Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Assembling triazolated calix[4]semitubes by means of copper(I)-catalyzed azide–alkyne cycloaddition

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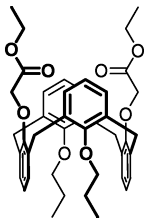
Supplementary Information

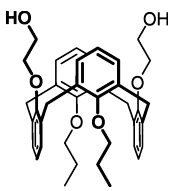
Contents

Synthesis and characterization of novel compounds

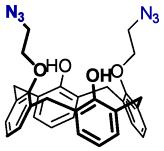
General experimental methods: NMR spectra were acquired on Bruker Avance 400 and Avance 600 instruments at 20 ºC if not stated otherwise, and chemical shifts are reported as ppm referenced to solvent signals. ESI mass spectra were obtained from Sciex TripleTOF 5600+ spectrometers. Chemicals received from commercial sources were used without further purification. Calixarenes **1**,[S1] **2**,[S2] **5**,[S3] **A**,[S4] **B**,[S5] **D**,[S6] and complex CuI·P(OEt)$_3$,[S7] were prepared according to the published procedures.



*1,3-Alternate calix[4]arene diester **3***. A suspension of calixarene **1** (1.02 g, 2.0 mmol) and anhydrous Cs_2CO_3 (2.61 g, 8.0 mmol) in dry DMF (50 ml) was stirred at room temperature for 1 h. Ethyl 2-bromoacetate (1.33 ml, 12.0 mmol) was added and the reaction mixture was stirred at room temperature for 24 h. The solvent was removed under reduced pressure and the residue was dissolved in dichloromethane. The solution was washed with 2 M HCl, water, dried and concentrated to dryness. The resultant oil was purified by column chromatography (gradient from dichloromethane to dichloromethane/ethanol (50:1)). Yield 0.670 g (49%), white solid. For analytical data see Ref. S8.



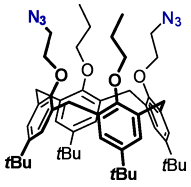
*1,3-Alternate calix[4]arene diol **4***. To a cooled (0–5 °C) suspension of $LiAlH_4$ (0.210 g, 5.40 mmol) in dry diethyl ether (50 ml) a solution of calixarene **3** (0.370 g, 0.54 mmol) in dry THF was added dropwise. The reaction mixture was stirred at room temperature for 24 h, and then quenched at cooling (0–5 °C) by dropwise addition of 0.5 M HCl (20 ml) under vigorous stirring. The organic layer was separated, the aqueous layer was washed with diethyl ether. The combined organic fractions were washed with water, dried by $MgSO_4$ and evaporated. Yield 0.210 g (65%), white solid. M.p. >250 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.06 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 7.03 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.88 (t, 2H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.85 (t, 2H, $^3J_{HH}$ = 7.5 Hz; ArH), 3.88 (d, 4H, $^2J_{HH}$ = 16.7 Hz; $ArCH_2Ar$), 3.84 (d, 4H, ^2J = 16.7 Hz; $ArCH_2Ar$), 3.64–3.59 (m, 4H; $C\underline{H}_2CH_2OH$), 3.38–3.31 (m, 4H; $C\underline{H}_2CH_2CH_3$), 3.31–3.25 (m, 4H; $C\underline{H}_2OH$), 2.37 (t, 2H, $^3J_{HH}$ = 6.7 Hz; OH), 1.05–0.94 (m, 4H; $C\underline{H}_2CH_3$), 0.62 (t, 6H, $^3J_{HH}$ = 7.5 Hz; $CH_2C\underline{H}_3$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 156.98, 156.07, 133.66, 133.58 (C_{Ar}), 129.26, 129.22, 122.79, 122.71 (CH_{Ar}), 71.85, 71.00 (OCH_2), 61.19 (CH_2OH), 38.20 ($ArCH_2Ar$), 22.15 ($\underline{C}H_2CH_3$), 9.93 (CH_3) ppm. ESI-MS *m*/*z*: 597.3209 $[M+H]^+$ for $C_{38}H_{45}O_6$ (597.3211).



