147	1	12.012841	1	19	18	17
C	1.523512	1	119.675117	1	-151.274826	1	19	18	17
C	1.532174	1	107.418938	1	58.715363	1	21	19	18
C	1.396116	1	119.003143	1	-101.104980	1	22	21	19
C	1.390168	1	121.039528	1	171.042953	1	23	22	21
C	1.388387	1	119.581871	1	-0.775441	1	24	23	22
C	1.400723	1	121.793640	1	2.298658	1	25	24	23
C	1.406794	1	117.583061	1	-0.652522	1	26	25	24
C	1.533658	1	116.908920	1	173.701385	1	26	25	24
O	1.370269	1	116.883957	1	21.650879	1	13	8	7
C	1.436049	1	118.768150	1	149.542969	1	29	13	8
C	1.522838	1	108.536102	1	-150.151688	1	30	29	13
C	1.530185	1	113.908463	1	65.667587	1	31	30	29
O	1.384196	1	119.305244	1	16.416828	1	20	15	14
C	1.436320	1	113.511299	1	98.962067	1	33	20	15
C	1.520233	1	108.833054	1	-177.803894	1	34	33	20
C	1.531474	1	112.227394	1	-179.626953	1	35	34	33
O	1.380414	1	118.992859	1	8.845088	1	27	22	21
C	1.435604	1	114.743073	1	87.604141	1	37	27	22
C	1.519716	1	108.609818	1	-179.243011	1	38	37	27
C	1.531393	1	112.151611	1	-179.790359	1	39	38	37
O	1.384663	1	119.570587	1	10.073675	1	1	2	7
C	1.437153	1	114.269028	1	83.375946	1	41	1	2
C	1.521385	1	109.041916	1	-173.830429	1	42	41	1
C	1.530122	1	113.930092	1	-62.797260	1	43	42	41
H	1.092404	1	111.672974	1	131.524872	1	7	2	3
H	1.092524	1	107.985939	1	13.749455	1	7	2	3
H	1.084214	1	118.321175	1	-18.055758	1	9	8	7
H	1.083574	1	120.068367	1	-172.707703	1	10	9	8
H	1.091149	1	112.364105	1	133.766281	1	14	12	11
H	1.097430	1	113.018761	1	-104.351166	1	14	12	11
H	1.083968	1	121.326340	1	-27.452114	1	17	16	11
H	1.084880	1	118.802757	1	-168.611786	1	18	17	16

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H    1.093806 1  111.805328 1  -60.311344 1      21   19   18
H    1.089023 1  109.389687 1 -179.724884 1      21   19   18
H    1.085272 1  119.102692 1   -7.731718 1      23   22   21
H    1.084243 1  120.280548 1 -179.651077 1      24   23   22
H    1.084634 1  119.446465 1 -178.731247 1      25   24   23
H    1.096056 1  107.009140 1  -97.291832 1      28   26   25
H    1.093224 1  105.734764 1   14.313111 1      28   26   25
H    1.084911 1  118.823517 1   -3.507266 1       5    6   28
H    1.084376 1  120.203949 1 -178.953979 1       4    5    6
H    1.083351 1  118.768639 1   -5.780649 1       3    2    7
H    1.098207 1  109.531372 1   61.041283 1      34   33   20
H    1.098129 1  109.512894 1  -56.732868 1      34   33   20
H    1.094626 1  108.734009 1  -57.582230 1      35   34   33
H    1.094522 1  108.679398 1   58.244976 1      35   34   33
H    1.092478 1  110.941177 1  179.878830 1      36   35   34
H    1.094217 1  111.415863 1   60.042477 1      36   35   34
H    1.094234 1  111.472382 1  -60.243797 1      36   35   34
H    1.098748 1  109.599945 1   59.527023 1      38   37   27
H    1.098261 1  109.749626 1  -58.092926 1      38   37   27
H    1.093438 1  108.430023 1  -57.662502 1      39   38   37
H    1.091884 1  107.943878 1   57.839417 1      39   38   37
H    1.092829 1  110.942291 1 -179.845978 1      40   39   38
H    1.094890 1  111.668251 1   60.306087 1      40   39   38
H    1.094845 1  111.579460 1  -60.034134 1      40   39   38
H    1.093263 1  110.976486 1  178.220703 1      44   43   42
H    1.094769 1  110.981804 1  -62.173332 1      44   43   42
H    1.090848 1  110.827744 1   57.706871 1      44   43   42
H    1.096394 1  107.504700 1  174.846405 1      43   42   41
H    1.094554 1  108.447868 1   59.866985 1      43   42   41
H    1.099207 1  109.601173 1   64.888374 1      42   41    1
H    1.096486 1  109.762558 1  -52.713470 1      42   41    1
H    1.093979 1  109.879036 1   89.529060 1      30   29   13
H    1.096270 1  109.228157 1  -29.179258 1      30   29   13
H    1.095040 1  108.408455 1  -57.491692 1      31   30   29
H    1.096340 1  107.428436 1 -172.175095 1      31   30   29
H    1.093002 1  111.104225 1 -179.483215 1      32   31   30
H    1.091681 1  110.927917 1  -59.275677 1      32   31   30
H    1.094487 1  111.086082 1   60.564022 1      32   31   30
```