Supporting Information for

Unprecedented *meta*-Substitution of Calixarenes: Direct Way to Inherently Chiral Derivatives

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Table of Contents

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) and on Bruker Advance DRX 500 (^{1}H: 500 MHz, ^{13}C: 125 MHz) spectrometers. 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 aluminum sheets with Silica gel 60 F_{254} (Merck). The column chromatography was performed using Silica gel 60 (Merck).

General remark: All organomercury derivatives are considered potentially hazardous and require special consideration!

The corresponding trifluoroacetyloxymercurio derivatives **4**, **5** and **11** were not fully characterized as we were unable to purify them using chromatographic separation – these compounds do not move on silica gel or alumina and possess instability upon the contact with sorbent material. All these compounds were characterized after their transformation into the chloromercurio derivatives **4'**, **5'** and **11'**.

11,23-di-*tert*-butyl-4-(trifluoroacetyloxymercurio)-25,26,27,28-tetrapropoxycalix[4]arene (4)

A mixture of calixarene **1** (0.20 g, 0.28 mmol) and $Hg(CF_3COO)_2$ (0.13 g, 0.30 mmol) was dissolved in dry chloroform and stirred overnight at room temp. Solvent was removed under a reduced pressure to yield the crude product. As this compound could not be purified using column chromatography, it was immediately transformed into the corresponding HgCl- derivative and characterized as compound **4'** (see the next procedure). Analytical sample (few milligrams) was obtained as a white powder (mp: 291-293.5 °C) by crystallization from CH_2Cl_2/methanol mixture (10/1) and basic characterization was made using ^{1}H NMR and MS spectroscopy: ^{1}H-NMR($CDCl_3$, 300 MHz): δ = 7.25 (d, 1H, J = 2.1 Hz, Ar-**H**), 7.15-7.06 (m, 3H, Ar-**H**), 6.31-6.17 (m, 2H, Ar-**H**), 6.07-5.94 (m, 3H, Ar-**H**), 4.67 (d, 1H, J = 14.2 Hz, Ar-**CH$_2$**-Ar), 4.47 (d, 1H, J = 13.6 Hz, Ar-**CH$_2$**- Ar), 4.44 (d, 2H, J = 13.5 Hz, Ar-**CH$_2$**- Ar), 4.08-3.91 (m, 4H, CH_3CH_2**CH$_2$**), 3.75-3.59 (m, 4H, CH_3CH_2**CH$_2$**), 3.16 (t, 3H, J = 14.6 Hz, Ar-**CH$_2$**-Ar), 3.01 (d, 1H, J = 14.3 Hz, Ar-**CH$_2$**-Ar), 1.96-1.80 (m, 8H, CH_3**CH$_2$**CH_2), 1.41 (s, 9H, C(C**H$_3$**)$_3$), 1.37 (s, 9H, C(C**H$_3$**)$_3$), 1.14-1.09 (m, 6H, **CH$_3$**CH_2CH_2), 0.94-0.79 (m, 6H, **CH$_3$**CH_2CH_2) ppm. IR (KBr) ν 1711 cm^{-1}. HRMS (TOF MS ESI$^+$) calcd for $C_{50}H_{63}O_6F_3HgNa$ 1041.4175 [(M+Na)$^+$], found m/z 1041.4185 [(M+Na)$^+$].

11,23-di-*tert*-butyl-4-(chloromercurio)-25,26,27,28-tetrapropoxycalix[4]arene (4')

A mixture of calixarene **1** (0.100 g, 0.14 mmol) and $Hg(CF_3COO)_2$ (0.073 g, 0.17 mmol) was dissolved in dry chloroform and stirred overnight at room temp. Aqueous 1M HCl (10 ml) was then added and the reaction mixture was stirred for 3 h. The organic layer was separated, washed three times with water and dried over $MgSO_4$. Solvent was removed under a reduced pressure, and the crude product was purified using column chromatography on a silica gel using CH_2Cl_2:hexane mixture (1:1 v/v) as en eluent. Product was obtained as a white powder in 44% yield (58 mg), mp: 264-266 °C. ^{1}H-NMR ($CDCl_3$, 300 MHz) δ 7.21 (d, 1H, *J*=2,1 Hz, Ar-**H**), 7.14-7.10 (m, 2H, Ar-**H**), 7.07-7.04 (m, 1H, Ar-**H**), 6.25-6.14 (m, 2H, Ar-**H**), 6.09-5.97 (m, 3H, Ar-**H**), 4.62 (d, 1H, *J*=14,1 Hz, Ar-**CH$_2$**-Ar), 4.50-4.39 (m, 3H, Ar-**CH$_2$**-Ar), 4.08-3.86 (m, 4H, CH_3CH_2**CH$_2$**), 3.73-3.58 (m, 4H, CH_3CH_2**CH$_2$**), 3.20-3.06 (m, 3H, Ar-**CH$_2$**-Ar), 2.97 (d, 1H, *J*=14,4 Hz, Ar-**CH$_2$**-Ar), 2.00-1.77 (m, 8H, CH_3**CH$_2$**CH_2), 1.42 (s, 9H, C(C**H$_3$**)$_3$), 1.40 (s, 9H, C(C**H$_3$**)$_3$), 1.14-1.05 (m, 6H, **CH$_3$**CH_2CH_2), 0.91-0.83 (m, 3H, **CH$_3$**CH_2CH_2), 0.83-0.76 (m, 3H, **CH$_3$**CH_2CH_2) ppm. ^{13}C-NMR ($CDCl_3$, 75 MHz) δ 157.0, 156.2, 155.9, 155.7, 155.5, 148.0, 145.5, 144.8, 144.4, 138.6, 138.5, 136.3, 136.1, 135.9, 135.3, 134.2, 133.8, 133.5, 130.5, 128.0, 127.7, 127.5, 127.4, 127.1, 126.2, 126.1, 125.9, 124.6, 122.6, 122.2, 77.2, 77.0, 76.6, 75.8, 34.6, 34.5, 34.4, 34.3, 32.0, 31.6, 31.5, 31.4, 31.2, 23.8, 23.7, 23.3, 22.5 ppm. HRMS (ESI+): calcd for $C_{48}H_{63}O_4ClHgNa$ 963.4013 [$(M+Na)^+$]; found *m/z* 963.4012 [$(M+Na)^+$]. Elemental analysis (%) calcd for $C_{48}H_{63}O_4ClHg$: C 61.33, H 6.75; found: C 61.66, H 6.57.

11,23-di-*tert*-butyl-4,18-bis(trifluoracetyloxymercurio)-25,26,27,28-tetrapropoxycalix[4]arene (5)

A mixture of calixarene **1** (0.20 g, 0.28 mmol) and $Hg(CF_3COO)_2$ (0.25 g, 0.58 mmol) was dissolved in dry chloroform and stirred overnight at room temp. Solvent was removed under a reduced pressure to yield the crude product. Analytical sample was obtained by the crystallization from CH_2Cl_2/methanol mixture (10:1 v/v). Title compound was obtained as a white powder, mp: 267-280 °C. ^{1}H-NMR ($CDCl_3$, 300 MHz) δ 7.27 (d, 2H, J=2.1 Hz, Ar-**H**), 7.11 (d, 2H, *J* = 2.2 Hz, Ar-**H**), 6.33 (d, 2H, *J* = 7.7 Hz, Ar-**H**), 6.03 (d, 2H, *J* = 7.8 Hz, Ar-**H**), 4.69 (d, 2H, *J* = 14.2 Hz, Ar-**CH$_2$**-Ar), 4.46 (d, 2H, *J* = 13.8 Hz, Ar-**CH$_2$**-Ar), 4.10-3.98 (m, 2H, CH_3CH_2**CH$_2$**), 3.94-3.83 (m, 2H, CH_3CH_2**CH$_2$**), 3.75-3.61 (m, 4H, CH_3CH_2**CH$_2$**), 3.23 (d, 2H, *J* = 14.2 Hz, Ar-**CH$_2$**-Ar), 2.99 (d, 2H, *J* = 14.3 Hz, Ar-**CH$_2$**-Ar), 1.92-1.76 (m, 8H, CH_3**CH$_2$**CH_2), 1.37 (bs, 18H, C(C**H$_3$**)$_3$), 1.11 (t, 6H, *J* = 7.3 Hz, **CH$_3$**CH_2CH_2), 0.81 (t, 6H, *J* = 7.4 Hz, **CH$_3$**CH_2CH_2) ppm. ^{13}C-NMR ($CDCl_3$, 75 MHz) δ 157.1, 156.5, 146.5, 139.6, 139.2, 138.0, 136.6, 136.4, 131.0, 127.9, 127.7, 124.7, 77.4, 76.7, 34.5, 34.3, 32.0, 31.5, 23.7, 22.7, 11.1, 9.7 ppm. IR (KBr) ν 1688 cm^{-1}. HRMS (TOF MS ESI$^-$): calcd for $C_{52}H_{62}F_6Hg_2O_8$ 1332.3761 [$(M)^-$]; found *m/z* 1331.3690 [$(M-H)^-$].

11,23-di-*tert*-butyl-4,18-bis(chloromercurio)-25,26,27,28-tetrapropoxycalix[4]arene (5')

A mixture of calixarene **1** (0.100 g, 0.14 mmol) and $Hg(TFA)_2$ (0.15 g, 0.35 mmol) was dissolved in dry chloroform and stirred 2 days at room temp. Aqueous 1M HCl (15 ml) was then added and the reaction mixture was stirred for 3 h. The organic layer was separated, washed three times with water and dried over MgSO4. Solvent was removed under a reduced pressure, and the crude product was purified on a silica gel column using a mixture of CH_2Cl_2:hexane (2:1 v/v) as en eluent. The title compound was obtained as a white powder in 42% yield (61 mg) together with 19 mg of calixaren **4'** (14%) which was formed as byproduct. Mp: 286-291 °C. ^{1}H-NMR($CDCl_3$, 300 MHz) δ 7.23 (d, 2H, *J*=2.3 Hz, Ar-**H**), 7.09 (d, 2H, *J*=2.0 Hz, Ar-**H**), 6.22 (d, 2H, *J*=7.6 Hz, Ar-**H**), 6.01 (d, 2H, *J*= 7.6 Hz, Ar-**H**), 4.64 (d, 1H, *J*=14.0 Hz, Ar-**CH_2**-Ar), 4.50-4.41 (m, 3H, Ar-**CH_2**-Ar), 4.13-3.82 (m, 4H, CH_3CH_2**CH_2**), 3.72-3.59 (m, 4H, CH_3CH_2**CH_2**), 3.24-3.05 (m, 3H, Ar-**CH_2**-Ar), 2.99 (d, 1H, *J*=14.0 Hz, Ar-**CH_2**-Ar), 1.98-1.73 (m, 8H, CH_3**CH_2**CH_2), 1.44 (bs, 18H, C(C**H_3**)$_3$), 1.11 (t, 6H, *J*=7.3 Hz, **CH_3**CH_2CH_2), 0.92-0.76 (m, 6H, **CH_3**CH_2CH_2) ppm. ^{13}C-NMR ($CDCl_3$, 75 MHz) δ 157.3, 156.2, 148.4, 146.0, 138.4, 138.3, 136.1, 136.0, 130.7, 127.9, 127.8, 125.1, 77.2, 76.6, 34.6, 34.5, 31.9, 31.6, 23.7, 22.6, 11.2, 9.8 ppm. HRMS (ESI^+): calcd for $C_{48}H_{62}Cl_2Hg_2O_4Na$ 1199.3330 [$(M+Na)^+$]; found *m/z* 1199.3323 [$(M+Na)^+$]. Elemental analysis (%) calcd for $C_{48}H_{62}O_4Cl_2Hg_2$: C 49.06, H 5.32; found: C 49.41, H 5.54.

11,23-di-*tert*-butyl-4-iodo-25,26,27,28-tetrapropoxycalix[4]arene (6a)

A mixture of calixarene **4'** (26 mg, 0.028 mmol) and I_2 (8.0 mg, 0.032 mmol) was dissolved in dry acetonitrile and stirred overnight at room temp. Aqueous solution of Na_2SO_3 (10%, 20 ml) was then added to quench the reaction. The organic layer was separated, washed three times with 1M HCl, three times with water, and dried over $MgSO_4$. Solvent was removed on vacuum evaporator to yield the crude product which was purified by column chromatography (silica gel, eluent = CH_2Cl_2:hexane 1:5 v/v). Title compound was obtained as a white powder in 36% yield (8.4 mg), mp: 204-209 °C. ^{1}H-NMR ($CDCl_3$, 300 MHz) δ 7.23 (d, 1H, *J*=7.9 Hz, Ar-**H**), 6.98 (d, 1H, *J*=2,3 Hz, Ar-**H**), 6.75-6.51 (m, 6H, Ar-**H**), 6.44 (d, 1H, *J*= 8.2, Ar-**H),** 4.56 (d, 1H, *J* = 13.5 Hz, Ar-**CH_2**-Ar), 4.49-4.33 (m, 3H, Ar-**CH_2**-Ar), 3.96-3.63 (m, 8H, CH_3CH_2**CH_2**), 3.49 (d, 1H, *J*=13.5 Hz, Ar-**CH_2**-Ar), 3.23-3.03 (m, 3H, Ar-**CH_2**-Ar), 2.12-1.79 (m, 8H, CH_3**CH_2**CH_2), 1.04 (s, 9H, C(**CH_3**)$_3$), 1.02 (s, 9H, C(**CH_3**)$_3$), 1.01-0.90 (m, 12H, **CH_3**CH_2CH_2) ppm. ^{13}C-NMR ($CDCl_3$, 75 MHz) δ 157.3, 156.8, 154.1, 153.9, 144.5, 143.6, 139.3, 136.2, 136.1, 135.4, 133.9, 133.8, 133.5, 132.7, 131.6, 129.9, 128.3, 128.2, 126.9, 125.5, 125.4, 125.0, 122.4, 122.1, 97.9, 77.5, 77.0, 76.9 (2x), 34.8, 34.0, 31.6, 31.4, 31.2, 30.9, 29.9, 23.6, 23.5, 23.4, 23.2 (2x), 10.6 (2x), 10.5, 10.4. HRMS (TOF MS ESI+): calcd for $C_{48}H_{63}IO_4$ 830.3771 [$(M)^+$]; found *m/z* 830.3746 [$(M)^+$]. Elemental analysis (%) calcd for $C_{48}H_{63}O_4I$: C 69.38, H 7.64; found: C 69.19, H 7.76.

11,23-di-*tert*-butyl-4-bromo-25,26,27,28-tetrapropoxycalix[4]arene (6b)

A mixture of calixarene **4** (0.110 g, 0.11 mmol) and NBS (0.019 g, 0.11 mmol) was dissolved in dry acetonitrile and stirred overnight at room temp. Solution of Na_2SO_3 (10%, 30 ml) was then added to quench the reaction. The organic layer was separated, washed three times with 1M HCl, three times with water and dried over $MgSO_4$. Solvent was removed under a reduced pressure to yield the crude product

which was purified using column chromatography (silica gel, eluent = CH_2Cl_2:hexane 7:5 v/v). Product was obtained as a white powder in 47% yield (39 mg), mp: 265-269 °C. ^{1}H-NMR ($CDCl_3$, 300 MHz) δ 7.21 (d, 1H, *J* = 2.1 Hz, Ar-**H**), 7.13-7.02 (m, 3H, Ar-**H**), 6.25-6.13 (m, 2H, Ar-**H**), 6.07-5.94 (m, 3H, Ar-**H**), 4.64 (d, 2H, *J* = 14.1 Hz, Ar-**CH$_2$**-Ar), 4.45 (d, 2H, *J* = 13.2 Hz, Ar-**CH$_2$**- Ar), 4.00-3.90 (m, 4H, CH_3CH_2**CH$_2$**), 3.71-3.60 (m, 4H, CH_3CH_2**CH$_2$**), 3.20-2.93 (m, 4H, Ar-**CH$_2$**-Ar), 1.98-1.80 (m, 8H, CH_3**CH$_2$**CH_2), 1.34 (s, 18H, C(C**H$_3$**)$_3$), 1.13-1.06 (m, 6H, **CH$_3$**CH_2CH_2), 0.90-0.77 (m, 6H, **CH$_3$**CH_2CH_2) ppm. ^{13}C-NMR ($CDCl_3$, 75 MHz) δ 157.0, 156.2, 155.9, 155.7, 145.5, 144.8, 138.6, 138.5, 136.4, 136.3, 135.9, 134.2, 133.8, 133.5, 130.4, 128.0, 127.7, 127.5, 127.1, 126.2, 126.1, 125.9, 124.6, 122.6, 77.2, 77.0 (2x), 75.8, 34.6, 34.5, 34.4, 32.0 (2x), 31.6, 31.5, 31.4, 23.7 (2x), 23.3, 22.5, 11.2, 11.1, 10.0, 9.8 ppm. HRMS (TOF MS ESI+): calcd for $C_{48}H_{63}BrO_4$ 782.3910 [$(M)^+$]; found *m/z* 782.3934 [$(M)^+$]. Elemental analysis (%) calcd for $C_{48}H_{63}O_4Br$: C 73.54, H 8.10; found: C 73.22, H 7.86.

11,23-di-*tert*-butyl-4,18-diiodo-25,26,27,28-tetrapropoxycalix[4]arene 7a

A mixture of calixarene **5'** (0.098 g, 0.074 mmol) and I_2 (0.088 g, 0.35 mmol) was dissolved in dry acetonitrile and stirred overnight at room temp. Solution of Na_2SO_3 (10%, 30 ml) was then added to quench the reaction. The organic layer was separated, washed three times with 1M HCl, three times with water and dried over MgSO4. Solvent was removed under a reduced pressure to yield the crude product (70 mg). Analytical sample was obtained by crystallization from CH_2Cl_2 and methanol, mp: 276-283 °C. ^{1}H-NMR($CDCl_3$, 300 MHz) δ 7.43 (d, 2H, *J* = 8.0 Hz, Ar-**H**), 6.82-6.77 (m, 4H, Ar-**H**), 6.42 (d, 2H, *J* = 2.4 Hz, Ar-**H**), 4.51 (d, 2H, *J* = 13.2 Hz, Ar-**CH$_2$**-Ar), 4.36 (d, 2H, *J* = 12.9 Hz, Ar-**CH$_2$**-Ar), 4.07-3.91 (m, 4H, CH_3CH_2**CH$_2$**), 3.73-3.56 (m, 6H, CH_3CH_2**CH$_2$**, Ar-**CH$_2$**-Ar), 3.12 (d, 2H, *J* = 12.8 Hz, Ar-**CH$_2$**-Ar), 2.18-2.00 (m, 4H, CH_3**CH$_2$**CH_2), 1.92-1.80 (m, 4H, CH_3**CH$_2$**CH_2), 1.04 (t, 6H, *J* = 7.4 Hz, **CH$_3$**CH_2CH_2), 0.96-0.89 (m, 6H, **CH$_3$**CH_2CH_2), 0.88 (bs, 18H, C(C**H$_3$**)$_3$) ppm. ^{13}C-NMR ($CDCl_3$, 75 MHz) δ 157.8, 152.9, 144.6, 140.8, 137.5, 133.6, 131.6, 131.3, 130.2, 124.9, 124.5, 98.8, 76.9 (2x), 34.2, 34.0, 31.5, 31.1, 23.7, 23.1, 10.9, 10.0 ppm. HRMS (ESI+): calcd for $C_{48}H_{62}I_2O_4K$ 995.2369 [$(M+K)^+$]; found *m/z* 974.3088 [$(M+H_2O)^+$], 995.2376 [$(M+K)^+$]. Elemental analysis (%) calcd for $C_{48}H_{62}O_4I_2$: C 60.25, H 6.53; found: C 60.53, H 6.73.

4-(Chloromercurio)-25,26,27,28-tetrapropoxycalix[4]arene (11'): A mixture of calixarene **10** (0.100 g, 0.17 mmol) and $Hg(CF_3COO)_2$ (0.073 g, 0.17 mmol) was dissolved in dry chloroform and stirred overnight at room temp. Aqueous 1M HCl (5 ml) was then added and the reaction mixture was stirred for 3 h. The organic layer was separated, washed three times with water and dried over $MgSO_4$. Solvent was removed under a reduced pressure to yield the crude product which was purified by column chromatography on a silica gel (eluent = CH_2Cl_2:hexane 7:6, v/v). The title compound was obtained as a white powder in 71% yield (100 mg), m.p. 199 – 201 °C. ^{1}H NMR ($CDCl_3$, 300 MHz, 298 K) δ 7.10-6.84 (m, 6H, Ar-**H**), 6.34-6.17 (m, 5H, Ar-**H**), 4.70 (d, 1H, *J* = 14.1 Hz, Ar-**CH$_2$**-Ar ax.), 4.50-4.39 (m, 3H, Ar-**CH$_2$**-Ar ax.), 4.08-3.90 (m, 4H, O-**CH$_2$**), 3.78-3.63 (m, 4H, O-**CH$_2$**), 3.18 (d, 2H, *J* = 13.5 Hz, Ar-**CH$_2$**-Ar eq.), 3.15 (d, 1H, *J* = 13.5 Hz, Ar-**CH$_2$**-Ar eq.), 3.02 (d, 1H, *J* = 14.1 Hz, Ar-**CH$_2$**-Ar eq.), 1.99-

1.79 (m, 8H, O-CH_2**CH_2**), 1.11-1.03 (m, 6H, CH_2-**CH_3**), 0.94-0.82 (m, 6H, CH_2-**CH_3**). ^{13}C NMR ($CDCl_3$, 75 MHz, 298 K) δ 158.1, 158.0, 157.3, 156.0, 148.2 138.8, 138.7, 137.2, 137.0, 136.5, 135.9, 135.7, 134.3, 133.9, 130.5, 130.2, 129.2, 129.0, 128.8, 128.1, 127.9, 127.5, 123.8, 122.5, 122.4, 122.2, 34.3, 31.5, 31.2 (2x), 30.0, 23.7 (2x); 23.4, 22.9, 11.0 (2x), 10.3, 10.2, 10.0 ppm. MS ES+ *m/z* for $C_{40}H_{47}ClHgO_4Na$ calcd.: 851.2761 [$(M+Na)^+$]; found: 851.27542 [$(M+Na)^+$]. Elemental analysis (%) calcd for $C_{40}H_{47}O_4ClHg$: C 58.03, H 5.72; found: C 57.87, H 5.64.

Mercuration of propoxybenzene

A mixture of derivate **8** (0.072 g, 0.53 mmol) and $Hg(CF_3COO)_2$ (0.23 g, 0.54 mmol) was dissolved in dry chloroform and stirred overnight at room temperature. Aqueous 1M HCl (10 ml) was then added and the reaction mixture was stirred for 3 h. The organic layer was separated, washed three times with water and dried over MgSO4. Solvent was removed under a reduced pressure to yield the crude mixture of products which were separated by column chromatography on a silica gel (eluent = CH_2Cl_2:hexane 1:2 v/v). The chloromercurio derivatives were obtained in 37:63 ratio (*ortho*:*para*).

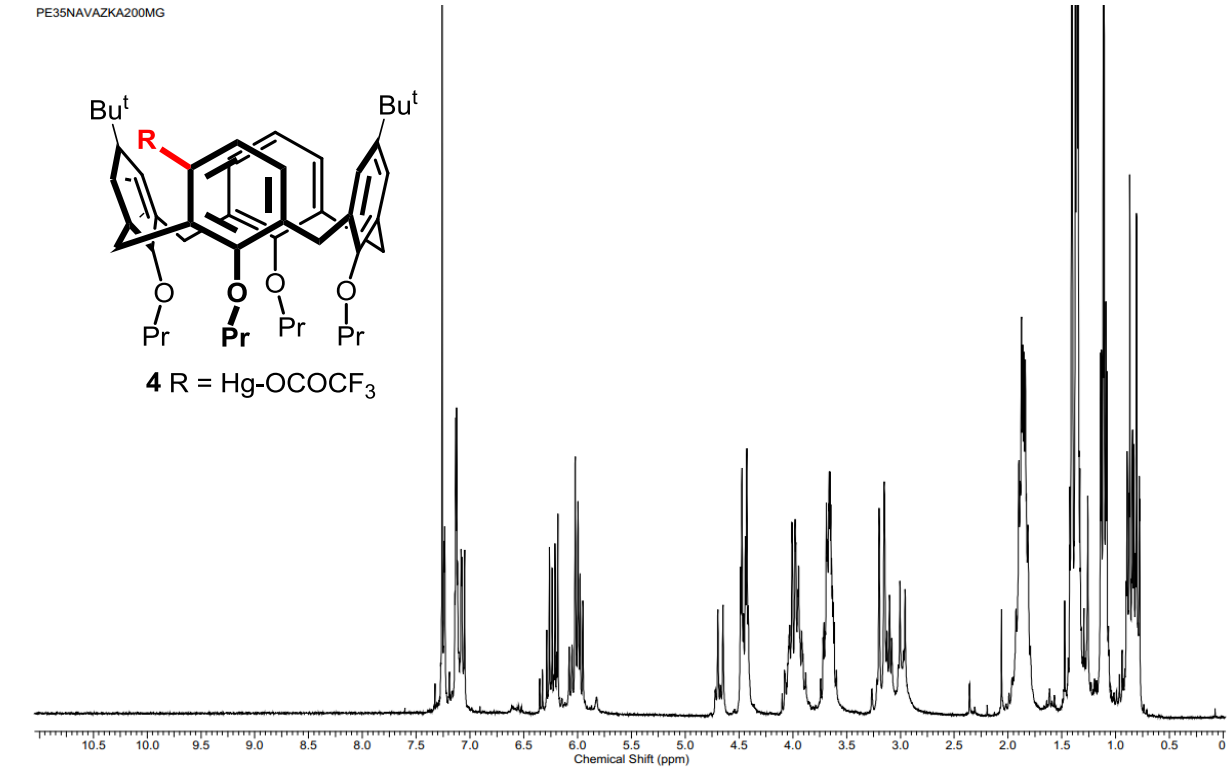
4-chloromercurio-1-propoxybenzene (8a-*para*): ^{1}H-NMR($CDCl_3$, 300 MHz) δ 7.23-7.18 (m, 2H), 6.97-6.92 (m, 2H), 3.92 (t, 2H, *J*=6.6 Hz), 1.89-1.75 (m, 2H), 1.04 (t, 3H, *J*=7.4 Hz) ppm.

2-chloromercurio-1-propoxybenzene (8b-*ortho*): ^{1}H-NMR($CDCl_3$, 300 MHz) δ 7.35-7.28 (m, 1H), 7.25-7.22 (m, 1H), 7.04-6.98 (m, 1H), 6.94-6.90 (m, 1H), 3.97-3.91 (m, 2H), 1.87-1.75 (m, 2H), 1.07-1.02 (m,3H) ppm.