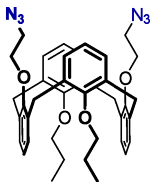
Cone calix[4]arene bis(azide) ***6***. A mixture of bromoethylated calix[4]arene **5** (1.56 g, 2.45 mmol) and NaN_3 (0.637 g, 9.80 mmol) in dry DMF (65 ml) was stirred at 60 °C for 8 h. The solvent was removed under reduced pressure, and the residue was parted between dichloromethane and aqueous 2 M HCl. The organic layer was separated, washed with water, dried with $MgSO_4$ and concentrated to dryness. The residue was purified by re-crystallization from dichloromethane/methanol. Yield 1.22 g (89%), white solid. M.p. 227–229 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.50 (s, 2H; OH), 7.07 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.87 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.76–6.71 (m, 2H; ArH), 6.67 (t, 2H, $^3J_{HH}$ = 7.5 Hz; ArH), 4.35 (d, 4H, $^2J_{HH}$ = 13.1 Hz; $ArCH_2Ar$), 4.10–4.06 (m, 4H; OCH_2), 3.90–3.85 (m, 4H; CH_2N_3), 3.39 (d, 4H; $^2J_{HH}$ = 13.1 Hz; $ArCH_2Ar$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$+CD_3OD): δ = 152.75, 151.20, 132.76 (C_{Ar}), 128.79, 128.60 (CH_{Ar}), 127.63 (C_{Ar}), 125.29, 118.88 (CH_{Ar}), 74.05 (OCH_2), 50.82 (CH_2N_3), 30.85 ($ArCH_2Ar$) ppm. ESI-MS *m*/*z*: 580.2667 $[M+NH_4]^+$ for $C_{32}H_{34}N_7O_4$ (580.2667).

1,3-Alternate calix[4]arene bis(alkyne) ***C***. *Method 1*. A mixture of calix[4]arene **1** (1.02 g, 2.0 mmol) and anhydrous Cs_2CO_3 (2.61 g, 8.0 mmol) in dry DMF (50 ml) was stirred at room temperature for 2 h. Propargyl bromide (80% in toluene, 0.89 ml, 8.0 mmol) was added and stirring was continued for 48 h at room temperature. The solvent was removed under reduced pressure without heating, and the residue was parted between dichloromethane and 2 M HCl. The organic layer was separated, washed with water, dried with $MgSO_4$ and concentrated to dryness. The residue was purified by column chromatography (gradient from hexane/dichloromethane (1:1) to dichloromethane). Yield 0.19 g (16%). *Method 2*. A mixture of calix[4]arene **2** (1.40 g, 2.8 mmol) and anhydrous Cs_2CO_3 (4.50 g, 14.0 mmol) in dry DMF (70 ml) was stirred at room temperature for 2 h. 1-Iodopropane (0.66 ml, 14.7 mmol) was added and stirring was continued for 24 h at 50 °C. The solvent was removed under reduced pressure (with heating at < 50 °C), and the residue was parted between dichloromethane and 2 M HCl. The organic layer was separated, washed with water, dried with $MgSO_4$, and concentrated to dryness. The residue was purified by re-crystallization from dichloromethane/methanol. Yield 0.61 g (37%), white solid. M.p. 206–208 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.11 (d, 4H, $^3J_{HH}$ = 7.6 Hz; ArH), 7.00 (d, 4H, $^3J_{HH}$ = 7.6 Hz; ArH), 6.76 (t, 2H, $^3J_{HH}$ = 7.6 Hz; ArH), 6.73 (t, 2H, $^3J_{HH}$ = 7.6 Hz; ArH), 4.04 (d, 4H, $^4J_{HH}$ = 2.4 Hz; $OC\underline{H}_2CCH$), 3.76 (d, 4H, $^2J_{HH}$ = 14.4 Hz; $ArCH_2Ar$), 3.63 (d, 4H, $^2J_{HH}$ = 14.4 Hz; $ArCH_2Ar$), 3.53–3.46 (m, 4H; OCH_2), 2.42 (t, 2H, $^4J_{HH}$ = 2.4 Hz; $CC\underline{H}$), 1.67–1.55 (m, 4H; $C\underline{H}_2CH_3$), 0.88 (t, 6H, $^3J_{HH}$ = 7.6 Hz; CH_3) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 156.45, 155.26, 134.26, 133.62 (C_{Ar}), 130.23, 130.08, 122.40, 122.18 (CH_{Ar}), 80.49 ($OCH_2\underline{C}$), 74.40, 73.53 (CH, OCH_2),