Mercuration of 2,6-dimethyl-1-propoxybenzene

A mixture of 2,6-dimethyl-1-dipropoxybenzene **9** (0.22 g, 1.34 mmol) and $Hg(CF_3COO)_2$ (0.58 g, 1.36 mmol) was dissolved in dry chloroform and stirred overnight at room temp. Aqueous 1M HCl (10 ml) was then added and the reaction mixture was stirred for 3 h. The organic layer was separated, washed three times with water and dried over MgSO4. Solvent was removed under a reduced pressure to yield the crude product. Products were obtained as a white powder in 65% yield (0.35 g), the mixture consists of **9-para** and **9-meta** isomers in 2:1 ratio (see 1H NMR spectrum of this mixture). Pure **9-para** isomer was obtained by crystallization from ethyl acetate, mp: 169.5-170 °C.

4-chloromercurio-2,6-dimethyl-1-propoxybenzene (9-para): ^{1}H-NMR($CDCl_3$, 300 MHz) δ 6.95 (s, 2H), 3.72 (t, 2H, *J*=6.6 Hz), 2.26 (s, 6H), 1.82 (sex, 2H, *J*=6.6, 7.4 Hz), 1.07 (t, 3H, *J*=7.4 Hz) ppm.^{13}C-NMR ($CDCl_3$, 75 MHz) δ 157.5, 143.6, 136.1, 132.3, 74.2, 23.9, 16.6, 10.9. HRMS (ESI+): calcd for $C_{11}H_{15}ClHgO$ 400.0517 [$(M)^+$]; found *m/z* 400.0509 [$(M)^+$].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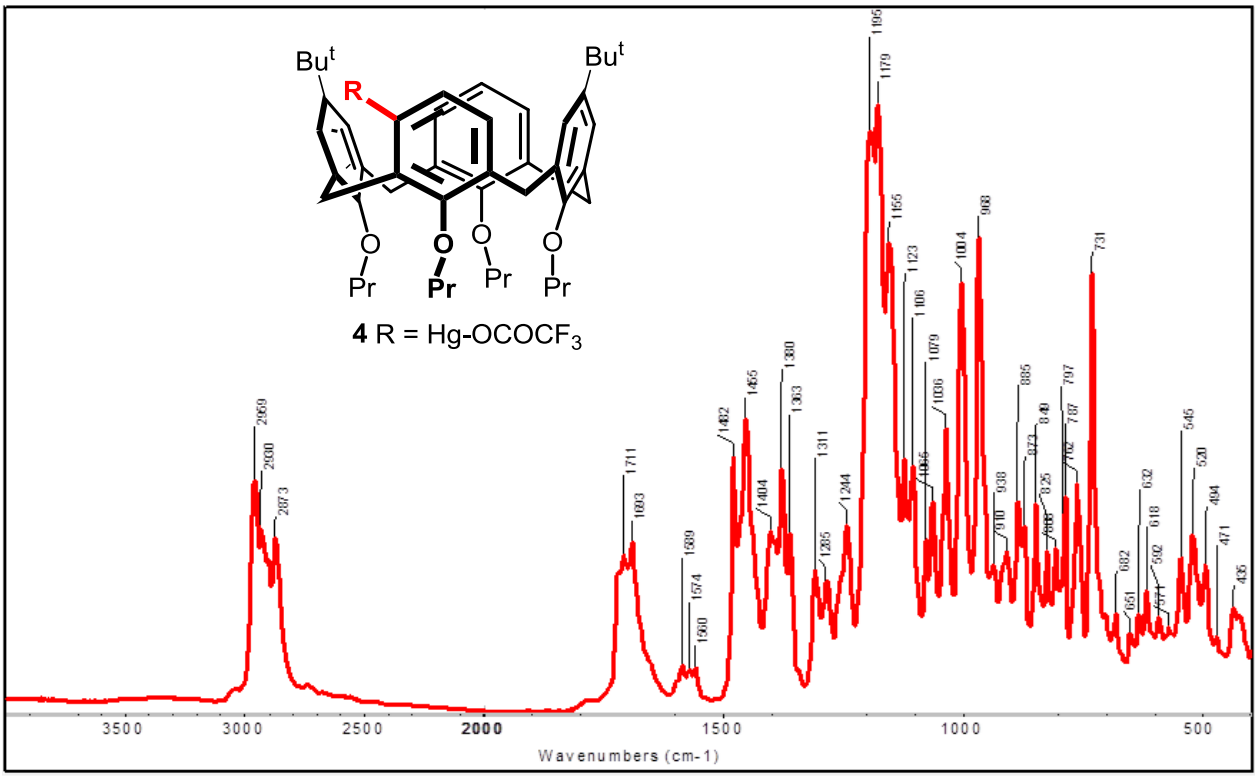
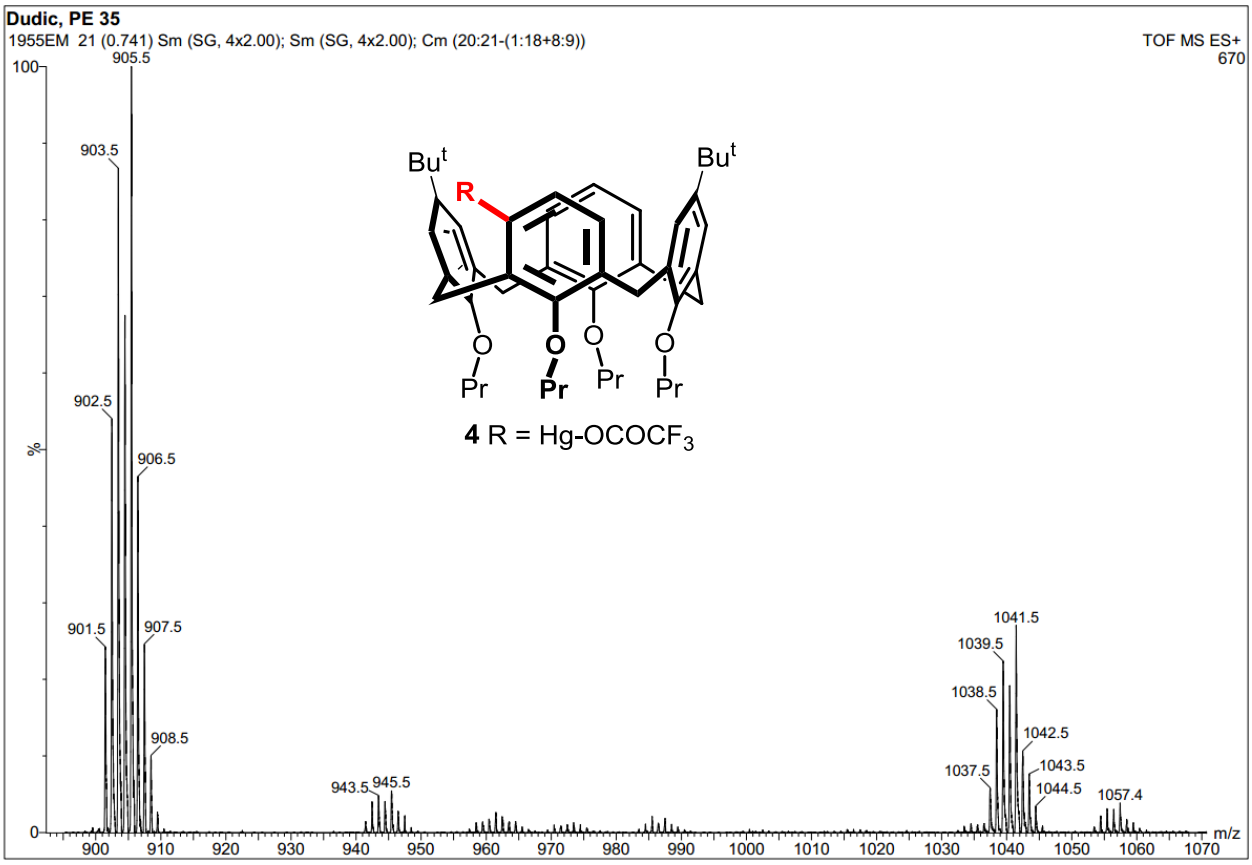
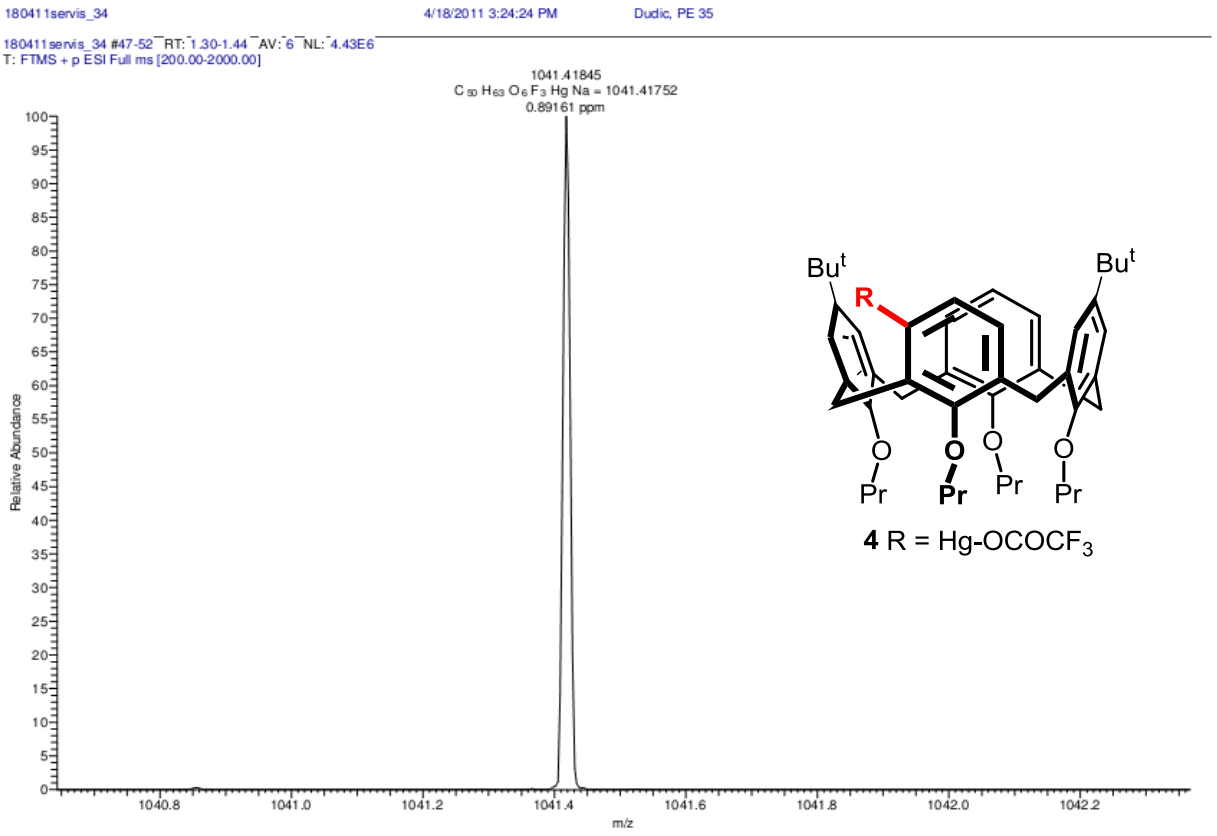
Pr
4 R = Hg-OCOCF3
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)


Bu^t
R
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
4 R = Hg-OCOCF3
2969
2930
2873
1711
1693
1689
1574
1500
1482
1455
1404
1380
1363
1311
1285
1244
1196
1179
1155
1123
1106
1079
1036
1004
968
938
910
885
840
825
797
787
731
682
651
632
618
592
545
520
494
471
436
3500 3000 2500 2000 1500 1000 500
Wavenumbers (cm-1)

Compound 4



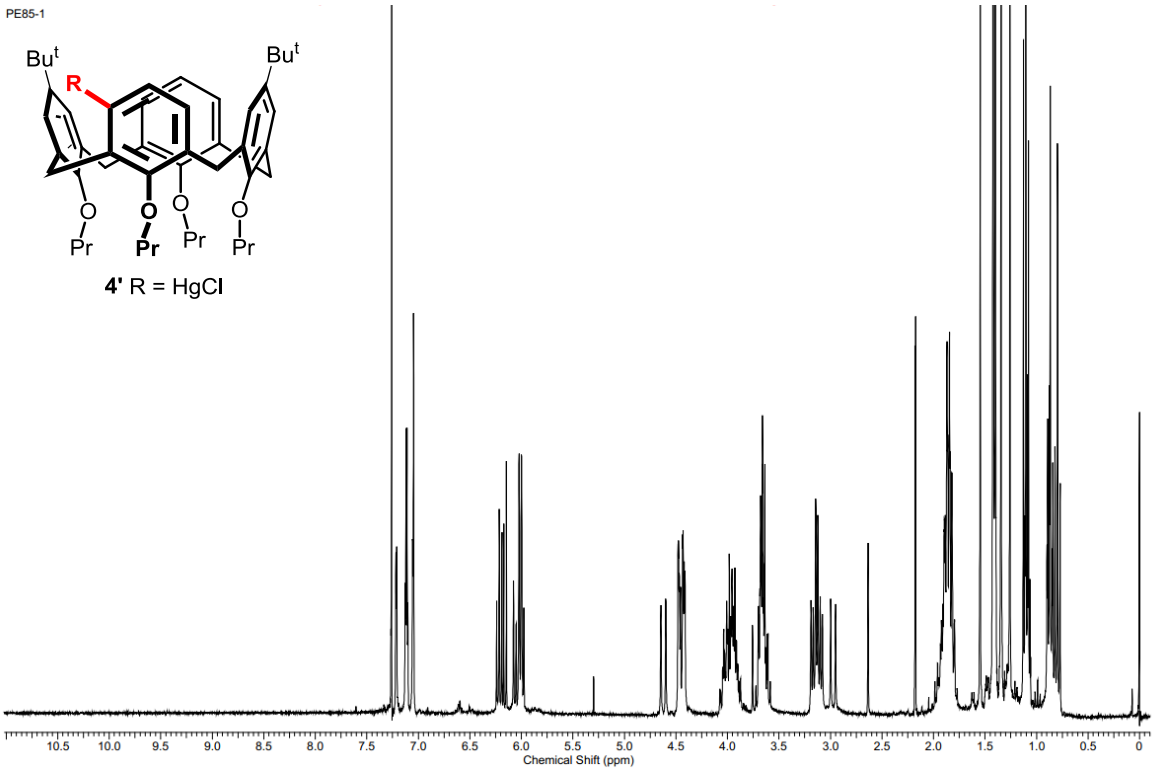
4 R = Hg-OCOCF$_3$

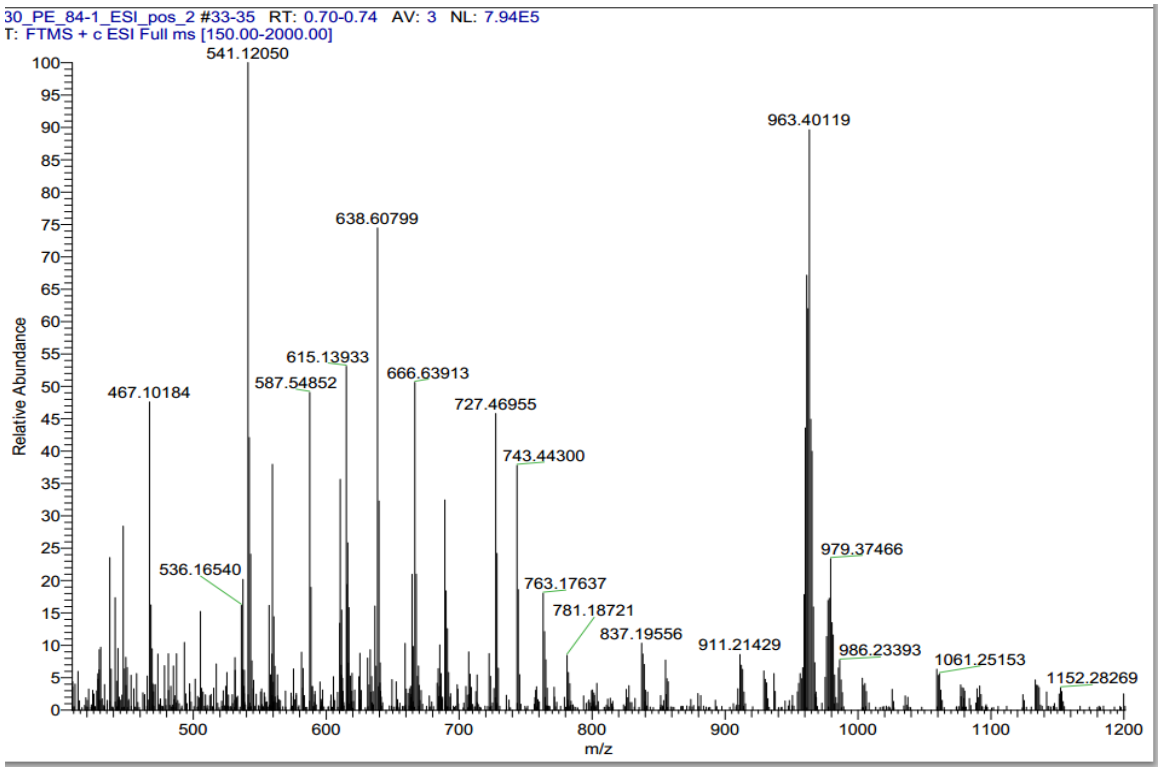


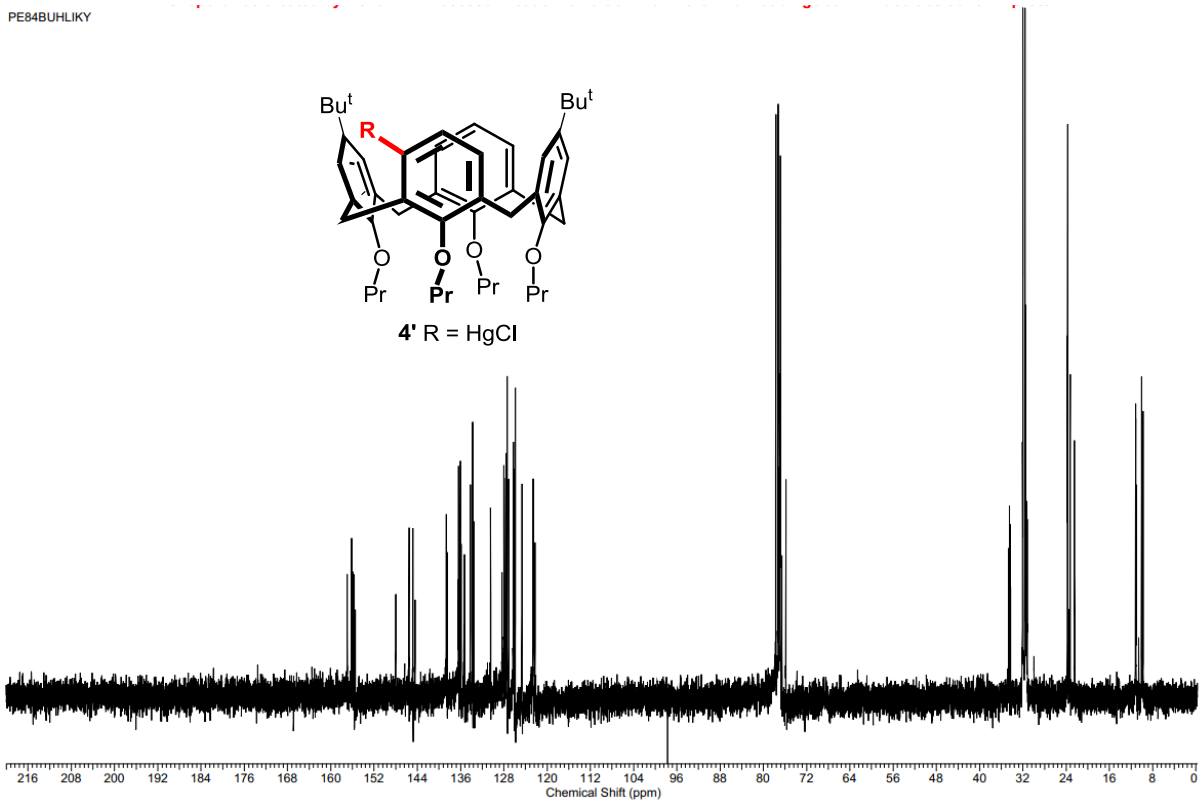
4 R = Hg-OCOCF$_3$

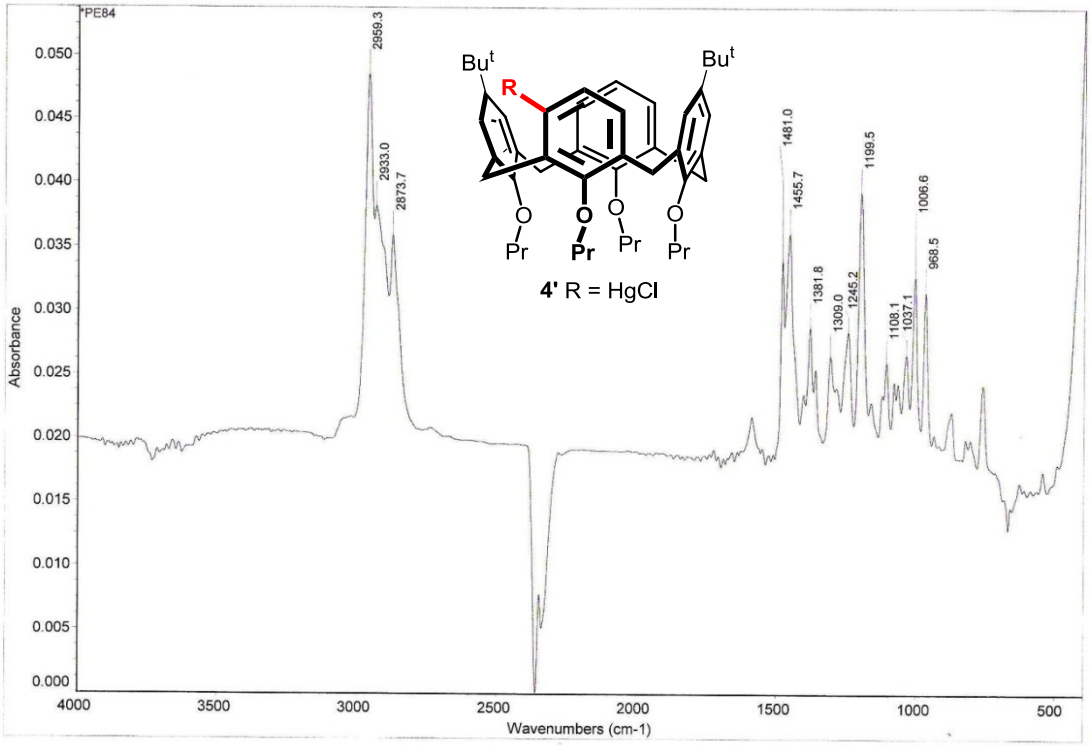
Compound 4

Compound 4‘

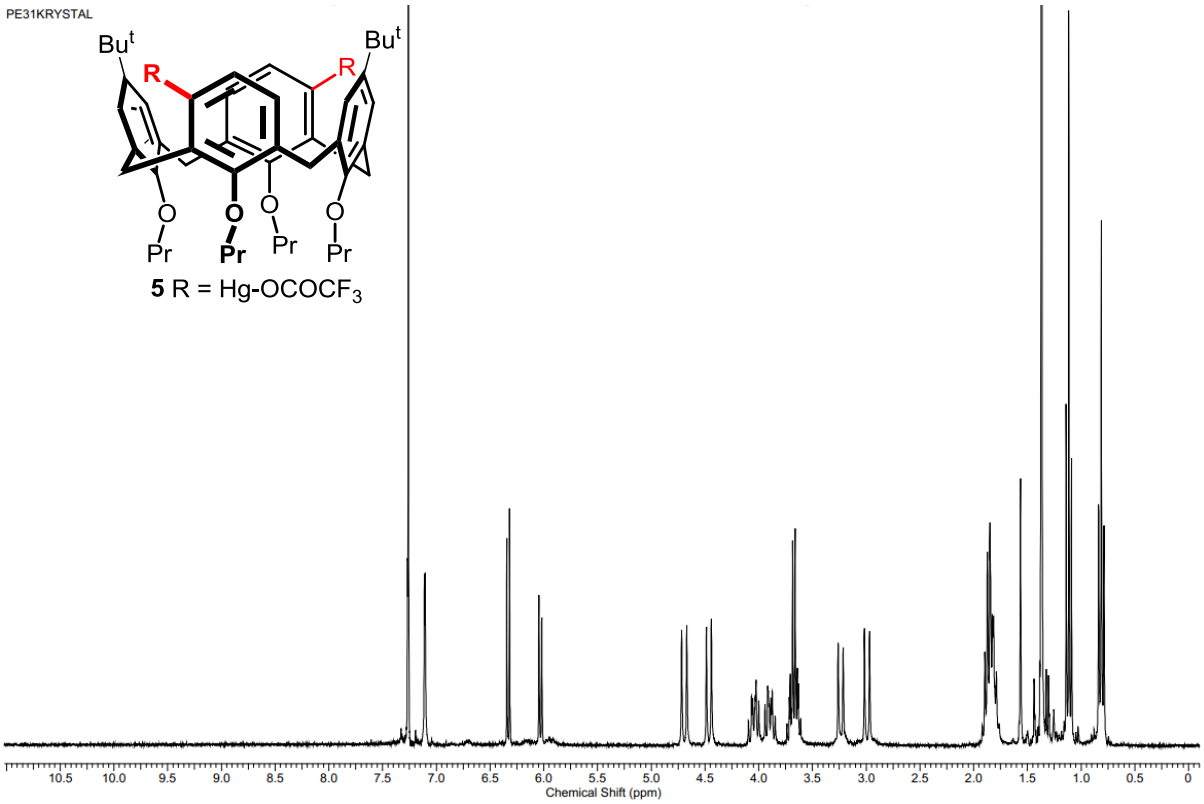

PE85-1
Bu^t
R
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
4' R = HgCl
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)

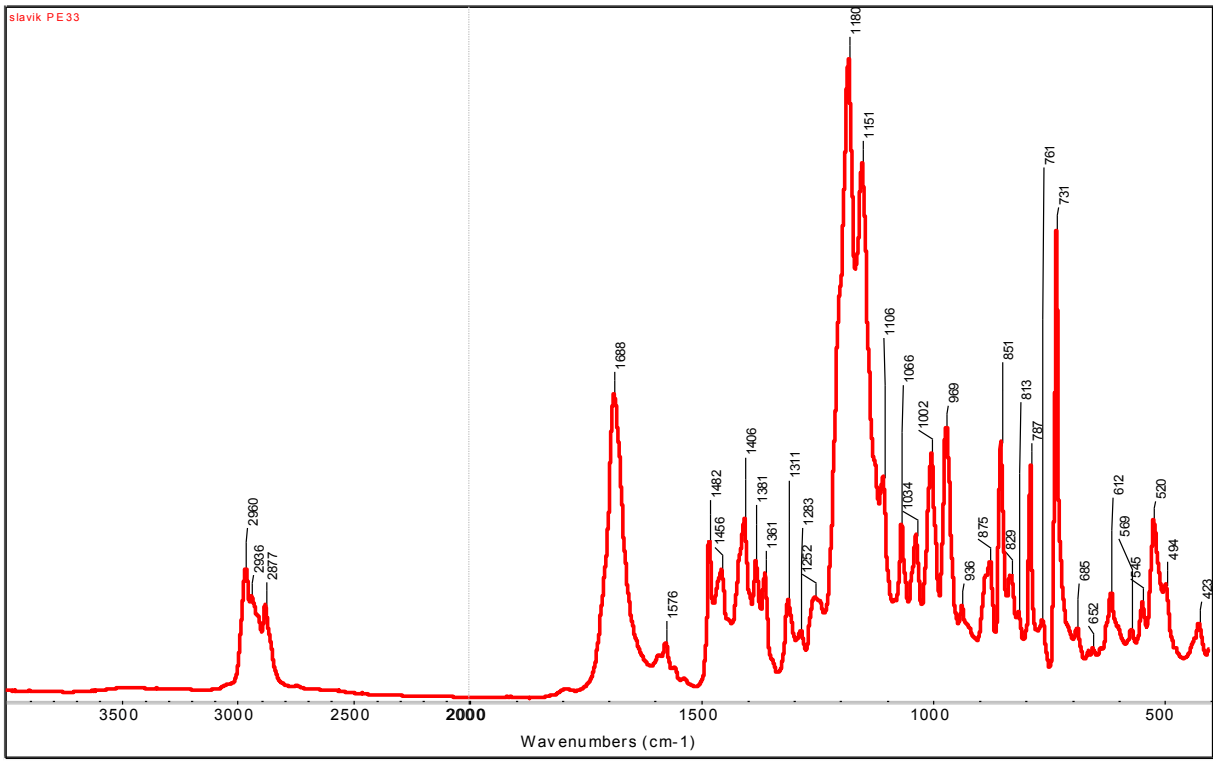

30_PE_84-1_ESI_pos_2 #33-35 RT: 0.70-0.74 AV: 3 NL: 7.94E5
T: FTMS + c ESI Full ms [150.00-2000.00]
Relative Abundance
m/z
541.12050
963.40119
638.60799
615.13933
587.54852
666.63913
467.10184
727.46955
743.44300
979.37466
536.16540
763.17637
781.18721
837.19556
911.21429
986.23393
1061.25153
1152.28269
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
500 600 700 800 900 1000 1100 1200


PE84BUHLIKY
Bu^t
R
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
4' R = HgCl
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)

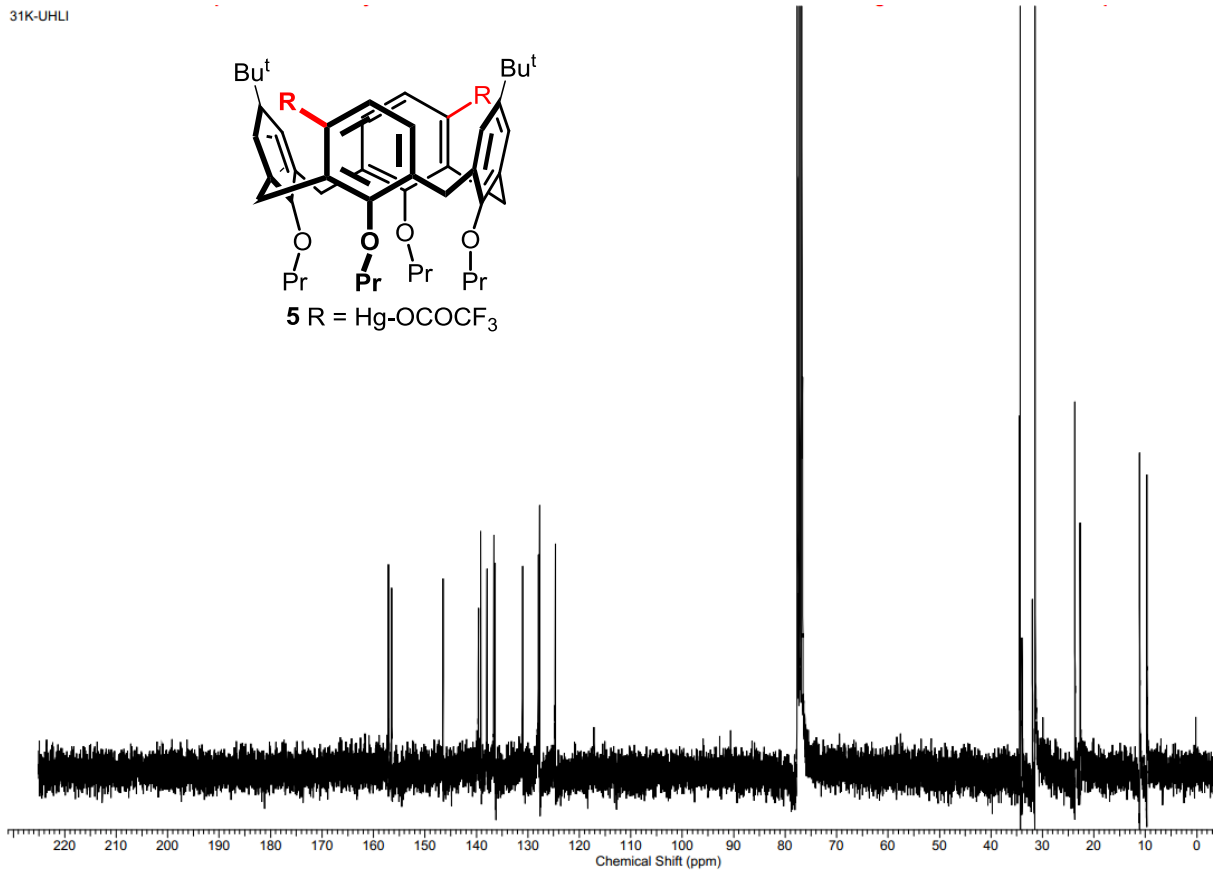

PE84
2959.3
2933.0
2873.7
1481.0
1455.7
1381.8
1309.0
1245.2
1199.5
1108.1
1037.1
1006.6
968.5
Bu^t
R
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
4' R = HgCl
Absorbance
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
4000 3500 3000 2500 2000 1500 1000 500
Wavenumbers (cm-1)

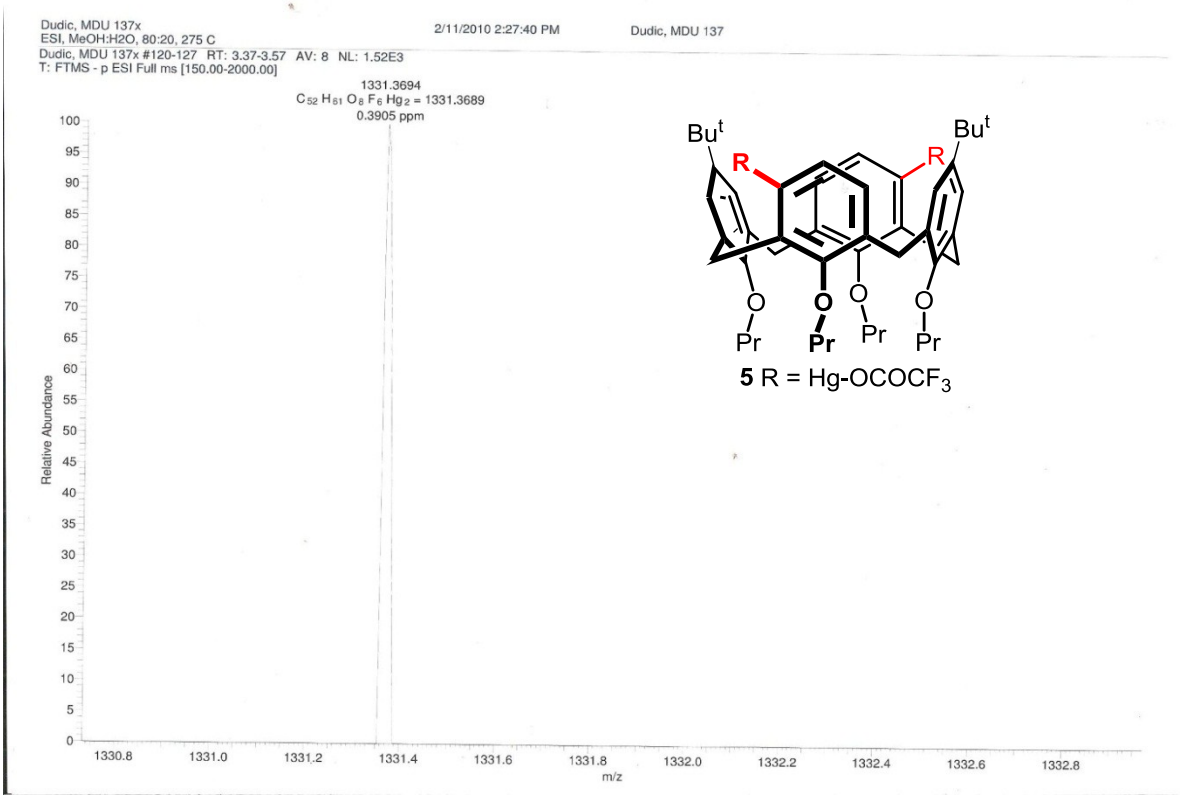
Compound 4‘


PE31KRYSTAL
Bu^t
Bu^t
R
R
O
Pr
O
Pr
O
Pr
O
Pr
5 R = Hg-OCOCF$_3$
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)

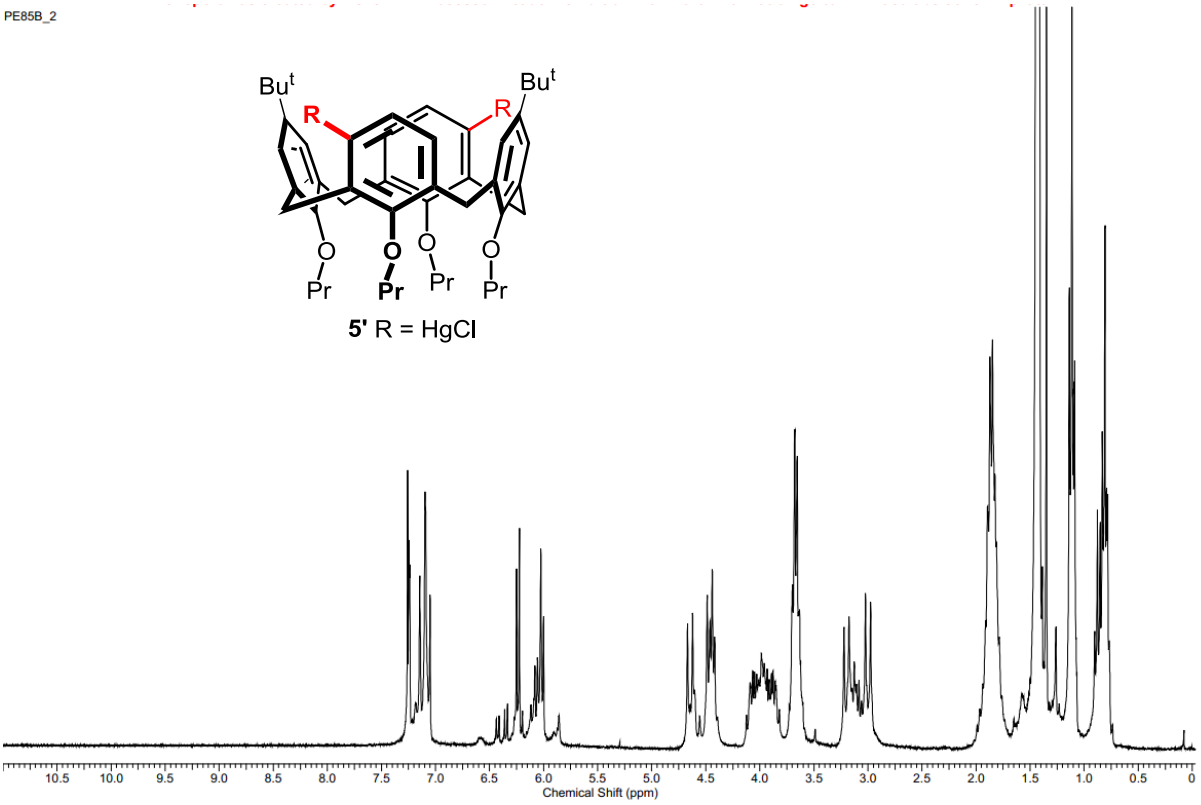

slavik PE33
2960
2936
2877
1688
1576
1482
1456
1406
1381
1361
1311
1283
1252
1180
1151
1106
1066
1034
1002
969
936
875
851
829
813
787
761
731
685
652
612
589
545
520
494
423
3500 3000 2500 2000 1500 1000 500
Wavenumbers (cm-1)

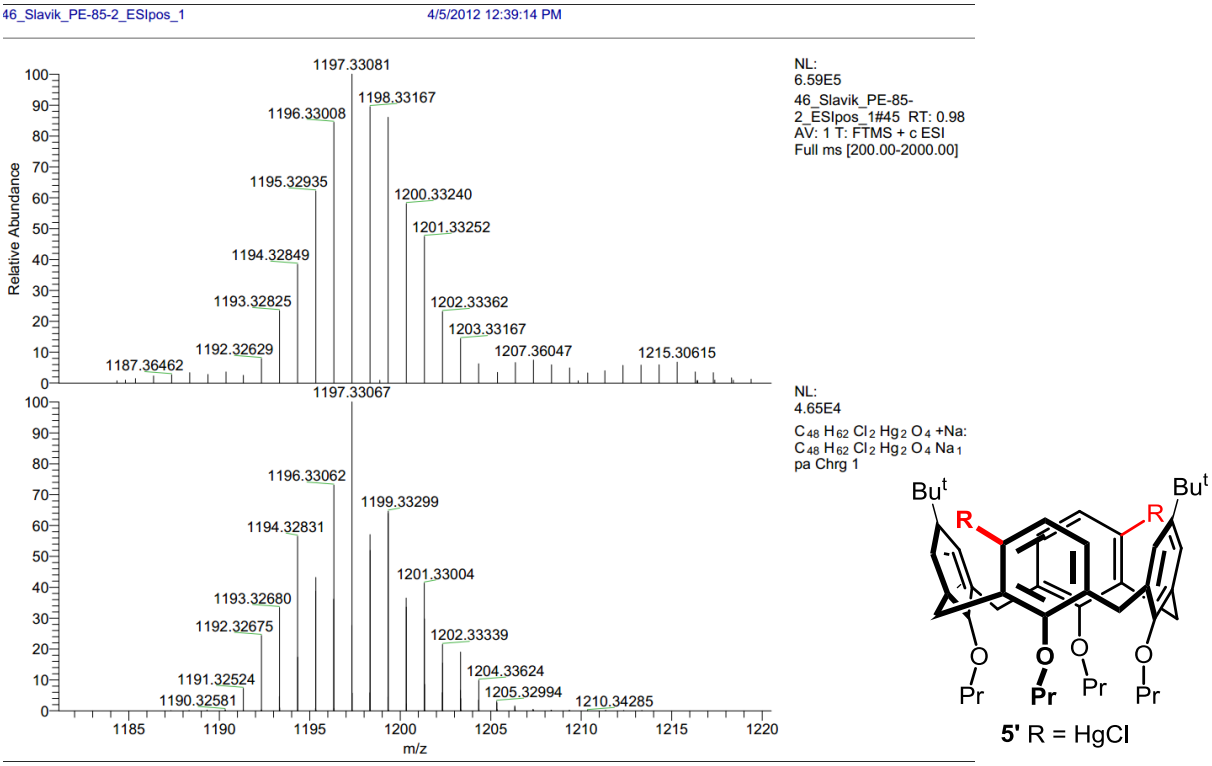
Compound 5


31K-UHLI
Bu^t
R
R
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
5 R = Hg-OCOCF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

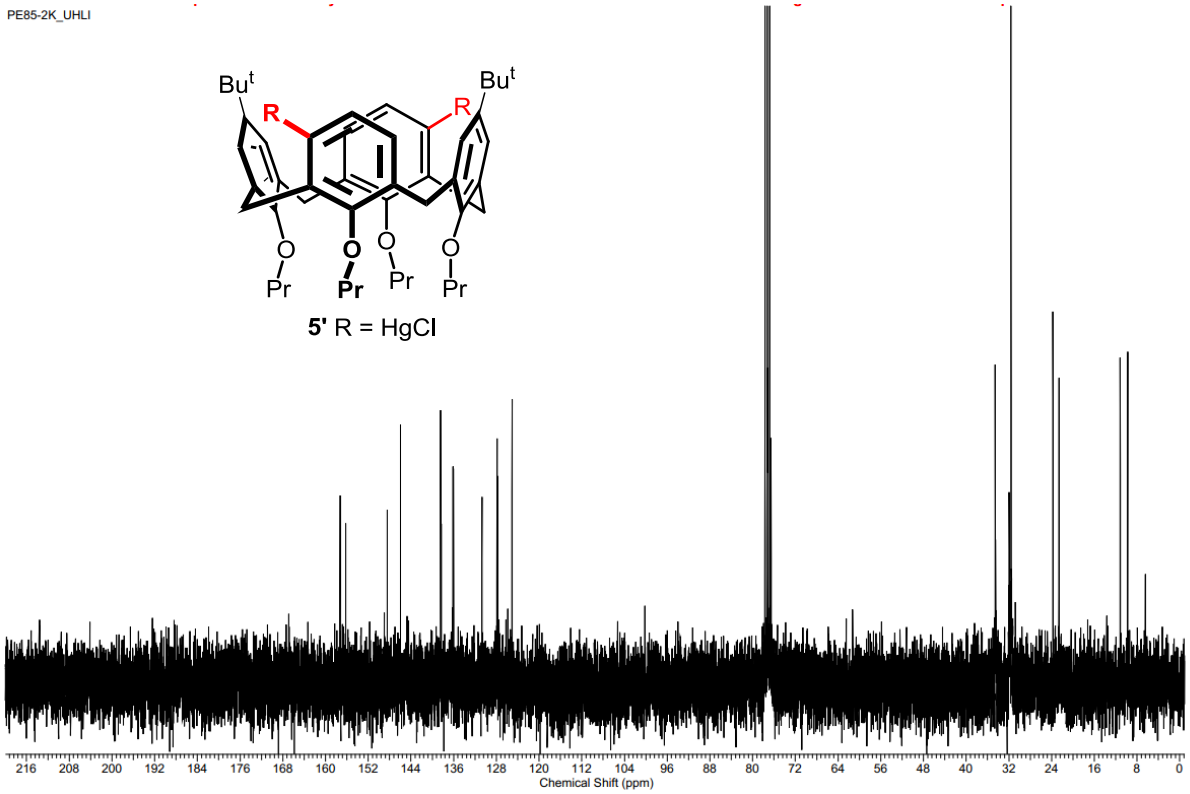

Dudic, MDU 137x
ESI, MeOH:H2O, 80:20, 275 C
Dudic, MDU 137x #120-127 RT: 3.37-3.57 AV: 8 NL: 1.52E3
T: FTMS - p ESI Full ms [150.00-2000.00]
2/11/2010 2:27:40 PM
Dudic, MDU 137
1331.3694
C52 H81 O8 F6 Hg2 = 1331.3689
0.3905 ppm
Relative Abundance
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
1330.8 1331.0 1331.2 1331.4 1331.6 1331.8 1332.0 1332.2 1332.4 1332.6 1332.8
m/z
Bu^t
R
R
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
5 R = Hg-OCOCF3

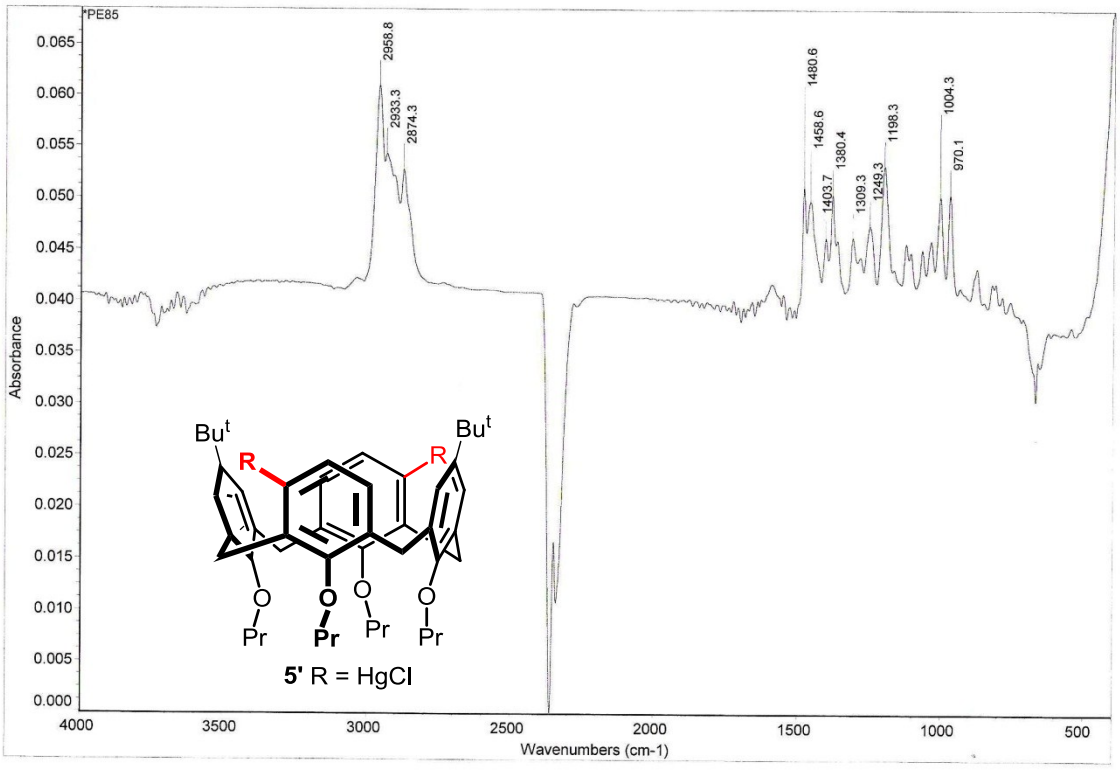
Compound 5


PE85B_2
Bu^t
R
Bu^t
R
O
Pr
O
Pr
O
Pr
O
Pr
5' R = HgCl
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)


46_Slavik_PE-85-2_ESIpos_1
4/5/2012 12:39:14 PM
Relative Abundance
m/z
1197.33081
1198.33167
1196.33008
1195.32935
1200.33240
1201.33252
1194.32849
1193.32825
1202.33362
1203.33167
1192.32629
1207.36047
1215.30615
1187.36462
NL:
6.59E5
46_Slavik_PE-85-2_ESIpos_1#45 RT: 0.98 AV: 1 T: FTMS + c ESI Full ms [200.00-2000.00]
1197.33067
1196.33062
1199.33299
1194.32831
1201.33004
1193.32680
1192.32675
1202.33339
1204.33624
1191.32524
1205.32994
1190.32581
1210.34285
NL:
4.65E4
C48 H62 Cl2 Hg2 O4 +Na: C48 H62 Cl2 Hg2 O4 Na1 pa Chrg 1
Bu^t
R
Bu^t
R
O
Pr
O
Pr
O
Pr
O
Pr
5' R = HgCl