58.96 (O<u>C</u>H$_2$CCH), 36.75 (ArCH$_2$Ar), 23.45 (<u>C</u>H$_2$CH$_3$), 10.35 (CH$_3$) ppm. ESI-MS *m*/*z*: 585.2997 $[M+H]^+$ for $C_{40}H_{41}O_4$ (585.2999).

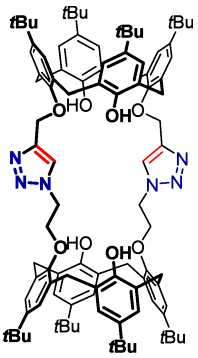


Cone calix[4]arene bis(azide) ***E***. To a solution of calix[4]arene **D** (1.96 g, 2.5 mmol) in dry DMF (100 ml) NaH (60%, 0.60 g, 15.0 mmol) was added. The mixture was stirred for 1 h at room temperature and 1-iodopropane (1.22 ml, 12.5 mmol) was added. The mixture was stirred at room temperature for 48 h. The reaction was quenched by a dropwise addition of water and the solution was concentrated under reduced pressure. Water (100 ml) was added to the residue, the precipitate was filtered and washed with water. The residue was purified by re-crystallization from dichloromethane/methanol. Yield 1.54 g (71%), white solid. For analytical data see Ref. S9.

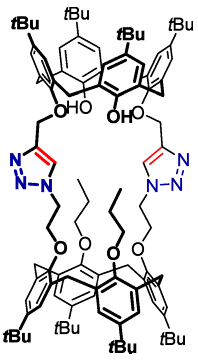


1,3-Alternate calix[4]arene bis(azide) ***F***. <u>*Method 1*</u>. Diisopropyl azodicarboxylate (0.270 ml, 1.38 mmol) was added dropwise at stirring to a cooled (0–5 °C) solution of Ph_3P (0.270 g, 1.03 mmol) in dry THF (4 ml). After a solid formed, the mixture was stirred at cooling for 1 h. A solution of calix[4]arene **4** (0.205 g, 0.34 mmol) and diphenyl phosphoryl azide (0.296 ml, 1.38 mmol) in THF (10 ml) was added dropwise. The reaction mixture was stirred at cooling for 1 h and then allowed to stay at room temperature for 48 h. The solution was concentrated under reduced pressure and the resultant oil was treated with cold methanol. The solid formed was collected, washed with methanol and dried. Yield 0.093 g (42%). <u>*Method 2*</u>. A suspension of calix[4]arene **6** (0.560 g, 1.0 mmol) and anhydrous Cs_2CO_3 (1.30 g, 4.0 mmol) in dry DMF (30 ml) was stirred at room temperature for 2 h. 1-Iodopropane (0.39 ml, 4.0 mmol) was added to the mixture and stirring was continued for 48 h at room temperature. The solvent was removed under reduced pressure, and the residue was parted between dichloromethane and 2 M HCl. The organic layer was separated, washed with water, dried with $MgSO_4$ and concentrated to dryness. The residue was purified by column chromatography (gradient from hexane/dichloromethane (3:2) to dichloromethane). Yield 0.350 g (54%), white solid. M.p. 118–120 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.05 (d, 4H, $^3J_{HH}$ = 7.6 Hz; ArH), 7.02 (d, 4H, $^3J_{HH}$ = 7.6 Hz; ArH), 6.81 (t, 2H, $^3J_{HH}$ = 7.6 Hz; ArH), 6.77 (t, 2H, $^3J_{HH}$ = 7.6 Hz; ArH), 3.77 (d, 4H, $^2J_{HH}$ = 15.3 Hz; ArCH$_2$Ar), 3.71 (d, 4H, $^2J_{HH}$ = 15.3 Hz; ArCH$_2$Ar), 3.51–3.48 (m, 4H; OCH$_2$), 3.47–3.44 (m, 4H; OCH$_2$), 3.04–3.01 (m, 4H; CH$_2$N$_3$), 1.42–1.35 (m, 4H; CH$_2$<u>C</u>H$_2$CH$_3$), 0.76 (t, 6H, $^3J_{HH}$ = 7.6 Hz; CH$_3$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 156.94, 155.42, 133.91, 133.60 (C_{Ar}), 129.76, 129.31, 122.49, 122.26 (CH_{Ar}), 72.65, 68.31 (OCH$_2$), 50.34 (CH$_2$N$_3$), 37.20 (ArCH$_2$Ar), 22.96 (<u>C</u>H$_2$CH$_3$), 10.24 (CH$_3$) ppm. ESI-MS *m*/*z*: 664.3602 $[M+NH_4]^+$ for $C_{38}H_{46}N_7O_4$ (664.3606).