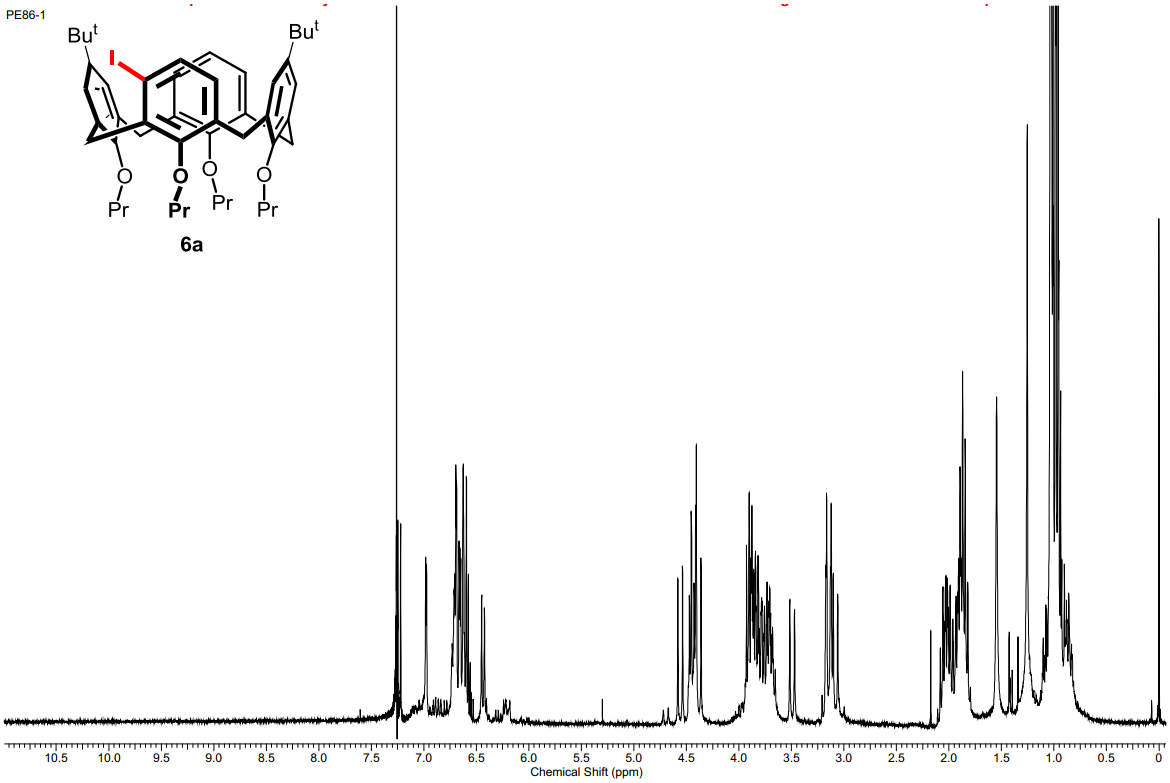
Compound 5‘

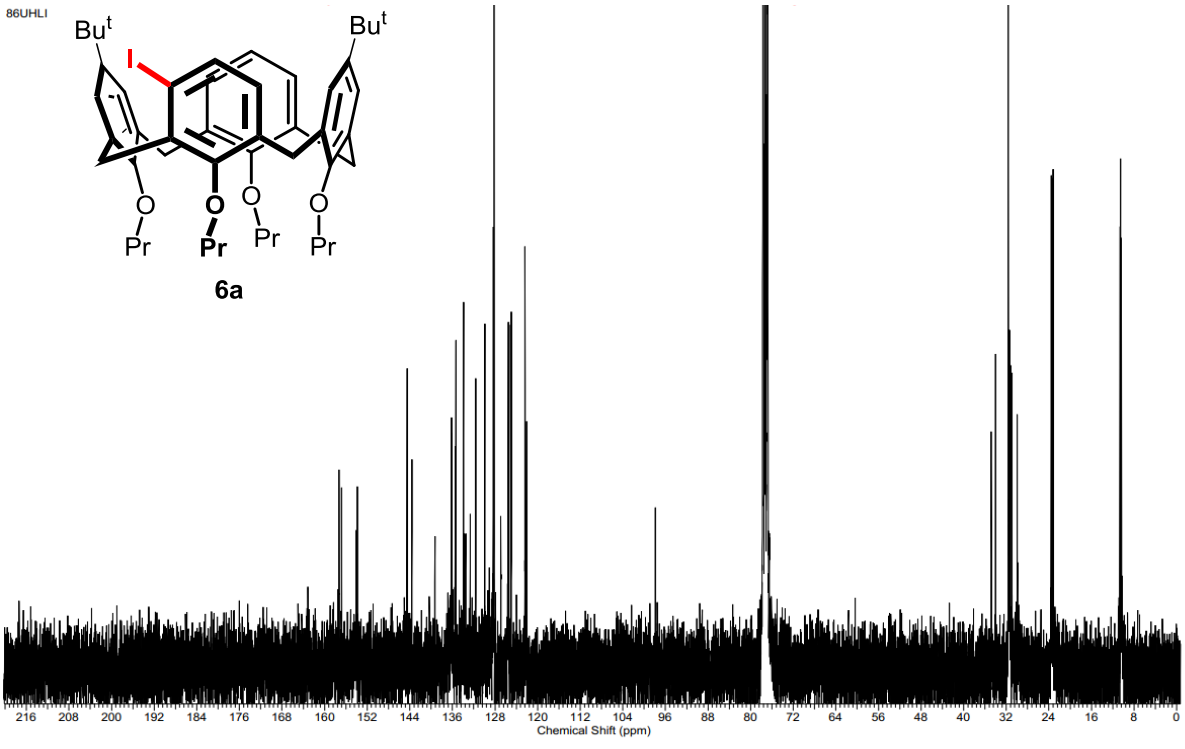

PE85-2K_UHLI
Bu^t
R
R
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
5' R = HgCl
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)


PE85
2958.8
2933.3
2874.3
1480.6
1458.6
1380.4
1403.7
1309.3
1249.3
1198.3
1004.3
970.1
Absorbance
0.065
0.060
0.055
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
Bu^t
R
R
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
5' R = HgCl
4000 3500 3000 2500 2000 1500 1000 500
Wavenumbers (cm-1)

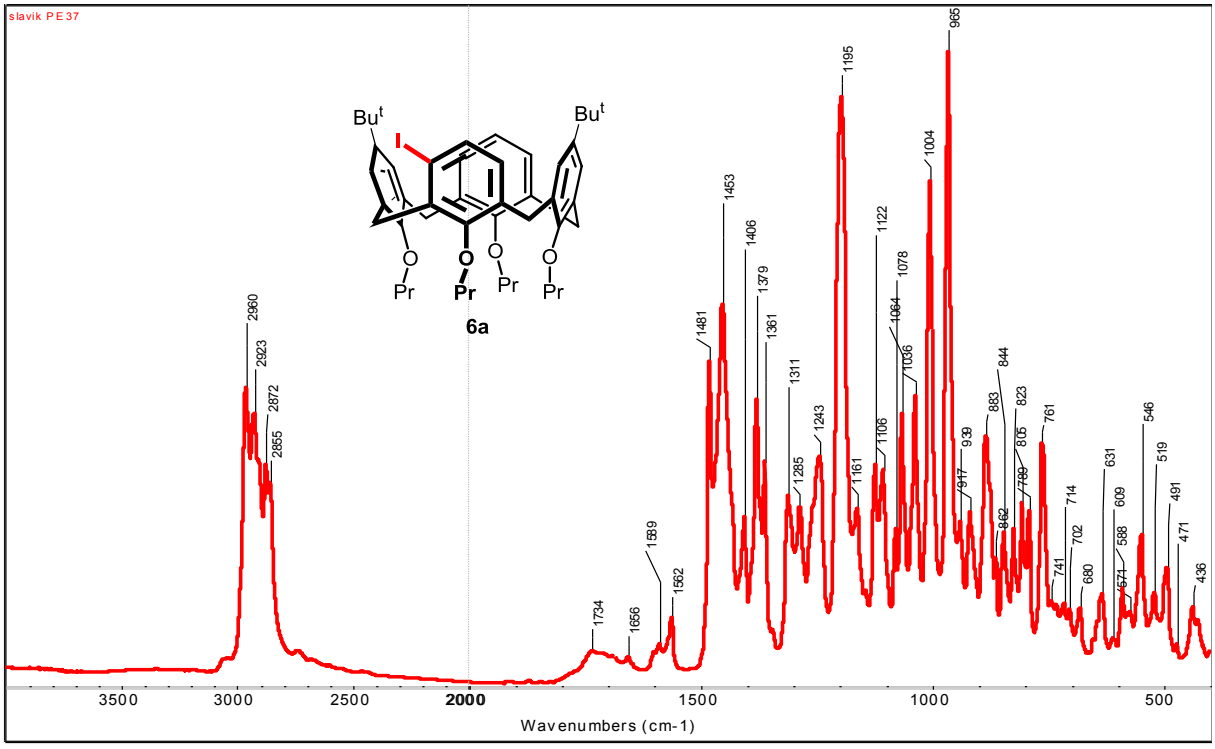
.

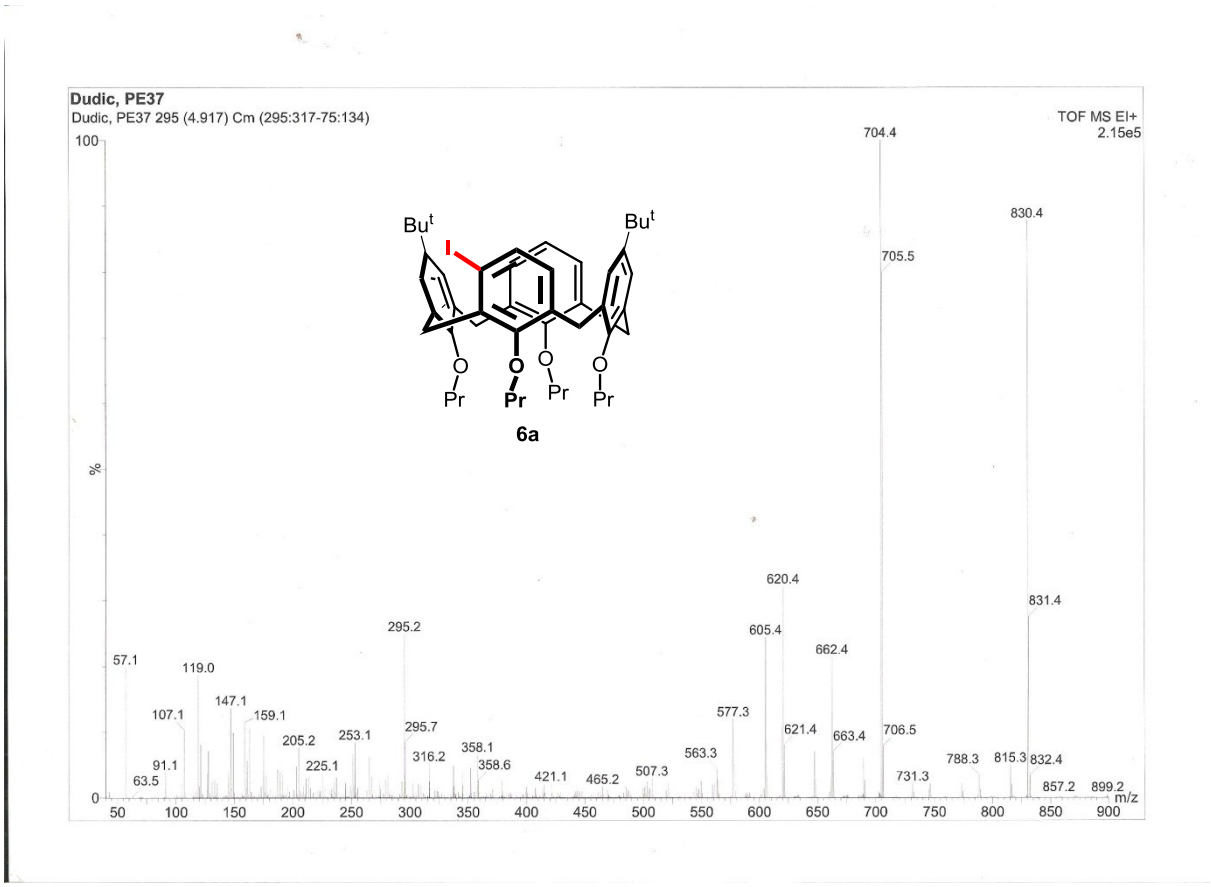
Compound 5‘


PE86-1
But
But
I
O
Pr
O
Pr
O
Pr
O
Pr
6a
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)


86UHLI
But
But
I
O
Pr
O
Pr
O
Pr
O
Pr
6a
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)

Compound 6a


slavik PE37
Bu^t
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
6a
2960
2923
2872
2855
1734
1656
1589
1562
1481
1453
1406
1379
1361
1311
1285
1243
1195
1161
1122
1106
1078
1064
1036
1004
965
939
917
883
862
844
823
805
788
761
741
714
702
680
671
631
609
588
546
519
491
471
436
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)


Dudic, PE37
Dudic, PE37 295 (4.917) Cm (295:317-75:134)
TOF MS EI+
2.15e5
100
%
0
Bu^t
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
6a
704.4
830.4
705.5
620.4
831.4
605.4
662.4
295.2
57.1
119.0
147.1
107.1
159.1
205.2
253.1
295.7
316.2
358.1
358.6
225.1
91.1
63.5
421.1
465.2
507.3
563.3
577.3
621.4
663.4
706.5
731.3
788.3
815.3
832.4
857.2
899.2
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
m/z

Compound 6a

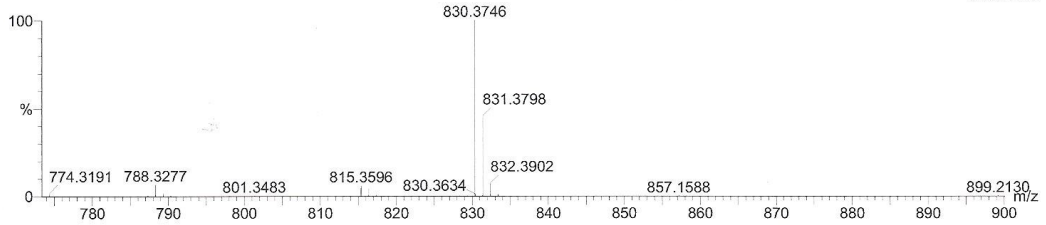
Elemental Composition Report Page 1

Single Mass Analysis (displaying only valid results)
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 500.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-48 H: 0-64 O: 0-4 I: 0-1

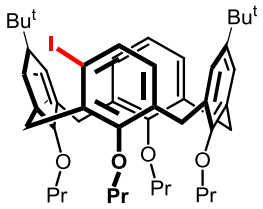
Dudic, PE37
Dudic, PE37 207 (3.450) Cm (191:207-110:157)

TOF MS EI+
8.10e+003

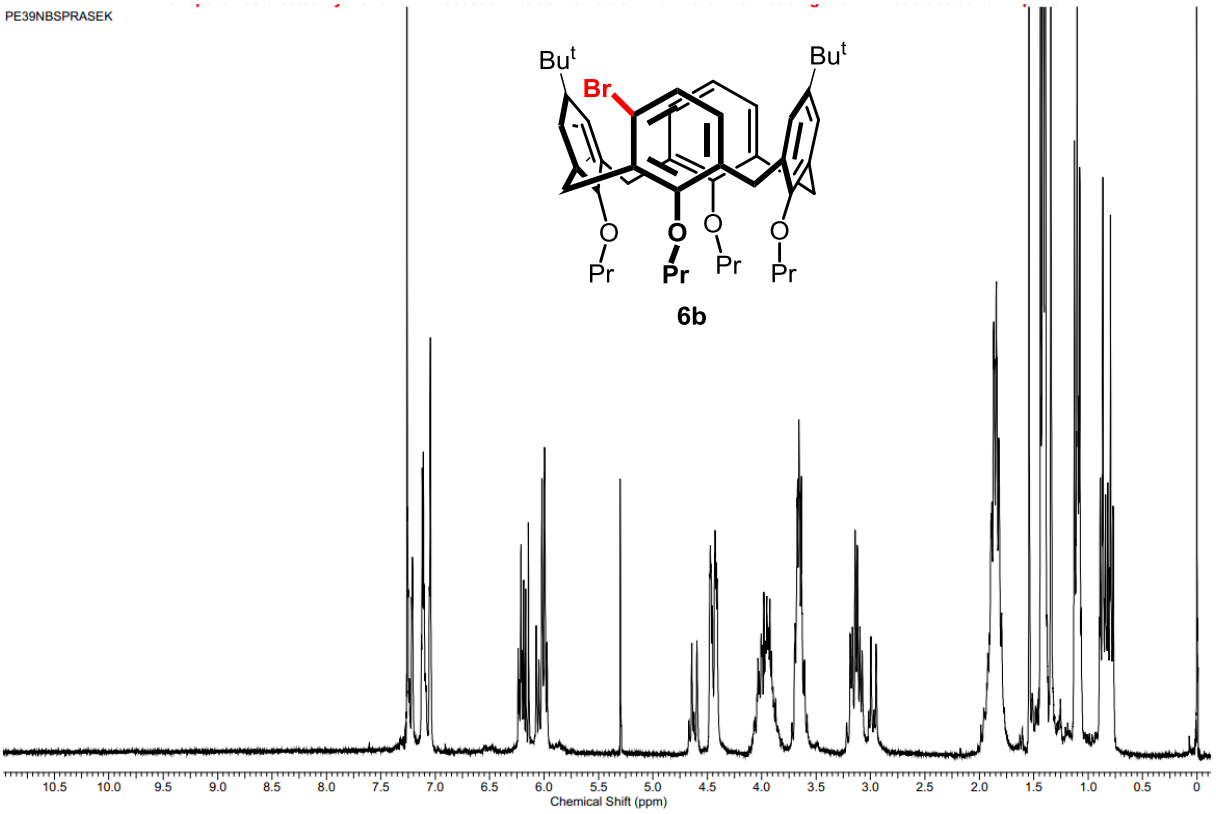


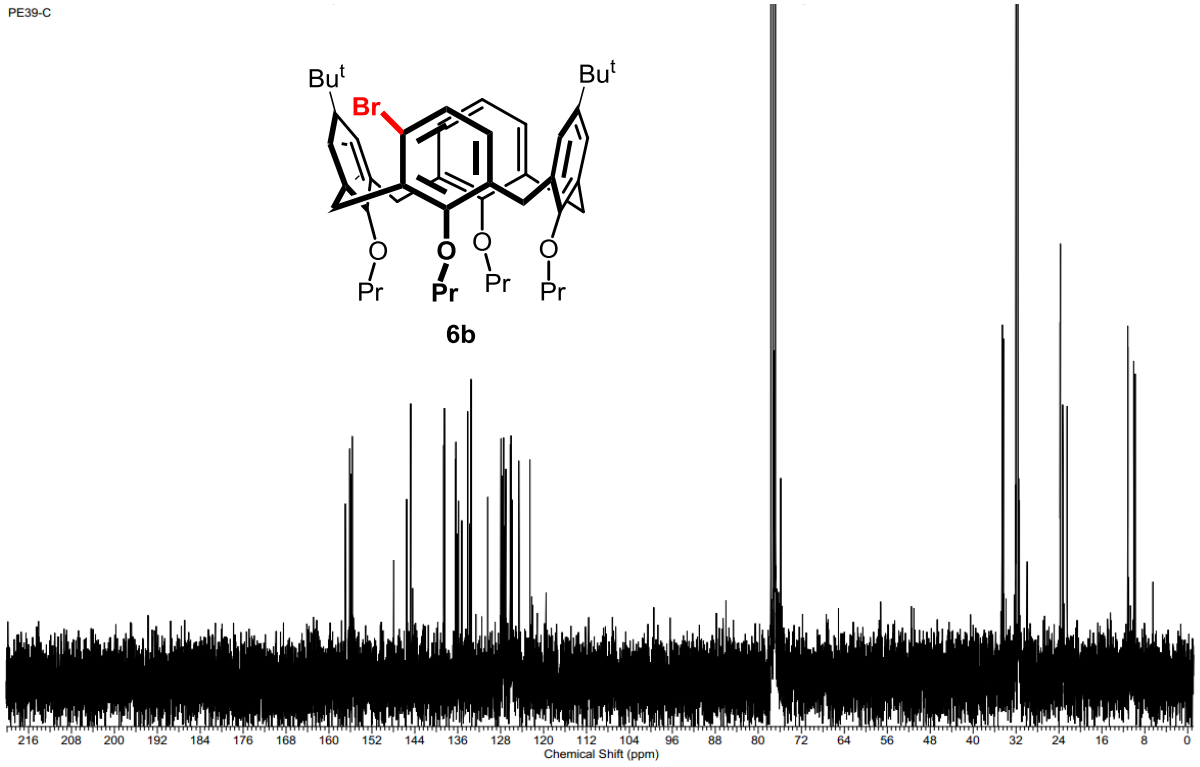
Minimum:				-10.0		
Maximum:		5.0	50.0	500.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
830.3746	830.3771	-2.5	-3.0	17.0	296.0	C48 H63 O4 I

Compound 6a

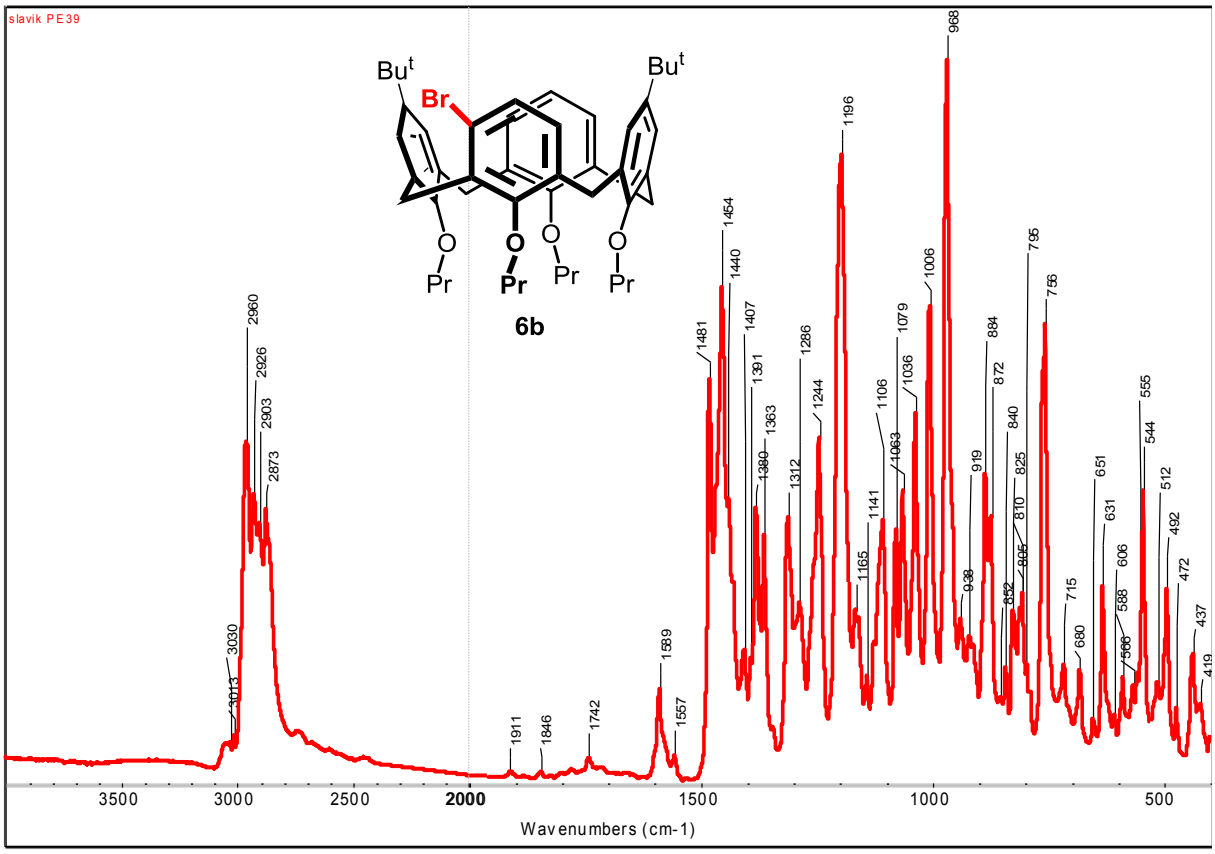


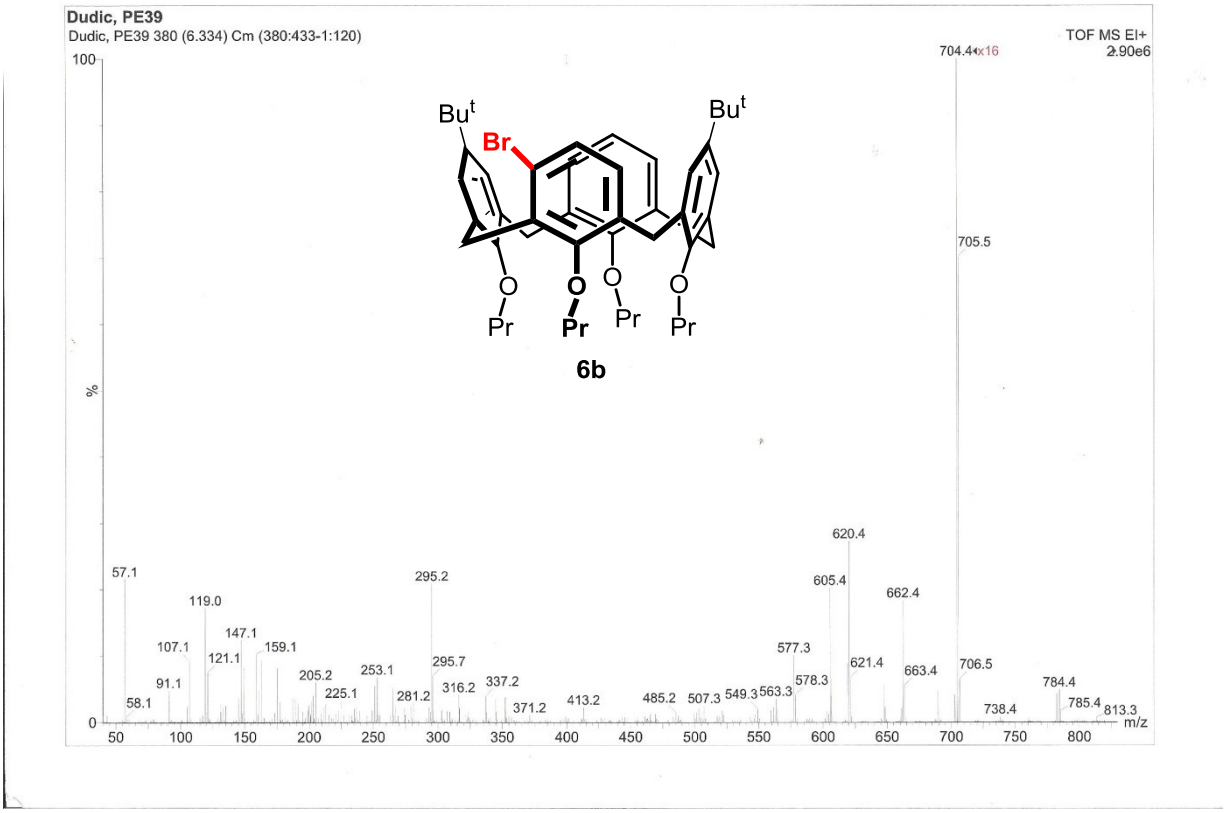
6a


PE39NBSPRASEK
Bu^t
Br
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
6b
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)


PE39-C
Bu^t
Br
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
6b
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)

Compound 6b


slavik PE39
Bu^t
Br
Bu^t
O
Pr
O
Pr
O
Pr
6b
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)


Dudic, PE39
Dudic, PE39 380 (6.334) Cm (380:433-1:120)
TOF MS EI+
2.90e6
704.4
705.5
Bu^t
Br
Bu^t
O
Pr
O
Pr
O
Pr
6b
%
m/z

Compound 6b

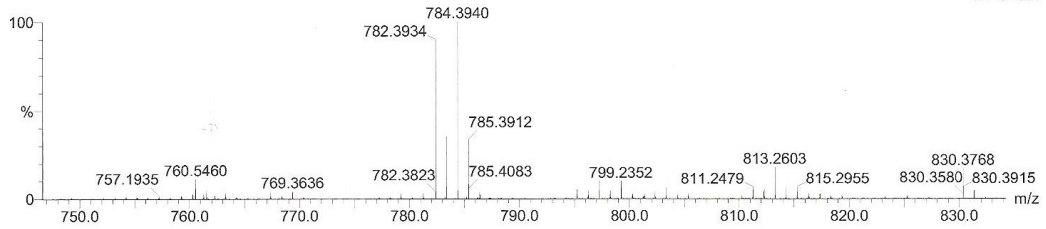
Elemental Composition Report Page 1

Single Mass Analysis (displaying only valid results)
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 500.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-48 H: 0-63 O: 0-4 Br: 0-1

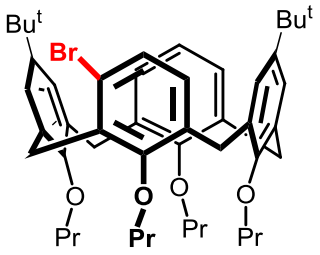
Dudic, PE39
Dudic, PE39 428 (7.134) Cm (405:429-21:103)