General procedure for the preparation of calix[4]semitubes. To a stirred mixture of calixarene (bis)alkyne and (bis)azide in toluene or THF, Cu(I)-catalyst was added (CuI dissolved in a small portion of toluene by addition of Et_3N, or $CuSO_4 \cdot 5H_2O$/sodium ascorbate mixture dissolved in water). The mixture was stirred at room temperature or at heating, and then concentrated under reduced pressure. The residue was parted between dichloromethane and 2 M HCl at vigorous stirring for at least 2 h. The organic layer was separated, washed with aqueous Na_2SO_3 (5%, for CuI-catalyzed reactions only), water and dried with $MgSO_4$. The solvent was removed and the residue was subjected to column chromatography. The two-step column separation was applied in several cases: from the first column, a polymeric material was first eluted followed by a semitube-containing fraction, which was then evaporated to dryness and subjected to the second column (with the same or different eluent) for the final purification.

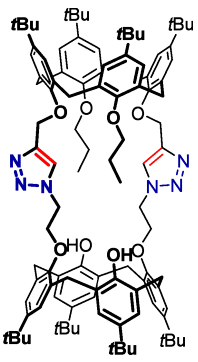


Calix[4]semitube ***AD*** was prepared according to *General procedure* from calixarene **A** (0.145 g, 0.20 mmol), calixarene **D** (0.157 g, 0.20 mmol), CuI (0.012 g, 0.06 mmol) and Et_3N (0.170 ml, 1.20 mmol) in toluene (15 ml). The reaction mixture was stirred at room temperature for 48 h. Column 1: gradient from dichloromethane to dichloromethane/ethanol (50:1), column 2: gradient from hexane to hexane/ethyl acetate (3:1). Yield 0.095 g (31%), white solid. For analytical data see Ref. S10.