TOF MS EI+
4.24e+003

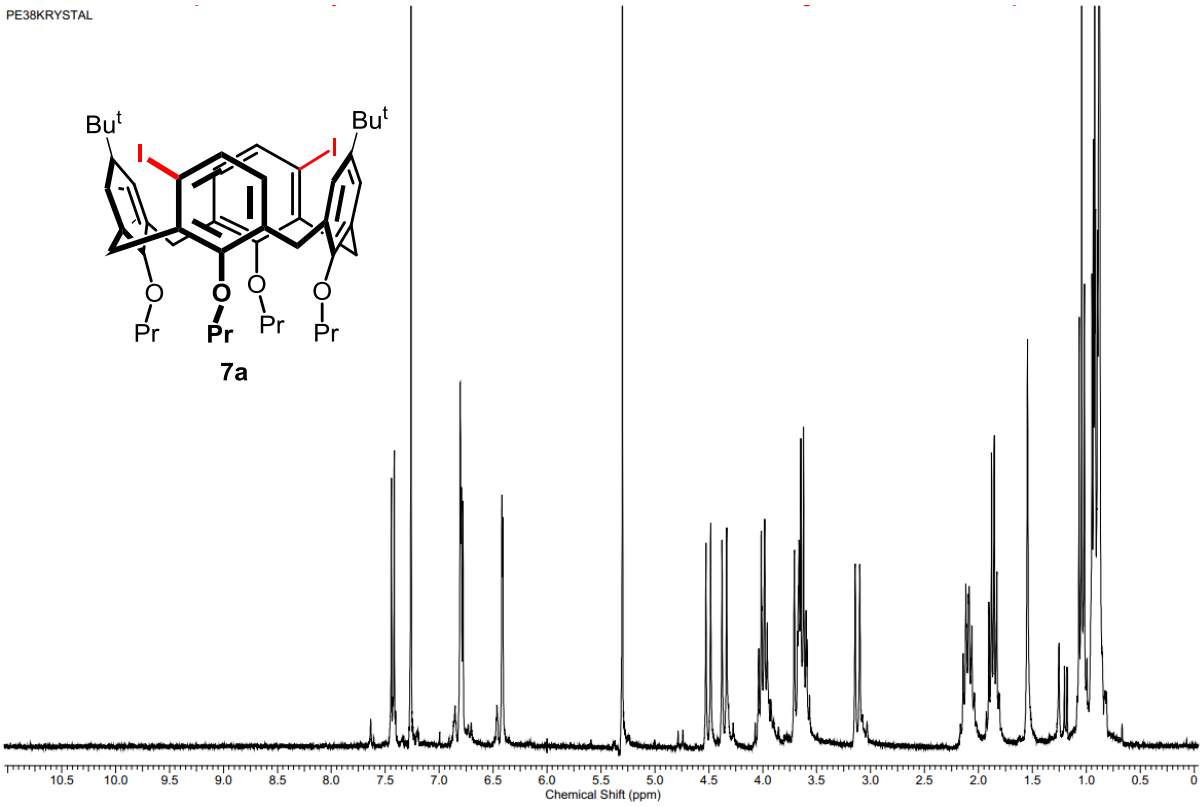


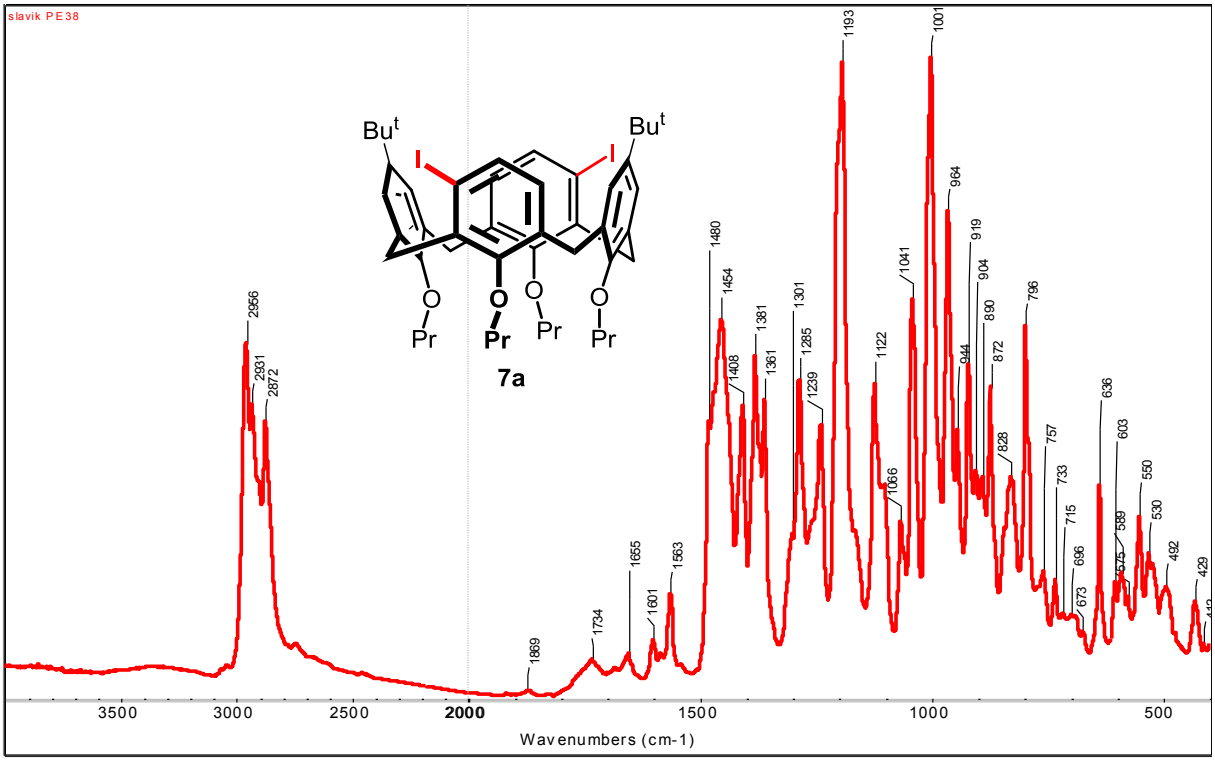
Minimum:				-10.0		
Maximum:		5.0	50.0	500.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
782.3934	782.3910	2.4	3.1	17.0	81.3	C48 H63 O4 Br

Compound 6b

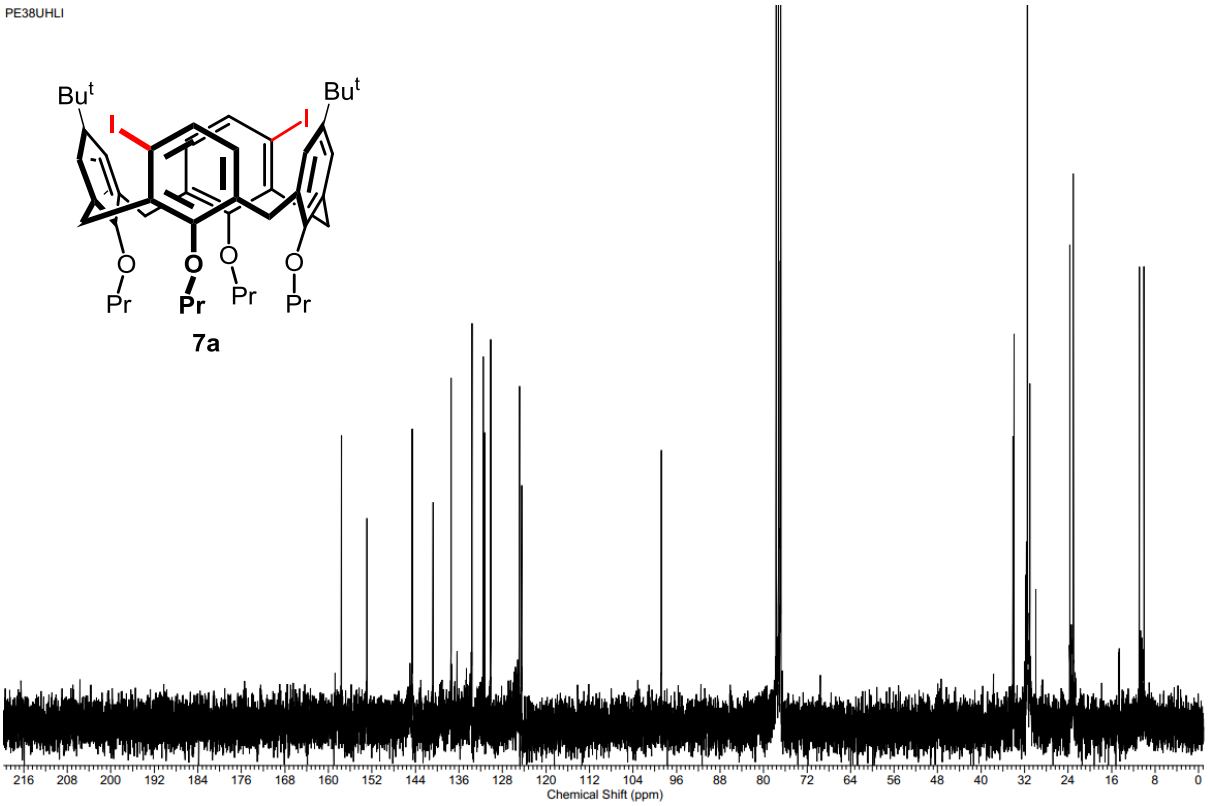


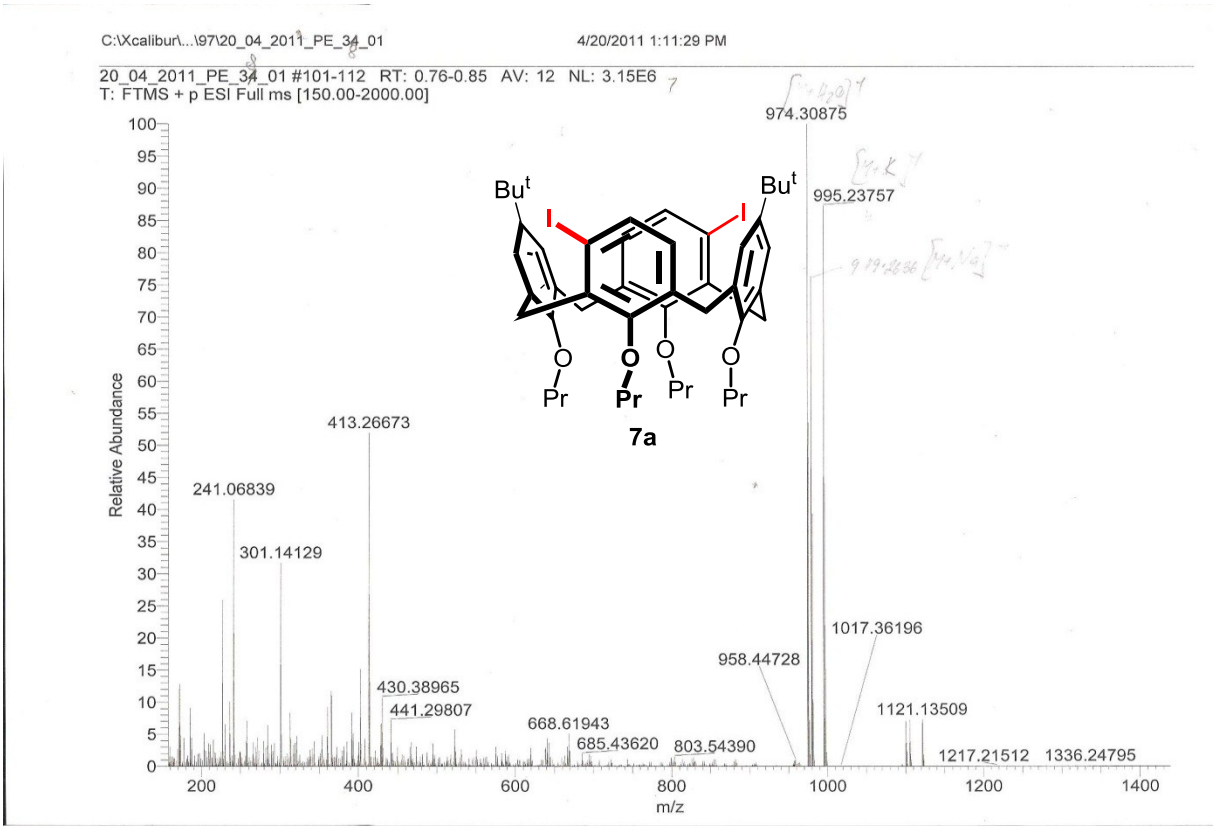
6b


PE38KRYSTAL
Bu^t
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
7a
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)

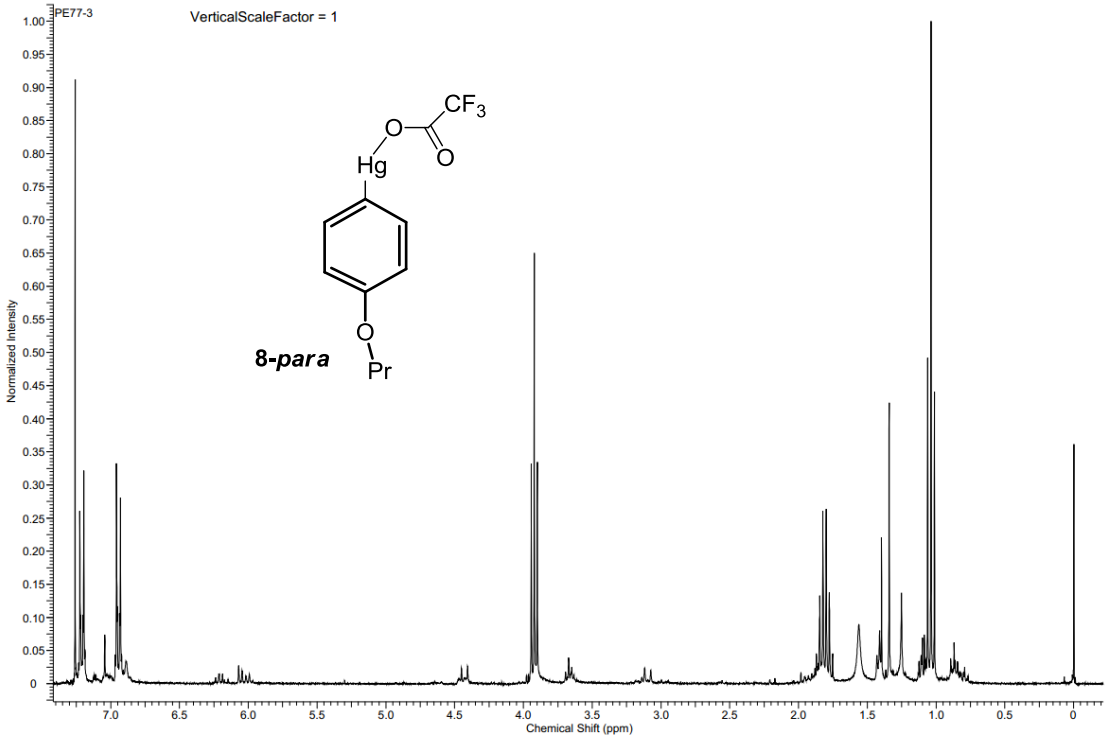

slavik PE38
Bu^t
Bu^t
O
Pr
O
Pr
O
Pr
O
Pr
7a
2956
2931
2872
1869
1734
1655
1601
1563
1480
1454
1408
1381
1361
1301
1285
1239
1193
1122
1066
1041
1001
964
944
919
904
890
872
828
796
757
733
715
696
673
636
603
589
575
550
530
492
429
3500 3000 2500 2000 1500 1000 500
Wavenumbers (cm-1)

Compound 7

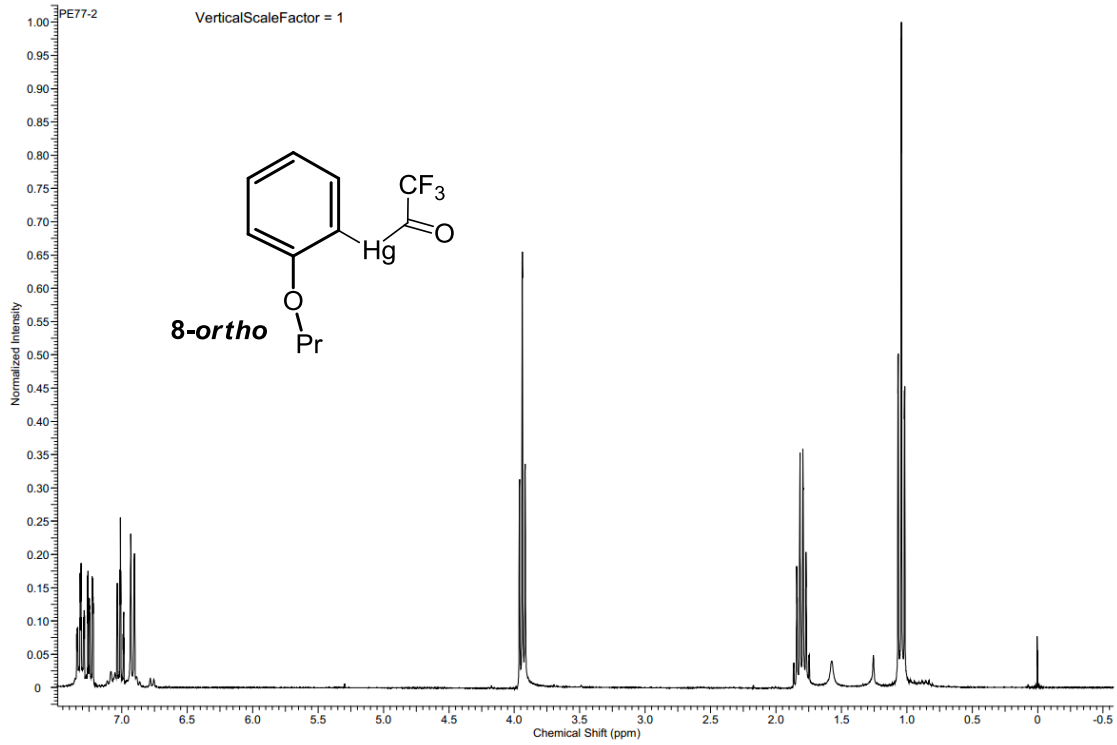

PE38UHLI
Bu^t
Bu^t
I
I
O
Pr
O
Pr
O
Pr
O
Pr
7a
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)


C:\Xcalibur\...\97\20_04_2011_PE_34_01
4/20/2011 1:11:29 PM
20_04_2011_PE_34_01 #101-112 RT: 0.76-0.85 AV: 12 NL: 3.15E6
T: FTMS + p ESI Full ms [150.00-2000.00]
Bu^t
Bu^t
I
I
O
Pr
O
Pr
O
Pr
O
Pr
7a
974.30875
995.23757
413.26673
241.06839
301.14129
1017.36196
958.44728
430.38965
441.29807
668.61943
685.43620
803.54390
1121.13509
1217.21512
1336.24795
Relative Abundance
m/z
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
200 400 600 800 1000 1200 1400

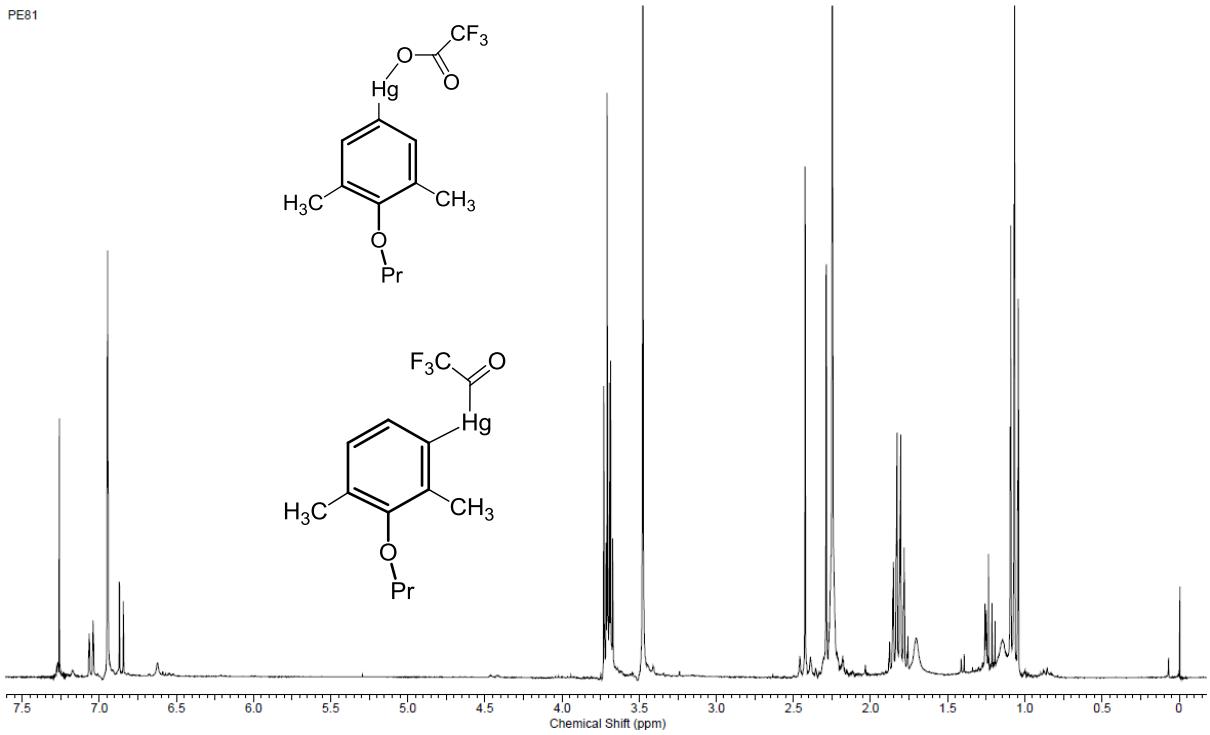
Compound 7a



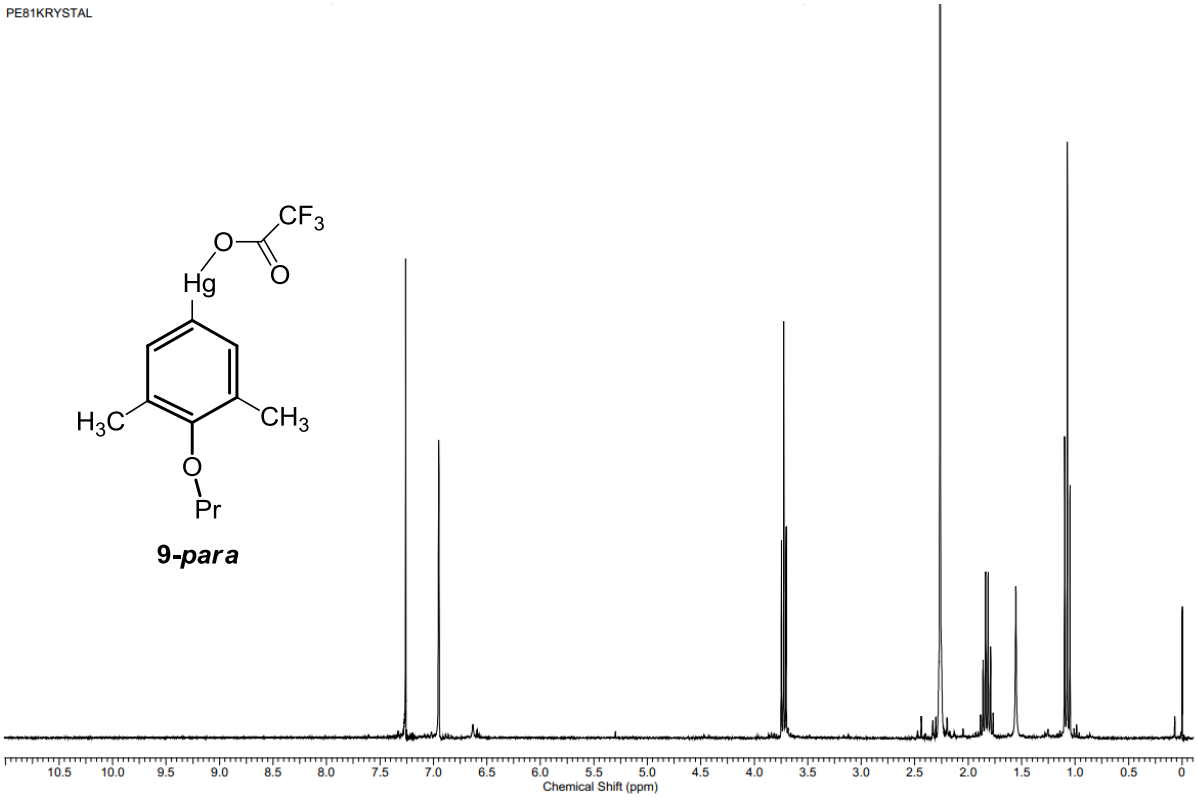
Compound 8-para



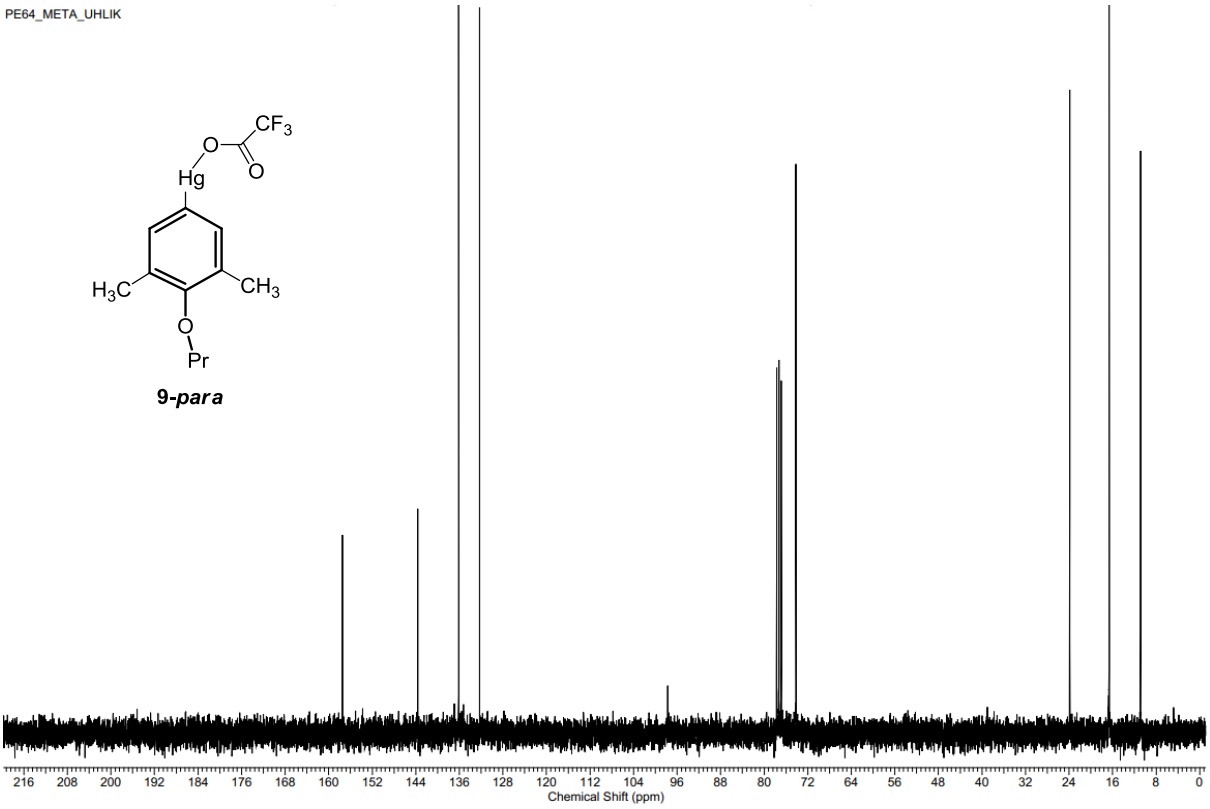
Compound 8-ortho

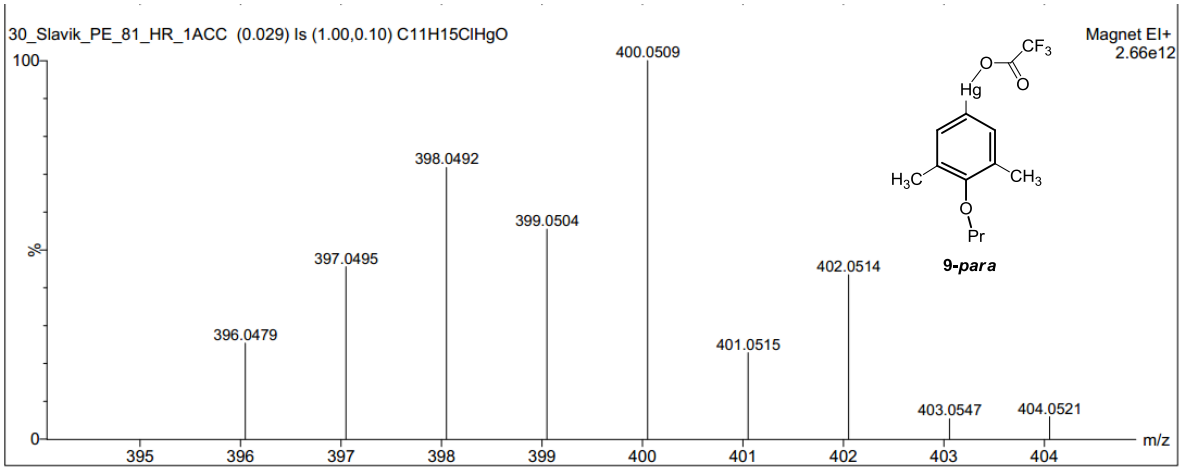


Mixture of 9-meta and 9-para isomers

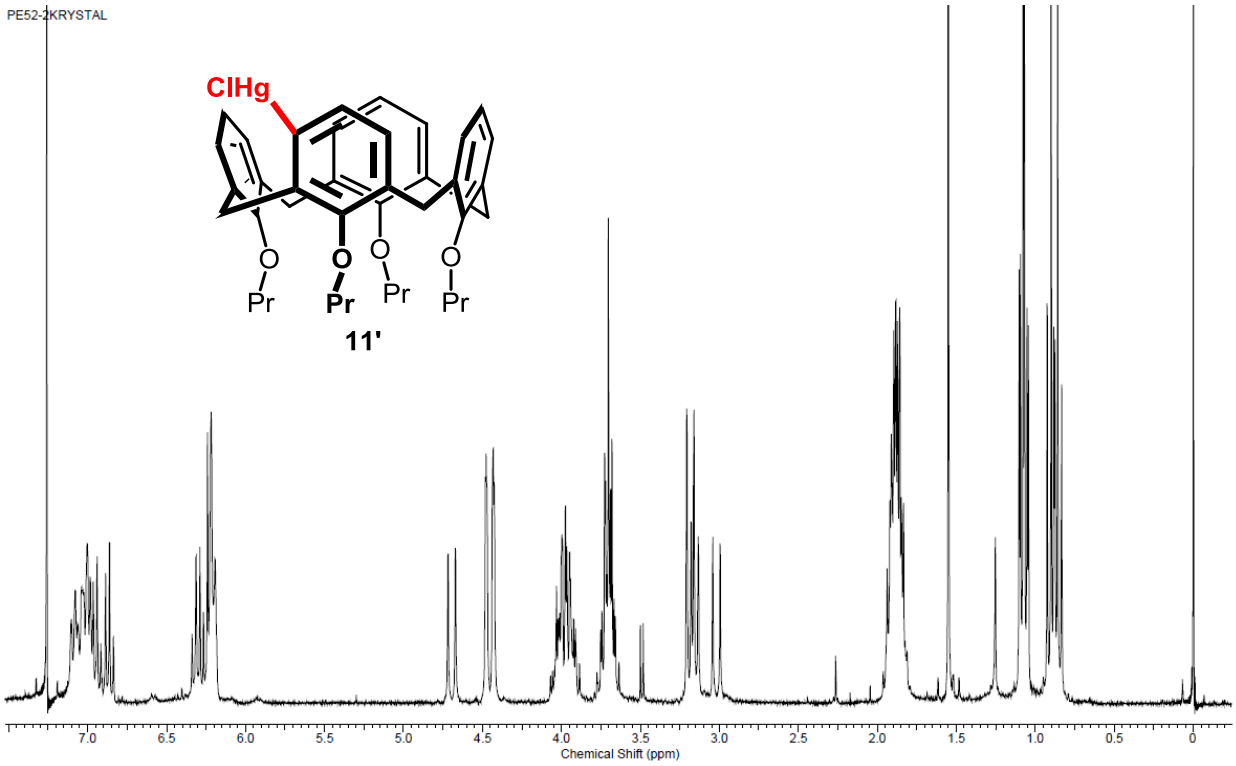


Pure isomer 9-para





Pure isomer 9-para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ClHg
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Pr
O
Pr
O
Pr
O
Pr
11'
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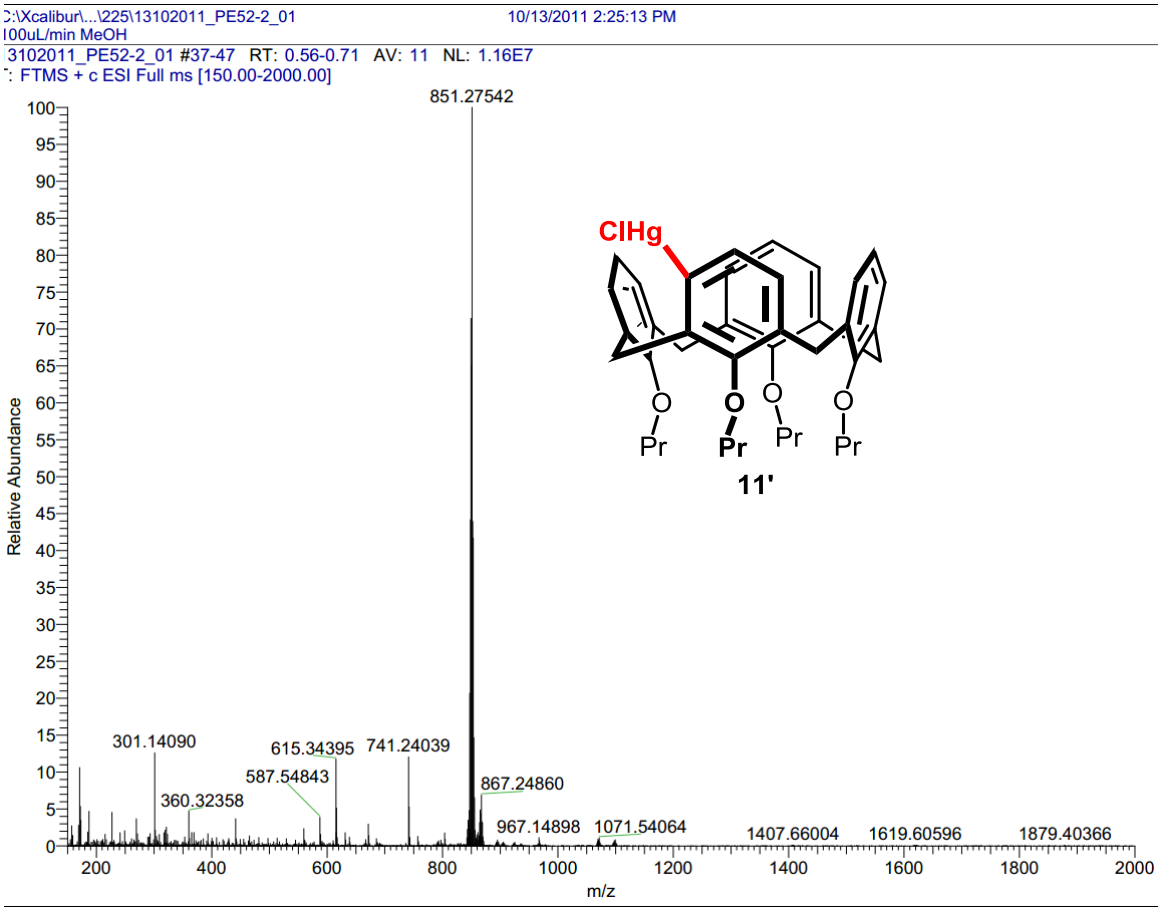
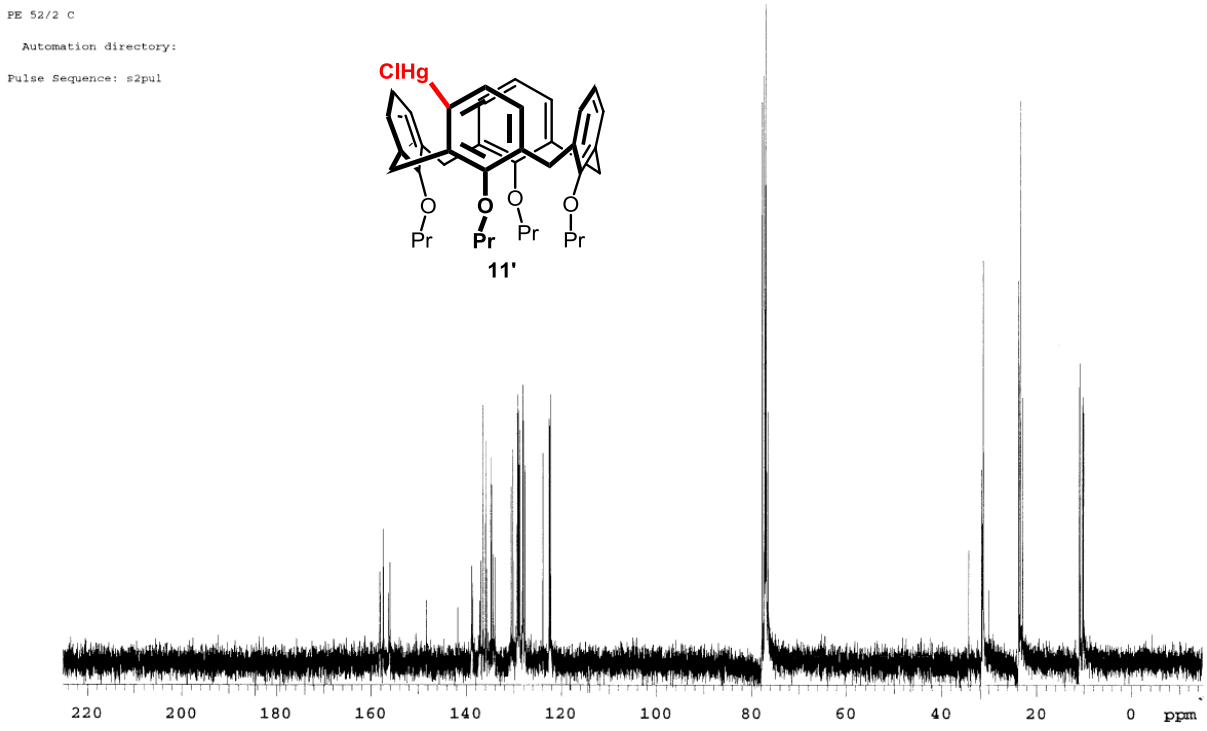
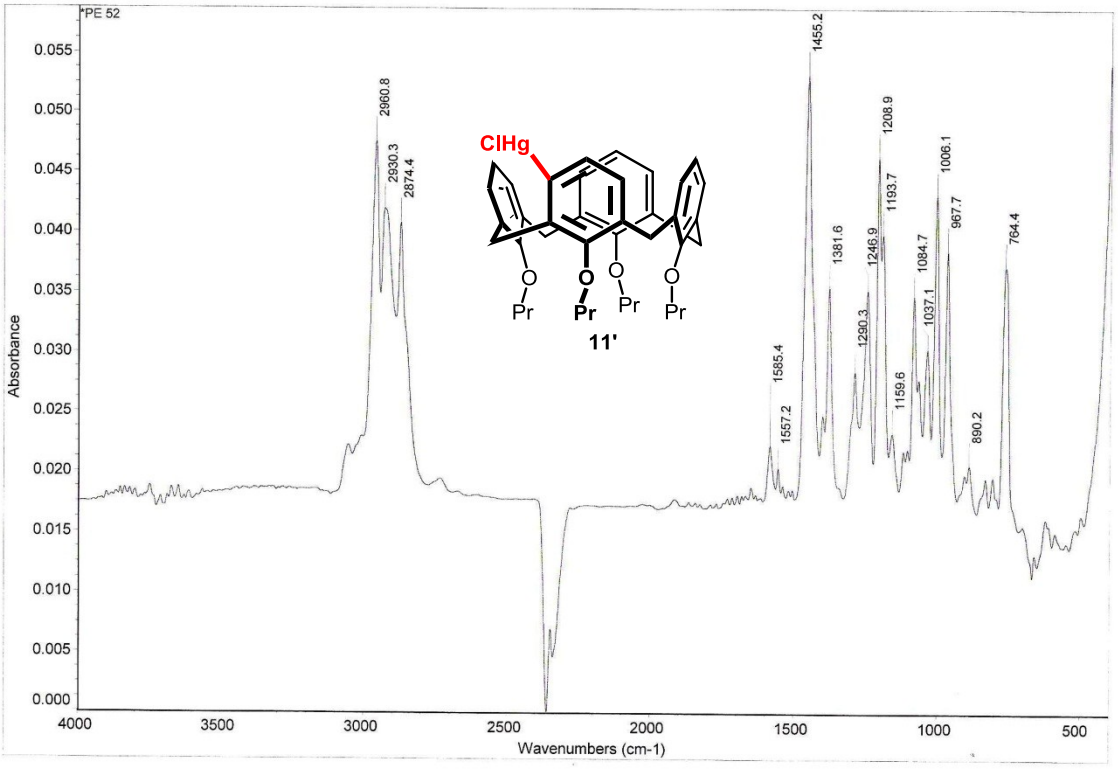
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)


C:\Xcalibur\...\225\13102011_PE52-2_01
10/13/2011 2:25:13 PM
100uL/min MeOH
13102011_PE52-2_01 #37-47 RT: 0.56-0.71 AV: 11 NL: 1.16E7
T: FTMS + c ESI Full ms [150.00-2000.00]
851.27542
ClHg
O
Pr
O
Pr
O
Pr
O
Pr
11'
Relative Abundance
301.14090
615.34395
741.24039
587.54843
867.24860
360.32358
967.14898
1071.54064
1407.66004
1619.60596
1879.40366
m/z

Compound 11‘

Compound 11‘


PE 52/2 C
Automation directory:
Pulse Sequence: s2pul
ClHg
O
Pr
11'
220
200
180
160
140
120
100
80
60
40
20
0
ppm


PE 52
Absorbance
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0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
2960.8
2930.3
2874.4
1455.2
1381.6
1585.4
1557.2
1290.3
1246.9
1208.9
1193.7
1159.6
1084.7
1037.1
1006.1
967.7
890.2
764.4
ClHg
11'
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

Crystallographic data

Diffraction data were collected at 150 K on a Nonius KappaCCD diffractometer (Enraf-Nonius) with the graphite monochromated Mo-Kα radiation. Cryostream Cooler (Oxford Cryosystem) was used for the low temperature measurements. The structures were solved by direct methods (SIR92[1], SHELXL97[2]) and refined by full-matrix least-squares on F^2 values (CRYSTALS[3]). ORTEP-3[4] and Accelrys DS Visualizer[5] were used for structure presentation.

The crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication. Copies of the data can be obtained free of charge on application to CCDC, e-mail: deposit@ccdc.cam.ac.uk.

X-ray of 5: $C_{52}H_{62}F_6Hg_2O_8$, M= 1330.2 g/mol, monoclinic system, space group *C2/c*, a=23.8873(6), b=16.1979(5), c=13.4171(4) Å, β=95.184(2)°, Z=4, V=5170.2(3) $Å^3$, Dc=1.71 $g.cm^{-3}$, μ(Mo Kα)=6.0 mm^{-1}, T=150 K, crystal dimensions of 0.1 x 0.1 x 0.1 mm. Half of the molecule was found in the asymmetric unit. All heavy atoms were refined anisotropically. Hydrogen atoms were localized from the expected geometry and difference electron density maps and were not refined. The structure converged to the final R=0.0313 and R_w=0.0363 using 3521 independent reflections (θ_{max}=27.5°) for 307 parameters. CCDC registration number 876019.

References

(1) Altomare, A.; Burla, M. C.; Camalli, M.; Cascarano, G.; Giacovazzo, C.; Guagliardi. A.; Polidori, G. *J. Appl. Crystallogr.*, **1994**, *27*, 435-435.

(2) Sheldrick, G. M.: SHELXL97. Program for Crystal Structure Refinement from Diffraction Data, University of Göttingen, Göttingen **1997**.

(3) Betteridge, P. W.; Carruthers, J. R.; Cooper, R. I.; Prout, K.; Watkin, D. J. *J. Appl. Cryst.* **2003**, 36, 1487.

(4) Farrugia L. J. *J. Appl. Cryst.* **1997**, *30*, 565.

(5) Accelrys Software Inc., Accelrys DS Visualizer version 1.7., www.accelrys.com, **2008**.

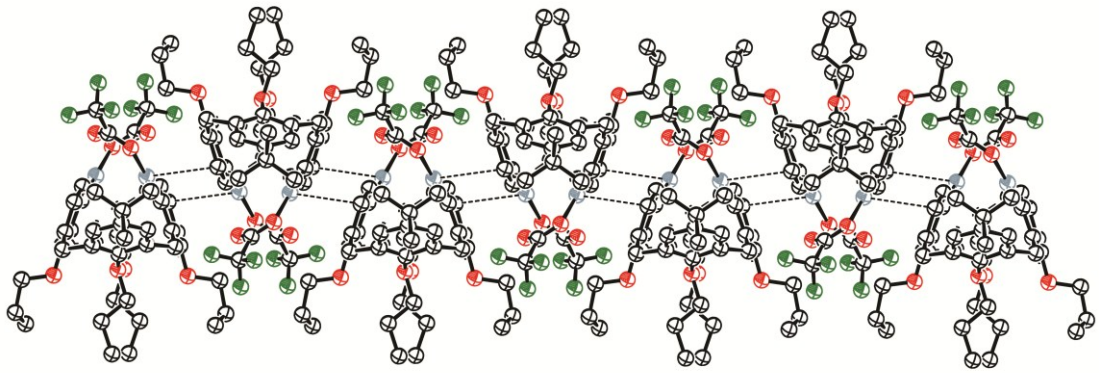

Figure S1. Molecular packing along [001] direction in the crystal structure of **5**. The intermolecular Hg-π interaction is represented by dashed line.

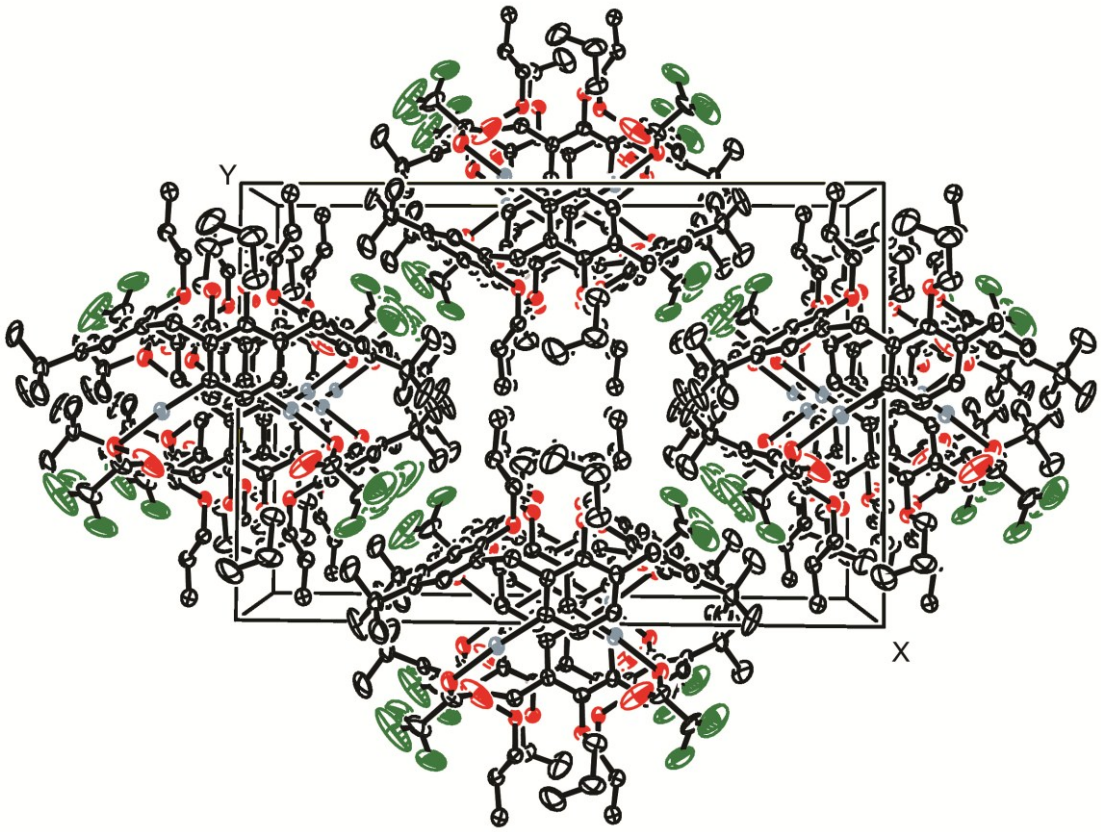

Figure S2. Molecular packing in the crystal structure of **5**; the XY plane.

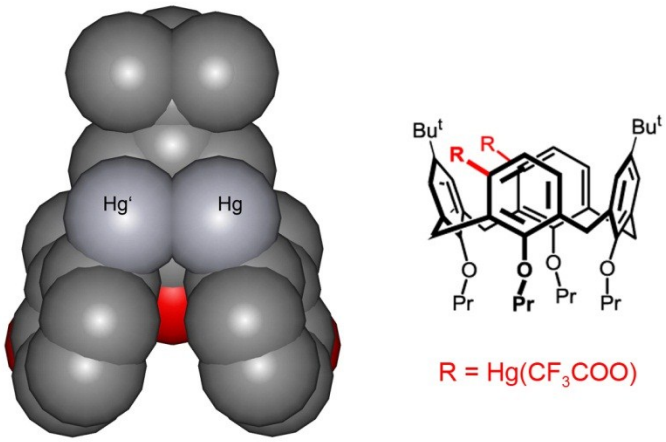

Figure S3. Computer simulation of the interference of two Hg atoms (van der Waals radii) in compound **5a** –possible explanation why this regioisomer does not formed in the mercuration reaction.

Theoretical calculations

Internal coordinates in standard MOPAC format.

meta-endo-in

```
scf done: -2563.348443

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 C    1.406485 1  121.106049 1    9.558606 1       4    3    2
 C    1.417924 1  118.789871 1   -3.465775 1       5    4    3
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 C    1.531604 1  111.544899 1   81.336960 1       8    7    3
 C    1.546130 1  110.709549 1  174.146866 1       9    8    7
 O    1.435896 1  118.337547 1   -5.335597 1       2    3    7
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 C    1.410313 1  122.366699 1  -11.154013 1      14   13   12
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 C    1.532615 1  110.875671 1  -71.247604 1      19   18   13
 C    1.546057 1  110.750839 1 -174.599060 1      20   19   18
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 O    2.482244 1  131.085739 1 -122.738838 1      22   17   12
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meta-endo-out

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 O    1.428481 1  118.400284 1 -175.197647 1      34   33   32
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 F    1.414896 1  109.196388 1  -70.238579 1      39   38   50
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 H    1.093694 1  119.002167 1    5.178627 1      33   34   41
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H    1.095047 1  121.370163 1 -171.415985 1      32   33   34
H    1.093721 1  120.035622 1   -1.735471 1      28   23   22
H    1.096295 1  120.507820 1  166.598389 1      16   17   12
H    1.094062 1  120.212418 1   -2.011098 1       5    4   41
H    1.102202 1  102.589256 1  170.559158 1      47   46   35
H    1.103061 1  109.374290 1   53.929089 1      47   46   35
H    1.102094 1  102.418861 1  171.085434 1      19   18   13
H    1.102351 1  109.511932 1   54.130703 1      19   18   13
H    1.093659 1  119.298370 1  179.804489 1      27   28   23
H    1.094112 1  119.322334 1  178.904343 1       6    5    4
H    1.100350 1  103.565613 1 -158.346481 1      43   42   24
H    1.107264 1  108.475739 1  -42.763168 1      43   42   24
H    1.094077 1  119.882111 1    1.577992 1       1    2   11
H    1.098683 1  103.531525 1 -161.101563 1       8    7    3
H    1.107144 1  108.293045 1  -46.010929 1       8    7    3
H    1.107097 1  109.892059 1   63.541473 1      20   19   18
H    1.105486 1  109.317802 1  -54.087261 1      20   19   18
H    1.105416 1  111.457741 1   60.260151 1      21   20   19
H    1.105443 1  111.590378 1  -60.653095 1      21   20   19
H    1.103352 1  110.325523 1  179.689499 1      21   20   19
H    1.107278 1  109.822929 1   64.377762 1      48   47   46
H    1.105678 1  109.207672 1  -53.035172 1      48   47   46
H    1.105436 1  111.401810 1   60.595943 1      49   48   47
H    1.105549 1  111.607689 1  -60.210205 1      49   48   47
H    1.103400 1  110.402519 1 -179.920166 1      49   48   47
H    1.104579 1  109.044029 1   51.832058 1      44   43   42
H    1.106639 1  109.857254 1  -64.698532 1      44   43   42
H    1.105883 1  111.717216 1   60.171646 1      45   44   43
H    1.106833 1  111.515381 1  -60.582024 1      45   44   43
H    1.103630 1  110.510017 1  179.781036 1      45   44   43
H    1.104424 1  109.280396 1   52.842209 1       9    8    7
H    1.106546 1  109.935555 1  -63.851463 1       9    8    7
H    1.105994 1  111.667076 1   60.113602 1      10    9    8
H    1.107159 1  111.551186 1  -60.529736 1      10    9    8
H    1.103694 1  110.567932 1  179.731033 1      10    9    8
H    1.097938 1  118.526672 1  -17.611359 1      31   30   29
H    1.094189 1  119.525948 1    0.642941 1      26   25   29
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meta-exo-in

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 C    1.431332 1    0.000000 0    0.000000 0       1    0    0
 C    1.456398 1  121.016510 1    0.000000 0       2    1    0
 C    1.449695 1  119.469116 1   -9.014670 1       3    2    1
 C    1.389907 1  119.082870 1    1.177751 1       4    3    2
 C    1.426917 1  120.781456 1    0.928131 1       5    4    3
 O    1.405202 1  118.869629 1  170.501175 1       2    3    4
 C    1.454770 1  111.822304 1  -46.117542 1       7    2    3
 C    1.416715 1  116.708908 1  -65.326073 1       8    7    2
 C    1.424389 1  118.203926 1  168.401138 1       9    8    7
 C    1.407918 1  120.364914 1   11.135006 1      10    9    8
 C    1.417533 1  119.384087 1   -3.978633 1      11   10    9
 C    1.417525 1  120.968803 1   -4.150561 1      12   11   10
 O    1.429155 1  118.140045 1 -168.025177 1      10    9    8
 C    1.453138 1  111.347809 1   63.152153 1      14   10    9
 C    1.427069 1  119.880836 1 -120.314606 1      15   14   10
 C    1.426169 1  116.538345 1  170.436340 1      16   15   14
 C    1.410723 1  121.573616 1    6.921006 1      17   16   15
 C    1.409619 1  120.120064 1   -1.904640 1      18   17   16
 C    1.410830 1  119.602097 1   -2.656628 1      19   18   17
 O    1.439106 1  119.860565 1 -173.392197 1      17   16   15
 C    1.422109 1  112.720192 1  123.385010 1      21   17   16
 C    1.411783 1  121.400475 1  120.654419 1      22   21   17
 C    1.417032 1  119.725929 1 -177.332153 1      23   22   21
 C    1.418915 1  121.378998 1    3.957962 1      24   23   22
 C    1.402965 1  117.495499 1   -4.127160 1      25   24   23
 C    1.418413 1  122.178352 1   -2.747977 1      26   25   24
 O    1.392921 1  121.376480 1  173.399811 1      27   22   23
 C    1.511293 1  112.327660 1 -106.948143 1      28   27   22
 C    1.531912 1  112.385323 1   76.215454 1      29   28   27
 C    1.545993 1  110.616989 1  175.146255 1      30   29   28
 O    1.457121 1  115.256599 1 -169.849411 1      26   27   22
 O    1.389470 1  119.449303 1    1.275846 1      16   17   21
 C    1.503112 1  116.765862 1  129.083878 1      33   16   17
 C    1.533899 1  111.611778 1  -71.492912 1      34   33   16
 C    1.545647 1  110.971954 1 -175.030380 1      35   34   33
 O    1.387234 1  121.610489 1    9.184915 1       9   10   14
 C    1.514222 1  112.595787 1   70.161194 1      37    9   10
 C    1.531889 1  110.875847 1   83.960518 1      38   37    9
 C    1.546000 1  110.882889 1  176.034836 1      39   38   37
Hg    2.395962 1   96.443588 1  -87.549652 1       3    2    7
 O    2.376492 1  158.707932 1  124.281723 1      41    3    2
 C    1.309224 1   91.127686 1  179.338837 1      42   41    3
 C    1.552873 1  116.965973 1 -178.572174 1      43   42   41
 F    1.396070 1  111.960281 1 -169.088257 1      44   43   42
 O    1.367862 1  117.500244 1    5.038253 1       1    2    7
 C    1.512411 1  120.502785 1  149.930328 1      46    1    2
 C    1.532738 1  111.440689 1  -63.670639 1      47   46    1
 C    1.546145 1  110.658974 1 -175.377884 1      48   47   46
 O    2.444489 1  144.393021 1  -56.476456 1      41    3    2
 F    1.407925 1  109.311249 1   46.843464 1      44   43   41
 F    1.401518 1  110.783371 1  -72.474129 1      44   43   41
 H    1.094725 1  118.943153 1   -2.920392 1      18   17   21
 H    1.093307 1  120.819160 1 -176.355164 1       5    4    3
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H    1.094728 1  119.172760 1 -176.576157 1      20   15   16
H    1.094155 1  119.654320 1 -174.806564 1       4    3    2
H    1.094231 1  119.404358 1   -3.713378 1      11   10   14
H    1.094492 1  120.208427 1 -177.336685 1      19   20   15
H    1.093763 1  120.914116 1  177.911133 1      25   26   27
H    1.094709 1  120.474846 1 -175.772614 1      13    8    9
H    1.101284 1  101.977661 1  177.275726 1      47   46    1
H    1.101714 1  109.312775 1   60.558399 1      47   46    1
H    1.103491 1  103.188179 1  169.238007 1      34   33   16
H    1.105149 1  109.394592 1   52.865997 1      34   33   16
H    1.094063 1  119.419083 1 -178.021790 1      12   13    8
H    1.094153 1  119.316116 1 -178.941498 1      24   23   22
H    1.098844 1  103.935265 1 -154.334229 1      38   37    9
H    1.105694 1  108.563583 1  -39.260399 1      38   37    9
H    1.094140 1  119.164734 1 -177.170990 1      23   22   27
H    1.099315 1  103.493889 1 -162.238571 1      29   28   27
H    1.108392 1  108.333092 1  -46.920826 1      29   28   27
H    1.107024 1  109.624481 1   63.630077 1      35   34   33
H    1.105770 1  109.056900 1  -53.346283 1      35   34   33
H    1.105823 1  111.394913 1   60.605412 1      36   35   34
H    1.105877 1  111.532333 1  -60.044621 1      36   35   34
H    1.103726 1  110.557350 1 -179.793655 1      36   35   34
H    1.108271 1  110.031769 1   63.959015 1      48   47   46
H    1.106173 1  109.414978 1  -54.124897 1      48   47   46
H    1.105147 1  111.382332 1   60.737701 1      49   48   47
H    1.105327 1  111.530518 1  -60.048332 1      49   48   47
H    1.103232 1  110.370438 1 -179.765060 1      49   48   47
H    1.106393 1  109.305626 1   54.036007 1      39   38   37
H    1.107006 1  109.778397 1  -62.561378 1      39   38   37
H    1.105743 1  111.545303 1   60.215603 1      40   39   38
H    1.106704 1  111.511871 1  -60.315498 1      40   39   38
H    1.103763 1  110.636841 1  179.912949 1      40   39   38
H    1.103965 1  109.062035 1   52.831890 1      30   29   28
H    1.106560 1  109.787682 1  -63.656013 1      30   29   28
H    1.106229 1  111.801857 1   60.597630 1      31   30   29
H    1.107230 1  111.519287 1  -60.118477 1      31   30   29
H    1.103757 1  110.500038 1 -179.734390 1      31   30   29
H    1.098727 1  117.196259 1   15.510961 1       3    2    7
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meta-exo-out

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 C    1.418677 1  120.314705 1    0.000000 0       2    1    0
 C    1.420815 1  118.514755 1  -11.400745 1       3    2    1
 C    1.406021 1  121.119896 1   11.711354 1       4    3    2
 C    1.417378 1  118.640015 1   -3.754976 1       5    4    3
 O    1.397025 1  121.217705 1  171.316284 1       3    2    1
 C    1.507399 1  111.971573 1 -109.608681 1       7    3    2
 C    1.533287 1  111.386871 1   82.656784 1       8    7    3
 C    1.545541 1  111.032394 1  176.030182 1       9    8    7
 O    1.435814 1  118.563187 1  -10.248104 1       2    3    7
 C    1.429272 1  111.252960 1  -67.974602 1      11    2    3
 C    1.425443 1  119.381088 1  129.307907 1      12   11    2
 C    1.424080 1  116.075058 1 -171.078705 1      13   12   11
 C    1.408238 1  123.089012 1   -8.674039 1      14   13   12
 C    1.408211 1  118.911591 1    3.237848 1      15   14   13
 C    1.408486 1  119.609161 1    3.010434 1      16   15   14
 O    1.390924 1  120.384666 1    2.169346 1      13   12   11
 C    1.503676 1  115.728661 1  121.193420 1      18   13   12
 C    1.533536 1  111.715630 1  -70.769279 1      19   18   13
 C    1.545615 1  111.094193 1 -175.608246 1      20   19   18
 O    1.467542 1  120.624451 1   -3.932563 1      14   13   18
 C    1.398160 1  112.271393 1 -118.081345 1      22   14   13
 C    1.433804 1  120.051865 1   47.830509 1      23   22   14
 C    1.415634 1  118.784348 1 -168.234528 1      24   23   22
 C    1.450261 1  120.243599 1  -13.475181 1      25   24   23
 C    1.454975 1  118.172401 1    4.935849 1      26   25   24
 C    1.397587 1  120.983292 1    2.747117 1      27   26   25
 O    1.403241 1  121.407158 1  173.519775 1      25   24   23
 C    1.458794 1  113.553749 1  -52.595249 1      29   25   24
 C    1.408582 1  116.885864 1  -61.162117 1      30   29   25
 C    1.407468 1  119.183907 1  179.052017 1      31   30   29
 C    1.409436 1  119.319275 1   -3.142668 1      32   31   30
 C    1.410912 1  120.803238 1    1.730721 1      33   32   31
 C    1.429013 1  121.238029 1    4.257940 1      34   33   32
 O    1.441977 1  118.484612 1 -173.503067 1      34   33   32
 O    1.375371 1  119.681900 1   -7.126396 1      24   25   29
 C    1.523845 1  112.523186 1 -110.232170 1      37   24   25
 C    1.530053 1  111.383614 1   73.167236 1      38   37   24
 C    1.546150 1  110.952499 1  172.906006 1      39   38   37
 O    1.387139 1  118.474152 1    1.720187 1      35   30   29
 C    1.506732 1  117.689987 1  139.139145 1      41   35   30
 C    1.533644 1  111.620956 1  -68.958824 1      42   41   35
 C    1.545839 1  110.838173 1 -176.697723 1      43   42   41
Hg    2.422990 1   93.060631 1   65.857246 1      26   25   29
 O    2.426907 1  148.733398 1   55.895058 1      45   26   25
 C    1.302487 1   89.302368 1  174.655334 1      46   45   26
 C    1.552787 1  117.366402 1  179.725174 1      47   46   45
 F    1.394015 1  112.458557 1 -177.990921 1      48   47   46
 O    2.404565 1  154.220444 1 -134.722153 1      45   26   25
 F    1.405801 1  109.839615 1 -118.584541 1      48   47   50
 F    1.406574 1  109.859276 1  122.519379 1      48   47   50
 H    1.093962 1  118.892410 1   -3.380810 1      17   12   11
 H    1.094155 1  118.646446 1    4.611719 1      33   34   36
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H    1.093879 1  118.911697 1   -1.265317 1      28   23   22
H    1.093802 1  120.179688 1  177.475372 1      16   17   12
H    1.094273 1  119.901024 1   -4.694245 1       5    4   36
H    1.101084 1  117.696632 1  -28.822298 1      26   25   29
H    1.103037 1  102.902916 1  171.705811 1      42   41   35
H    1.102874 1  109.131294 1   55.091835 1      42   41   35
H    1.102937 1  103.328331 1  169.606705 1      19   18   13
H    1.107765 1  109.305664 1   53.367859 1      19   18   13
H    1.094632 1  119.951347 1 -176.235382 1      27   28   23
H    1.094251 1  119.544800 1  178.788361 1       6    5    4
H    1.094267 1  102.593719 1 -165.159714 1      38   37   24
H    1.104954 1  108.470551 1  -50.889954 1      38   37   24
H    1.094351 1  119.320396 1    4.640792 1       1    2   11
H    1.102518 1  104.393211 1 -156.353806 1       8    7    3
H    1.106769 1  108.913910 1  -40.721828 1       8    7    3
H    1.107060 1  109.639420 1   62.947002 1      20   19   18
H    1.105422 1  108.861046 1  -53.849445 1      20   19   18
H    1.105714 1  111.447304 1   60.514938 1      21   20   19
H    1.105996 1  111.577438 1  -60.212044 1      21   20   19
H    1.103660 1  110.510345 1 -179.922775 1      21   20   19
H    1.107035 1  109.612892 1   62.228985 1      43   42   41
H    1.106614 1  109.381180 1  -55.128414 1      43   42   41
H    1.105711 1  111.477303 1   60.377609 1      44   43   42
H    1.105428 1  111.399353 1  -60.266788 1      44   43   42
H    1.103637 1  110.565552 1 -179.948853 1      44   43   42
H    1.104378 1  109.079445 1   50.316254 1      39   38   37
H    1.113059 1  110.033356 1  -67.546394 1      39   38   37
H    1.105556 1  111.708527 1   57.581417 1      40   39   38
H    1.106141 1  111.160507 1  -62.856060 1      40   39   38
H    1.103227 1  110.428246 1  177.300842 1      40   39   38
H    1.106154 1  109.266785 1   53.779984 1       9    8    7
H    1.106279 1  109.481483 1  -62.428795 1       9    8    7
H    1.105920 1  111.576767 1   60.250122 1      10    9    8
H    1.107124 1  111.543243 1  -60.357353 1      10    9    8
H    1.103764 1  110.633110 1  179.935791 1      10    9    8
H    1.094819 1  119.687820 1   -2.495684 1      31   30   29
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para-endo-in

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scf done: -2563.348255

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 C    1.408065 1    0.000000 0    0.000000 0       1    0    0
 C    1.418562 1  120.626701 1    0.000000 0       2    1    0
 C    1.420850 1  118.816101 1   -8.030765 1       3    2    1
 C    1.406291 1  121.063835 1    8.207994 1       4    3    2
 C    1.416850 1  118.617607 1   -2.619855 1       5    4    3
 O    1.395416 1  120.882416 1  173.975204 1       3    2    1
 C    1.510301 1  112.282791 1 -102.661552 1       7    3    2
 C    1.532493 1  112.521408 1   79.115753 1       8    7    3
 C    1.546130 1  110.584106 1  174.164520 1       9    8    7
 O    1.440005 1  117.874260 1   -5.390749 1       2    3    7
 C    1.419877 1  112.540649 1  -69.138313 1      11    2    3
 C    1.438074 1  119.716988 1  127.656059 1      12   11    2
 C    1.441579 1  116.791588 1 -169.532471 1      13   12   11
 C    1.403386 1  121.704163 1  -11.988162 1      14   13   12
 C    1.425421 1  120.021111 1    4.045387 1      15   14   13
 C    1.437265 1  118.927605 1    3.375767 1      16   15   14
 O    1.363288 1  117.562294 1    6.255542 1      13   12   11
 C    1.513728 1  120.300034 1  144.871933 1      18   13   12
 C    1.532537 1  110.539787 1  -72.397057 1      19   18   13
 C    1.546151 1  110.516281 1 -174.818527 1      20   19   18
 O    1.433208 1  119.927101 1   -8.972165 1      14   13   18
 C    1.443720 1  111.900101 1 -119.145317 1      22   14   13
 C    1.419019 1  117.291718 1   63.244087 1      23   22   14
 C    1.416929 1  118.904114 1 -172.275452 1      24   23   22
 C    1.408169 1  120.668877 1   -8.062214 1      25   24   23
 C    1.417228 1  118.930252 1    2.323311 1      26   25   24
 C    1.417559 1  121.275185 1    3.503415 1      27   26   25
 O    1.437380 1  117.640137 1  172.938461 1      25   24   23
 C    1.419489 1  112.722382 1  -67.174278 1      29   25   24
 C    1.404323 1  119.454529 1  -53.786045 1      30   29   25
 C    1.430414 1  120.486717 1  179.190781 1      31   30   29
 C    1.433223 1  118.948769 1   -3.689832 1      32   31   30
 C    1.405463 1  120.014168 1    1.885417 1      33   32   31
 C    1.437673 1  121.292519 1    6.805592 1      34   33   32
 O    1.434075 1  118.369186 1 -171.650208 1      34   33   32
 O    1.394383 1  120.577835 1   -4.947375 1      24   25   29
 C    1.511514 1  112.251480 1 -103.741875 1      37   24   25
 C    1.532194 1  112.518105 1   77.083466 1      38   37   24
 C    1.546347 1  110.479828 1  174.820038 1      39   38   37
 O    1.363628 1  117.510628 1    6.575437 1      35   30   29
 C    1.514226 1  119.685257 1  148.471909 1      41   35   30
 C    1.526382 1  106.579094 1 -165.670425 1      42   41   35
 C    1.546177 1  110.702141 1  178.304581 1      43   42   41
Hg    2.516208 1   91.346138 1  105.027878 1      32   33   34
 O    2.464548 1   96.841095 1  117.202652 1      45   32   33
 C    1.302785 1   90.181152 1 -109.102531 1      46   45   32
 C    1.552960 1  117.453278 1 -178.539383 1      47   46   45
 F    1.401363 1  111.980141 1 -155.234024 1      48   47   46
 O    2.475543 1  109.655289 1   61.339661 1      45   32   33
 F    1.413089 1  109.297737 1  -93.083275 1      48   47   50
 F    1.400483 1  111.922791 1  147.408401 1      48   47   50
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 H    1.095237 1  119.084709 1    9.141784 1      33   34   36
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H    1.094366 1  119.107193 1    6.843694 1      15   14   22
H    1.098130 1  119.966492 1 -164.410324 1      32   33   34
H    1.094131 1  120.109055 1   -1.964415 1      28   23   22
H    1.097934 1  119.757004 1  163.930756 1      16   17   12
H    1.094092 1  120.106445 1   -1.973571 1       5    4   36
H    1.101363 1  109.052406 1   72.352692 1      42   41   35
H    1.106746 1  107.366249 1  -45.697823 1      42   41   35
H    1.101945 1  102.476654 1  168.783157 1      19   18   13
H    1.101789 1  109.480499 1   51.647373 1      19   18   13
H    1.094141 1  119.348961 1  178.803284 1      27   28   23
H    1.093851 1  119.355423 1  179.531937 1       6    5    4
H    1.099523 1  103.518745 1 -161.506943 1      38   37   24
H    1.107626 1  108.353394 1  -46.054581 1      38   37   24
H    1.094144 1  119.810837 1    1.858783 1       1    2   11
H    1.100860 1  103.674950 1 -159.446091 1       8    7    3
H    1.108067 1  108.416374 1  -43.776749 1       8    7    3
H    1.107248 1  109.814102 1   64.196533 1      20   19   18
H    1.105505 1  109.347984 1  -53.402416 1      20   19   18
H    1.105409 1  111.464737 1   60.687851 1      21   20   19
H    1.105470 1  111.630783 1  -60.244686 1      21   20   19
H    1.103363 1  110.282883 1 -179.904404 1      21   20   19
H    1.105170 1  109.367142 1   56.677174 1      43   42   41
H    1.106747 1  109.379486 1  -60.412964 1      43   42   41
H    1.105615 1  111.696617 1   59.847813 1      44   43   42
H    1.105351 1  111.489258 1  -61.030674 1      44   43   42
H    1.103206 1  110.279922 1  179.540421 1      44   43   42
H    1.104182 1  109.303299 1   52.534611 1      39   38   37
H    1.106437 1  109.923347 1  -64.145668 1      39   38   37
H    1.105974 1  111.658539 1   59.881294 1      40   39   38
H    1.107131 1  111.567039 1  -60.784828 1      40   39   38
H    1.103753 1  110.552864 1  179.469528 1      40   39   38
H    1.104402 1  109.254242 1   51.796097 1       9    8    7
H    1.106293 1  109.828072 1  -64.664658 1       9    8    7
H    1.106047 1  111.678177 1   59.549400 1      10    9    8
H    1.107095 1  111.587463 1  -61.158318 1      10    9    8
H    1.103671 1  110.533875 1  179.121613 1      10    9    8
H    1.094506 1  118.968491 1   -4.606179 1      31   30   29
H    1.094182 1  119.809906 1    1.943289 1      26   25   29
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para-endo-out

```
scf done: -2563.348409

 C    0.000000 0    0.000000 0    0.000000 0       0    0    0
 C    1.411743 1    0.000000 0    0.000000 0       1    0    0
 C    1.426025 1  120.347527 1    0.000000 0       2    1    0
 C    1.428822 1  118.742729 1   -8.654341 1       3    2    1
 C    1.406705 1  120.873009 1    9.398847 1       4    3    2
 C    1.418183 1  118.803093 1   -3.484073 1       5    4    3
 O    1.388997 1  120.636528 1  172.712830 1       3    2    1
 C    1.513204 1  112.854263 1 -106.916656 1       7    3    2
 C    1.531671 1  111.664146 1   80.497009 1       8    7    3
 C    1.546080 1  110.682701 1  173.735397 1       9    8    7
 O    1.434781 1  118.275787 1   -4.875767 1       2    3    7
 C    1.423691 1  113.634247 1  -68.977196 1      11    2    3
 C    1.425757 1  120.397972 1  124.856018 1      12   11    2
 C    1.442129 1  116.147469 1 -169.099930 1      13   12   11
 C    1.411246 1  122.330444 1  -10.874436 1      14   13   12
 C    1.407864 1  119.923622 1    2.572543 1      15   14   13
 C    1.434541 1  119.069084 1    4.406833 1      16   15   14
 O    1.371282 1  118.552208 1    5.014146 1      13   12   11
 C    1.510880 1  119.080612 1  139.717941 1      18   13   12
 C    1.532513 1  111.062500 1  -72.381844 1      19   18   13
 C    1.546135 1  110.608391 1 -175.390533 1      20   19   18
Hg    2.568629 1  109.933594 1   76.764275 1      17   12   11
 O    2.473186 1  131.850418 1 -123.213760 1      22   17   12
 C    1.300874 1   90.786705 1  -21.745092 1      23   22   17
 C    1.551447 1  117.469070 1  172.899857 1      24   23   22
 F    1.419304 1  108.563568 1  -83.857536 1      25   24   23
 O    1.428994 1  119.254463 1   -6.473829 1      14   13   18
 C    1.444433 1  111.934418 1 -120.628174 1      27   14   13
 C    1.417883 1  116.679031 1   64.102524 1      28   27   14
 C    1.415645 1  118.857071 1 -171.761002 1      29   28   27
 C    1.407437 1  120.791100 1   -8.186509 1      30   29   28
 C    1.417743 1  118.794067 1    2.245154 1      31   30   29
 C    1.417903 1  121.329651 1    3.656619 1      32   31   30
 O    1.437615 1  117.020172 1  172.776917 1      30   29   28
 C    1.415049 1  112.992828 1  -66.161789 1      34   30   29
 C    1.407887 1  119.718307 1  -50.776669 1      35   34   30
 C    1.416646 1  120.230820 1 -178.922943 1      36   35   34
 C    1.433815 1  119.208809 1   -5.062026 1      37   36   35
 C    1.415285 1  119.818985 1    0.689116 1      38   37   36
 C    1.427148 1  121.295097 1    8.861909 1      39   38   37
 O    1.440933 1  117.509521 1 -168.250626 1      39   38   37
 O    1.392468 1  120.404076 1   -4.824395 1      29   30   34
 C    1.511634 1  112.430031 1 -105.853455 1      42   29   30
 C    1.532049 1  112.220406 1   77.233673 1      43   42   29
 C    1.546474 1  110.590714 1  174.930527 1      44   43   42
 O    1.368501 1  117.616463 1    4.454436 1      40   35   34
 C    1.511649 1  119.035316 1  148.266266 1      46   40   35
 C    1.526646 1  106.651901 1 -167.800095 1      47   46   40
 C    1.546024 1  110.813774 1  177.950928 1      48   47   46
 O    2.498064 1   79.807114 1 -142.788071 1      22   17   12
 F    1.397670 1  112.532967 1  -26.031986 1      25   24   50
 F    1.399585 1  112.120956 1 -148.062256 1      25   24   50
 H    1.097802 1  118.535446 1  -17.563179 1      17   12   11
 H    1.096277 1  119.341438 1   16.888636 1      38   39   41
```

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H    1.093726 1  118.956261 1    5.025378 1      15   14   27
H    1.096420 1  119.660347 1 -170.679138 1      37   38   39
H    1.094083 1  120.200706 1   -2.220456 1      33   28   27
H    1.095223 1  119.575699 1  172.483978 1      16   17   12
H    1.093801 1  119.995415 1   -1.912385 1       5    4   41
H    1.102083 1  109.131882 1   70.344162 1      47   46   40
H    1.107068 1  107.443924 1  -47.822277 1      47   46   40
H    1.102417 1  102.611786 1  168.603561 1      19   18   13
H    1.102958 1  109.426826 1   51.976475 1      19   18   13
H    1.094109 1  119.330025 1  178.861664 1      32   33   28
H    1.093754 1  119.393822 1  179.870865 1       6    5    4
H    1.099060 1  103.478775 1 -161.158478 1      43   42   29
H    1.107217 1  108.348976 1  -46.008678 1      43   42   29
H    1.094018 1  119.592308 1    0.291534 1       1    2   11
H    1.100429 1  103.663361 1 -158.204697 1       8    7    3
H    1.107421 1  108.464027 1  -42.563572 1       8    7    3
H    1.107392 1  109.811882 1   63.566307 1      20   19   18
H    1.105576 1  109.339462 1  -53.881786 1      20   19   18
H    1.105512 1  111.456543 1   60.738716 1      21   20   19
H    1.105524 1  111.589012 1  -60.085831 1      21   20   19
H    1.103372 1  110.386848 1 -179.796555 1      21   20   19
H    1.105165 1  109.268066 1   56.286827 1      48   47   46
H    1.106952 1  109.345329 1  -60.705769 1      48   47   46
H    1.105707 1  111.662659 1   59.693302 1      49   48   47
H    1.105389 1  111.469337 1  -61.100128 1      49   48   47
H    1.103175 1  110.350426 1  179.440628 1      49   48   47
H    1.104248 1  109.239426 1   52.599495 1      44   43   42
H    1.106563 1  109.871162 1  -64.023987 1      44   43   42
H    1.105894 1  111.629456 1   59.976654 1      45   44   43
H    1.107206 1  111.601997 1  -60.680233 1      45   44   43
H    1.103778 1  110.563995 1  179.575302 1      45   44   43
H    1.104617 1  109.058357 1   51.407055 1       9    8    7
H    1.106641 1  109.805008 1  -65.034477 1       9    8    7
H    1.105915 1  111.725403 1   59.698193 1      10    9    8
H    1.106953 1  111.545967 1  -61.071613 1      10    9    8
H    1.103628 1  110.506790 1  179.297409 1      10    9    8
H    1.093664 1  119.055389 1   -2.429723 1      36   35   34
H    1.094083 1  119.928207 1    1.845400 1      31   30   34
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para-exo-in

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scf done: -2563.326356

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 C    1.411718 1    0.000000 0    0.000000 0       1    0    0
 C    1.419289 1  119.621216 1    0.000000 0       2    1    0
 C    1.418903 1  118.978958 1   -9.672796 1       3    2    1
 C    1.404005 1  121.813988 1    9.315623 1       4    3    2
 C    1.418684 1  117.778908 1   -2.358674 1       5    4    3
 O    1.395154 1  121.214996 1  173.374680 1       3    2    1
 C    1.508877 1  112.723625 1 -103.656174 1       7    3    2
 C    1.532827 1  112.670395 1   74.466682 1       8    7    3
 C    1.546358 1  110.582901 1  172.456558 1       9    8    7
 O    1.421401 1  119.235649 1   -5.426698 1       2    3    7
 C    1.437724 1  112.985626 1  -60.087688 1      11    2    3
 C    1.425967 1  119.644653 1  126.539719 1      12   11    2
 C    1.427403 1  116.687897 1 -173.725464 1      13   12   11
 C    1.409019 1  121.771622 1   -7.899728 1      14   13   12
 C    1.410944 1  119.803963 1    3.568861 1      15   14   13
 C    1.410150 1  119.669846 1    2.022073 1      16   15   14
 O    1.389047 1  119.298004 1    0.932859 1      13   12   11
 C    1.504149 1  116.901100 1  130.090240 1      18   13   12
 C    1.533852 1  111.401802 1  -71.702644 1      19   18   13
 C    1.545837 1  110.934181 1 -175.885101 1      20   19   18
 O    1.449975 1  119.753242 1   -4.739550 1      14   13   18
 C    1.433247 1  110.692886 1 -119.738991 1      22   14   13
 C    1.422220 1  117.966957 1   62.648087 1      23   22   14
 C    1.415887 1  118.271492 1 -166.376099 1      24   23   22
 C    1.406428 1  121.524734 1  -11.058082 1      25   24   23
 C    1.417813 1  118.386421 1    2.614413 1      26   25   24
 C    1.416936 1  120.972687 1    5.264412 1      27   26   25
 O    1.448491 1  116.491257 1  166.742493 1      25   24   23
 C    1.408317 1  111.498558 1  -67.279175 1      29   25   24
 C    1.398173 1  120.920418 1  -43.453510 1      30   29   25
 C    1.446055 1  120.734116 1  178.475723 1      31   30   29
 C    1.443447 1  118.364037 1   -6.102794 1      32   31   30
 C    1.397229 1  120.597588 1    4.643708 1      33   32   31
 C    1.448541 1  121.036667 1    4.173724 1      34   33   32
 O    1.425494 1  118.714966 1 -171.324982 1      34   33   32
 O    1.391393 1  120.083000 1   -9.789546 1      24   25   29
 C    1.511238 1  112.336449 1 -112.917336 1      37   24   25
 C    1.532256 1  111.078125 1   83.644806 1      38   37   24
 C    1.545379 1  110.978218 1 -179.919327 1      39   38   37
 O    1.348137 1  115.710403 1    6.294353 1      35   30   29
 C    1.516677 1  123.616455 1  159.413010 1      41   35   30
 C    1.532910 1  109.875366 1  -75.743729 1      42   41   35
 C    1.546589 1  110.346741 1 -172.080994 1      43   42   41
Hg    2.401379 1  101.902405 1 -102.420418 1      32   33   34
 O    2.373470 1  163.382446 1   34.818573 1      45   32   33
 C    1.311023 1   91.640976 1  167.073013 1      46   45   32
 C    1.553988 1  118.109756 1 -179.694595 1      47   46   45
 F    1.406526 1  109.627640 1 -112.957390 1      48   47   46
 O    2.470860 1  139.412750 1 -161.562225 1      45   32   33
 F    1.403967 1  110.220642 1  -52.264160 1      48   47   50
 F    1.395877 1  112.438408 1 -172.862366 1      48   47   50
 H    1.095002 1  118.940369 1   -2.939043 1      17   12   11
 H    1.094686 1  118.881302 1    2.044399 1      33   34   36
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H    1.094679 1  119.110100 1    5.581967 1      15   14   22
H    1.099270 1  117.661339 1  156.716919 1      32   33   34
H    1.094304 1  119.490730 1   -4.678059 1      28   23   22
H    1.095058 1  120.174194 1  175.949463 1      16   17   12
H    1.094174 1  120.649490 1   -3.316128 1       5    4   36
H    1.094286 1  120.183540 1    5.338533 1      26   25   29
H    1.101180 1  101.968269 1  165.801132 1      42   41   35
H    1.099946 1  109.502350 1   48.112278 1      42   41   35
H    1.103527 1  103.108147 1  169.049408 1      19   18   13
H    1.104583 1  109.324814 1   52.645794 1      19   18   13
H    1.094388 1  119.541885 1  178.994415 1      27   28   23
H    1.094553 1  119.254341 1  178.617264 1       6    5    4
H    1.099804 1  104.075989 1 -154.744736 1      38   37   24
H    1.106130 1  108.694778 1  -39.457462 1      38   37   24
H    1.094261 1  119.160751 1    1.862079 1       1    2   11
H    1.100351 1  103.256317 1 -164.438385 1       8    7    3
H    1.109166 1  108.465981 1  -48.572037 1       8    7    3
H    1.107328 1  109.540718 1   62.886040 1      20   19   18
H    1.105834 1  109.134621 1  -54.130306 1      20   19   18
H    1.105961 1  111.411316 1   60.490150 1      21   20   19
H    1.105858 1  111.475227 1  -60.159218 1      21   20   19
H    1.103849 1  110.576431 1 -179.898773 1      21   20   19
H    1.107977 1  109.825966 1   67.089279 1      43   42   41
H    1.105642 1  109.338577 1  -51.000782 1      43   42   41
H    1.105423 1  111.269272 1   60.866859 1      44   43   42
H    1.105458 1  111.695351 1  -60.140953 1      44   43   42
H    1.103791 1  110.194954 1 -179.888931 1      44   43   42
H    1.106188 1  109.495689 1   57.930450 1      39   38   37
H    1.106290 1  109.678085 1  -58.568249 1      39   38   37
H    1.105565 1  111.270599 1   61.381310 1      40   39   38
H    1.106828 1  111.613457 1  -59.031456 1      40   39   38
H    1.104121 1  110.670807 1 -179.004410 1      40   39   38
H    1.103852 1  108.991371 1   50.102322 1       9    8    7
H    1.106606 1  109.810196 1  -66.472969 1       9    8    7
H    1.106382 1  111.875755 1   59.707893 1      10    9    8
H    1.107443 1  111.517975 1  -61.083256 1      10    9    8
H    1.103887 1  110.440468 1  179.414429 1      10    9    8
H    1.094674 1  119.278831 1    1.691214 1      31   30   29
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para-exo-out

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scf done: -2563.323061

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 C    1.408937 1    0.000000 0    0.000000 0       1    0    0
 C    1.420299 1  120.453430 1    0.000000 0       2    1    0
 C    1.420806 1  118.828377 1   -9.816189 1       3    2    1
 C    1.405465 1  120.876060 1    9.963645 1       4    3    2
 C    1.418314 1  118.763199 1   -3.152369 1       5    4    3
 O    1.398110 1  120.458313 1  171.102692 1       3    2    1
 C    1.510113 1  111.575981 1 -109.907471 1       7    3    2
 C    1.533655 1  111.578918 1   77.129112 1       8    7    3
 C    1.545977 1  110.766861 1  178.002823 1       9    8    7
 O    1.430951 1  118.485718 1   -8.521161 1       2    3    7
 C    1.427922 1  111.250923 1  -59.441681 1      11    2    3
 C    1.425452 1  119.387268 1  124.183273 1      12   11    2
 C    1.422801 1  116.461510 1 -171.474747 1      13   12   11
 C    1.407915 1  122.305153 1   -8.091189 1      14   13   12
 C    1.410894 1  119.420418 1    3.215454 1      15   14   13
 C    1.406634 1  119.717880 1    2.723964 1      16   15   14
 O    1.392612 1  119.922127 1    2.197723 1      13   12   11
 C    1.504282 1  116.186874 1  122.202034 1      18   13   12
 C    1.533111 1  111.536827 1  -72.083702 1      19   18   13
 C    1.545624 1  111.016655 1 -176.208954 1      20   19   18
 O    1.463310 1  118.946220 1   -3.777504 1      14   13   18
 C    1.419339 1  111.179245 1 -127.499344 1      22   14   13
 C    1.452804 1  119.399673 1   66.520203 1      23   22   14
 C    1.453572 1  118.331352 1 -158.313171 1      24   23   22
 C    1.395356 1  119.005180 1  -20.732306 1      25   24   23
 C    1.451852 1  120.301186 1    5.919474 1      26   25   24
 C    1.453364 1  118.829422 1   10.030252 1      27   26   25
 O    1.401043 1  119.690208 1  164.670349 1      25   24   23
 C    1.457232 1  112.156403 1  -66.300140 1      29   25   24
 C    1.408788 1  117.437325 1  -61.544910 1      30   29   25
 C    1.408213 1  119.627182 1 -179.902420 1      31   30   29
 C    1.409683 1  119.411697 1   -2.818585 1      32   31   30
 C    1.408411 1  120.352394 1    1.695745 1      33   32   31
 C    1.430525 1  121.680542 1    3.714605 1      34   33   32
 O    1.441841 1  118.598625 1 -174.184174 1      34   33   32
 O    1.337626 1  116.560242 1  -15.059172 1      24   25   29
 C    1.527884 1  121.508186 1 -146.351471 1      37   24   25
 C    1.528994 1  106.607689 1  120.593277 1      38   37   24
 C    1.547189 1  109.742996 1  173.239182 1      39   38   37
 O    1.386428 1  119.070801 1    0.334943 1      35   30   29
 C    1.504993 1  117.371696 1  134.062073 1      41   35   30
 C    1.534082 1  111.439415 1  -69.433533 1      42   41   35
 C    1.545640 1  110.880379 1 -176.018097 1      43   42   41
Hg    2.462066 1   96.913109 1   95.614227 1      27   28   23
 O    2.589961 1  107.767250 1  -50.905643 1      45   27   28
 C    1.287852 1   84.842247 1  179.178726 1      46   45   27
 C    1.555445 1  119.817986 1 -179.987442 1      47   46   45
 F    1.403511 1  110.655075 1 -120.867012 1      48   47   46
 O    2.351610 1  163.220490 1  -48.619061 1      45   27   28
 F    1.404320 1  110.572823 1  -60.974480 1      48   47   50
 F    1.403451 1  111.578354 1  179.105988 1      48   47   50
 H    1.094050 1  118.932541 1   -3.140203 1      17   12   11
 H    1.094288 1  118.866875 1    4.138929 1      33   34   36
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H    1.094202 1  120.030289 1    4.741656 1      15   14   22
H    1.093731 1  120.255249 1 -178.837234 1      32   33   34
H    1.094960 1  119.402084 1   -2.057680 1      28   23   22
H    1.093831 1  120.195679 1  177.869247 1      16   17   12
H    1.094052 1  119.785652 1   -2.773287 1       5    4   36
H    1.094403 1  119.063568 1   -0.625173 1      26   25   29
H    1.102817 1  102.936317 1  171.393890 1      42   41   35
H    1.104006 1  109.418190 1   54.721344 1      42   41   35
H    1.103290 1  103.317200 1  168.401398 1      19   18   13
H    1.106570 1  109.268967 1   52.155285 1      19   18   13
H    1.098202 1  117.525360 1 -163.101318 1      27   28   23
H    1.094296 1  119.419922 1  179.141602 1       6    5    4
H    1.100163 1  105.132973 1 -117.755211 1      38   37   24
H    1.102594 1  108.554901 1   -0.324502 1      38   37   24
H    1.093961 1  119.466919 1    2.317056 1       1    2   11
H    1.098387 1  103.851746 1 -161.264069 1       8    7    3
H    1.106157 1  108.597107 1  -46.022976 1       8    7    3
H    1.107083 1  109.608719 1   62.377262 1      20   19   18
H    1.105382 1  108.972832 1  -54.458309 1      20   19   18
H    1.105732 1  111.460091 1   60.440094 1      21   20   19
H    1.105993 1  111.580315 1  -60.296295 1      21   20   19
H    1.103618 1  110.488113 1  179.987885 1      21   20   19
H    1.107136 1  109.572609 1   62.836624 1      43   42   41
H    1.105937 1  109.195137 1  -54.338715 1      43   42   41
H    1.105766 1  111.437279 1   60.473976 1      44   43   42
H    1.105645 1  111.458542 1  -60.152943 1      44   43   42
H    1.103761 1  110.567841 1 -179.880432 1      44   43   42
H    1.104782 1  109.684471 1   51.416836 1      39   38   37
H    1.103577 1  109.282211 1  -66.278419 1      39   38   37
H    1.104847 1  111.458572 1   60.738861 1      40   39   38
H    1.105864 1  111.743340 1  -60.631016 1      40   39   38
H    1.103436 1  109.936890 1  179.566940 1      40   39   38
H    1.105226 1  109.350754 1   55.364208 1       9    8    7
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H    1.105888 1  111.495201 1   60.788658 1      10    9    8
H    1.106712 1  111.677727 1  -59.782478 1      10    9    8
H    1.103955 1  110.590492 1 -179.614822 1      10    9    8
H    1.094736 1  119.452438 1   -1.505199 1      31   30   29
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meta-in product

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 C    1.419491 1  119.972710 1    0.000000 0       2    1    0
 C    1.421565 1  118.886520 1  -10.823324 1       3    2    1
 C    1.406631 1  120.970367 1   11.258442 1       4    3    2
 C    1.417398 1  118.649292 1   -3.760425 1       5    4    3
 O    1.391932 1  120.414803 1  172.619308 1       3    2    1
 C    1.499970 1  112.784325 1 -113.745483 1       7    3    2
 C    1.534570 1  110.885651 1   82.875320 1       8    7    3
 C    1.544903 1  111.155830 1  173.811096 1       9    8    7
 O    1.427676 1  119.187378 1   -7.366630 1       2    3    7
 C    1.439605 1  112.157127 1  -63.438789 1      11    2    3
 C    1.423441 1  119.827965 1  124.962135 1      12   11    2
 C    1.425850 1  116.791618 1 -173.169281 1      13   12   11
 C    1.408683 1  122.098763 1   -7.429635 1      14   13   12
 C    1.409960 1  119.357620 1    3.490411 1      15   14   13
 C    1.408775 1  119.900322 1    1.776696 1      16   15   14
 O    1.397522 1  119.444588 1    1.251453 1      13   12   11
 C    1.494202 1  115.893097 1  128.291214 1      18   13   12
 C    1.535789 1  111.695320 1  -70.028587 1      19   18   13
 C    1.544923 1  111.289787 1 -176.890945 1      20   19   18
 O    1.453890 1  119.655487 1   -4.303253 1      14   13   18
 C    1.430113 1  111.205864 1 -121.828171 1      22   14   13
 C    1.424069 1  118.085373 1   58.641590 1      23   22   14
 C    1.418867 1  119.037323 1 -167.334290 1      24   23   22
 C    1.417419 1  119.830925 1  -12.018411 1      25   24   23
 C    1.420834 1  119.393074 1    3.767207 1      26   25   24
 C    1.416062 1  120.845963 1    4.665720 1      27   26   25
 O    1.424298 1  119.699936 1  167.822021 1      25   24   23
 C    1.448278 1  113.787308 1  -57.315372 1      29   25   24
 C    1.412012 1  120.202095 1  -58.182255 1      30   29   25
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 C    1.408033 1  120.143234 1    1.201453 1      33   32   31
 C    1.426789 1  121.454407 1    5.057351 1      34   33   32
Hg    2.198457 1  120.498573 1    9.186952 1      31   30   29
 O    2.301131 1  174.804413 1 -119.009583 1      36   31   30
 C    1.320532 1  100.663536 1 -140.360275 1      37   36   31
 C    1.552354 1  113.990089 1 -173.197479 1      38   37   36
 F    1.402651 1  112.608147 1 -169.007187 1      39   38   37
 O    1.447572 1  118.145439 1 -172.046829 1      34   33   32
 O    1.387730 1  119.865814 1   -9.285225 1      24   25   29
 C    1.503432 1  112.488548 1 -112.643379 1      42   24   25
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 C    1.545416 1  111.017242 1  173.444656 1      44   43   42
 O    1.393582 1  119.281380 1   -0.489444 1      35   30   29
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 C    1.535302 1  111.528214 1  -71.698448 1      47   46   35
 C    1.545041 1  111.236717 1 -176.308105 1      48   47   46
 O    1.276240 1  120.106407 1   13.148741 1      38   39   40
 F    1.419327 1  109.971260 1 -106.111320 1      39   38   50
 F    1.407261 1  112.411156 1  134.481384 1      39   38   50
 H    1.094594 1  118.894287 1   -1.865678 1      17   12   11
 H    1.094413 1  119.127686 1    4.667603 1      33   34   41
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H    1.093725 1  119.636696 1   -2.112780 1      28   23   22
H    1.094555 1  120.376678 1  178.062881 1      16   17   12
H    1.094430 1  119.759659 1   -4.280267 1       5    4   41
H    1.095801 1  119.261116 1    6.306722 1      26   25   29
H    1.103890 1  103.434761 1  169.081253 1      47   46   35
H    1.105322 1  109.635193 1   52.656807 1      47   46   35
H    1.103966 1  103.520844 1  170.604111 1      19   18   13
H    1.105849 1  109.586952 1   54.157429 1      19   18   13
H    1.094366 1  119.741447 1  179.198013 1      27   28   23
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H    1.107179 1  109.176231 1  -40.513901 1       8    7    3
H    1.106858 1  109.282318 1   61.709404 1      20   19   18
H    1.106019 1  108.962990 1  -54.844452 1      20   19   18
H    1.106482 1  111.362770 1   60.013500 1      21   20   19
H    1.106156 1  111.304787 1  -60.322269 1      21   20   19
H    1.104464 1  110.787117 1  179.847702 1      21   20   19
H    1.107081 1  109.384148 1   62.311634 1      48   47   46
H    1.105956 1  108.964790 1  -54.330158 1      48   47   46
H    1.106395 1  111.372383 1   60.365280 1      49   48   47
H    1.106153 1  111.325951 1  -59.984180 1      49   48   47
H    1.104407 1  110.772987 1 -179.841705 1      49   48   47
H    1.105034 1  108.661095 1   51.012665 1      44   43   42
H    1.107281 1  109.680275 1  -65.113899 1      44   43   42
H    1.106544 1  111.527161 1   59.939625 1      45   44   43
H    1.107335 1  111.324081 1  -60.298988 1      45   44   43
H    1.104700 1  110.818520 1  179.845337 1      45   44   43
H    1.105538 1  108.715042 1   51.463676 1       9    8    7
H    1.106909 1  109.512321 1  -64.431763 1       9    8    7
H    1.106615 1  111.565384 1   59.918205 1      10    9    8
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meta-out product

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 C    1.420782 1  119.000458 1  -10.101167 1       3    2    1
 C    1.407193 1  120.837540 1   10.445842 1       4    3    2
 C    1.417249 1  118.744026 1   -3.450348 1       5    4    3
 O    1.392341 1  120.411125 1  173.014160 1       3    2    1
 C    1.500162 1  112.606850 1 -109.921837 1       7    3    2
 C    1.533986 1  111.097610 1   82.009964 1       8    7    3
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 O    1.429495 1  118.894424 1   -6.942582 1       2    3    7
 C    1.438248 1  111.937103 1  -63.704475 1      11    2    3
 C    1.424631 1  119.994820 1  123.594452 1      12   11    2
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 C    1.408732 1  121.864006 1   -7.569417 1      14   13   12
 C    1.409035 1  119.795998 1    3.629518 1      15   14   13
 C    1.408364 1  119.572273 1    1.682188 1      16   15   14
 O    1.395731 1  119.303093 1    1.628730 1      13   12   11
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 C    1.535660 1  111.723335 1  -71.384880 1      19   18   13
 C    1.544940 1  111.205635 1 -176.357330 1      20   19   18
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 C    1.433044 1  111.335602 1 -120.781105 1      22   14   13
 C    1.423584 1  118.242836 1   61.822563 1      23   22   14
 C    1.417824 1  118.415733 1 -168.761536 1      24   23   22
 C    1.409168 1  120.541061 1  -11.021639 1      25   24   23
 C    1.417026 1  119.767151 1    3.382885 1      26   25   24
 C    1.420299 1  120.034988 1    4.512304 1      27   26   25
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 C    1.408789 1  120.098015 1    1.567777 1      33   32   31
 C    1.427780 1  121.671432 1    3.528635 1      34   33   32
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 C    1.545389 1  111.021248 1  172.894653 1      39   38   37
 O    1.394277 1  119.354141 1    1.222297 1      35   30   29
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 C    1.545266 1  111.246155 1 -175.690094 1      43   42   41
Hg    2.197945 1  111.236534 1    4.111215 1      26   25   29
 O    2.320154 1  166.721085 1   86.739990 1      45   26   25
 C    1.319003 1   97.736191 1  176.352020 1      46   45   26
 C    1.550772 1  114.641563 1 -179.463364 1      47   46   45
 F    1.402122 1  112.609612 1 -174.103210 1      48   47   46
 O    2.675965 1  138.827957 1  -97.806198 1      45   26   25
 F    1.413847 1  110.697281 1 -113.569427 1      48   47   50
 F    1.410232 1  111.460281 1  127.059364 1      48   47   50
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 H    1.094407 1  118.899658 1    3.503431 1      33   34   36
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H    1.107368 1  108.978050 1  -42.268059 1      38   37   24
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H    1.107866 1  109.163857 1  -41.296669 1       8    7    3
H    1.106946 1  109.348320 1   62.206093 1      20   19   18
H    1.106011 1  108.984367 1  -54.393520 1      20   19   18
H    1.106406 1  111.331017 1   60.330685 1      21   20   19
H    1.106203 1  111.325851 1  -59.988453 1      21   20   19
H    1.104397 1  110.781555 1 -179.863876 1      21   20   19
H    1.107051 1  109.466614 1   62.934658 1      43   42   41
H    1.106263 1  109.009750 1  -53.849846 1      43   42   41
H    1.106267 1  111.354317 1   60.617218 1      44   43   42
H    1.106120 1  111.331596 1  -59.775639 1      44   43   42
H    1.104311 1  110.727791 1 -179.610306 1      44   43   42
H    1.104971 1  108.569855 1   50.592358 1      39   38   37
H    1.107341 1  109.697792 1  -65.536697 1      39   38   37
H    1.106629 1  111.604156 1   59.835991 1      40   39   38
H    1.107335 1  111.239815 1  -60.444801 1      40   39   38
H    1.104649 1  110.825928 1  179.781723 1      40   39   38
H    1.104931 1  108.621536 1   51.391193 1       9    8    7
H    1.106937 1  109.545143 1  -64.454674 1       9    8    7
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H    1.107546 1  111.351486 1  -60.389179 1      10    9    8
H    1.104744 1  110.819801 1  179.810272 1      10    9    8
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para-in product

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 C    1.421120 1  118.972939 1  -10.082828 1       3    2    1
 C    1.406636 1  120.934860 1   10.457354 1       4    3    2
 C    1.417575 1  118.652504 1   -3.478476 1       5    4    3
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 C    1.410002 1  119.792320 1    3.687305 1      15   14   13
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 O    1.394912 1  119.408096 1    1.288921 1      13   12   11
 C    1.494892 1  116.280632 1  129.385101 1      18   13   12
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 C    1.545020 1  111.266968 1 -176.483078 1      20   19   18
 O    1.449366 1  119.854248 1   -4.230703 1      14   13   18
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 C    1.417068 1  120.959145 1    4.435859 1      27   26   25
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 C    1.413735 1  118.328636 1  -51.467487 1      30   29   25
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 C    1.410047 1  119.944328 1   -1.726676 1      32   31   30
 C    1.411727 1  119.536911 1    0.469976 1      33   32   31
 C    1.426806 1  122.004150 1    4.195995 1      34   33   32
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 C    1.545453 1  111.055901 1  173.739441 1      39   38   37
 O    1.391917 1  118.887436 1    0.984906 1      35   30   29
 C    1.495686 1  117.054176 1  134.337051 1      41   35   30
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 C    1.544960 1  111.223351 1 -175.868561 1      43   42   41
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 O    2.693624 1  137.102722 1    5.537030 1      45   32   33
 C    1.279766 1   82.431320 1 -177.910004 1      46   45   32
 C    1.551189 1  120.427032 1  179.955276 1      47   46   45
 F    1.401907 1  112.597000 1    0.898224 1      48   47   46
 O    2.316388 1  168.564087 1 -165.518082 1      45   32   33
 F    1.412862 1  110.965370 1   60.512981 1      48   47   50
 F    1.411591 1  111.188705 1  -58.863461 1      48   47   50
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H    1.104085 1  103.424568 1  170.557770 1      19   18   13
H    1.105421 1  109.623985 1   54.137634 1      19   18   13
H    1.094833 1  119.507278 1  179.205475 1      27   28   23
H    1.094736 1  119.446861 1  179.475250 1       6    5    4
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H    1.107566 1  109.050957 1  -41.369408 1      38   37   24
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H    1.107615 1  109.066696 1  -41.904369 1       8    7    3
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H    1.104422 1  110.774193 1 -179.716751 1      21   20   19
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H    1.105413 1  108.717781 1   51.426723 1      39   38   37
H    1.106940 1  109.645355 1  -64.613312 1      39   38   37
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para-out product

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 C    1.409143 1  119.758736 1    3.562366 1      15   14   13
 C    1.408284 1  119.606232 1    1.757673 1      16   15   14
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