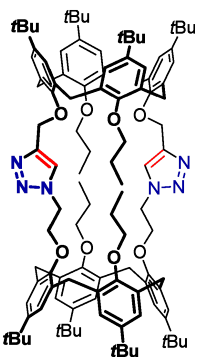


Calix[4]semitube ***AE*** was prepared according to *General procedure* from calixarene **A** (0.072 g, 0.10 mmol), calixarene **E** (0.087 g, 0.10 mmol), CuI (0.006 g, 0.03 mmol) and Et_3N (1 ml) in toluene (10 ml). The reaction mixture was stirred at 70 °C for 9 h. Column: gradient from dichloromethane to dichloromethane/ethanol (50:1). Yield 0.042 g (26%), white solid. M.p. >250 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.92 (s, 2H; ArH_{Trz}), 7.18 (s, 4H; ArH), 7.11 (s, 2H; OH), 7.08 (s, 4H; ArH), 6.82 (s, 4H; ArH), 6.52 (s, 4H; ArH), 5.36–5.28 (m, 4H; NCH_2), 5.20 (s, 4H; OCH_2Trz), 4.51–4.43 (m, 4H; $NCH_2C\underline{H}_2$), 4.39 (d, 4H, $^2J_{HH}$ = 12.8 Hz; $ArCH_2Ar$), 4.36 (d, 4H, $^2J_{HH}$ = 13.1 Hz; $ArCH_2Ar$), 3.80–3.74 (m, 4H; $OC\underline{H}_2CH_2CH_3$), 3.38 (d, 4H, $^2J_{HH}$ = 13.1 Hz; $ArCH_2Ar$), 3.25 (d, 4H, $^2J_{HH}$ = 12.8 Hz; $ArCH_2Ar$), 1.97–1.85 (m, 4H; $C\underline{H}_2CH_3$), 1.37 (s, 18H; $C(CH_3)_3$), 1.30 (s, 18H; $C(CH_3)_3$), 0.96 (s, 18H; $C(CH_3)_3$), 0.92 (t, 6H, $^3J_{HH}$ = 7.4 Hz; CH_3), 0.84 (s, 18H; $C(CH_3)_3$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 153.30, 151.81, 150.55, 149.87, 147.27, 146.20 (C_{Ar}), 144.69 ($C_{Ar\ Trz}$)*, 144.46, 141.58, 135.34, 132.49, 131.69, 127.71 (C_{Ar}), 125.84, 125.61, 124.99, 124.66 (CH_{Ar}), 122.25

($CH_{Ar\,Trz}$)*, 78.03, 71.85, 70.05 (OCH_2), 49.18 (NCH_2), 34.16, 33.92, 33.80, 33.60 ($\underline{C}(CH_3)_3$), 31.67, 31.08, 30.95 ($C(\underline{C}H_3)_3$), 30.90 ($ArCH_2Ar$), 23.58 ($\underline{C}H_2CH_3$), 10.38 (CH_3) ppm. ESI-MS *m*/*z*: 1597.0377 $[M+H]^+$ for $C_{104}H_{135}N_6O_8$ (1597.0369).

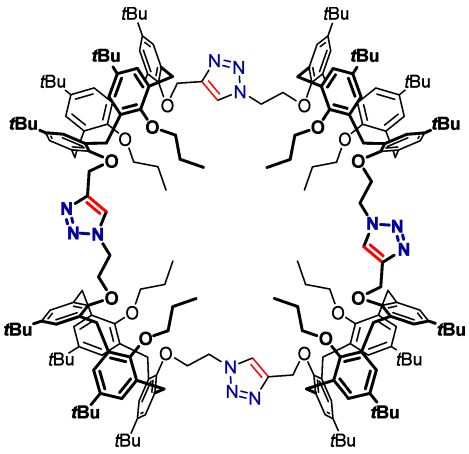


Calix[4]semitube ***BD*** was prepared according to *General procedure* from calixarene **B** (0.162 g, 0.20 mmol), calixarene **D** (0.157 g, 0.20 mmol), CuI (0.012 g, 0.06 mmol) and Et_3N (1 ml) in toluene (15 ml). The reaction mixture was stirred at 70 °C for 9 h. Column: gradient from dichloromethane to dichloromethane/ethanol (50:1), the product separated from the column was additionally washed with methanol. Yield 0.139 g (44%), white solid. M.p. >250 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.43 (s, 2H; ArH_{Trz}), 7.07 (s, 4H; ArH), 7.01 (s, 4H; ArH), 6.74 (s, 4H; ArH), 6.46 (s, 2H; OH), 6.43 (s, 4H; ArH), 5.27 (s, 4H; OCH_2Trz), 5.09–5.06 (m, 4H; NCH_2), 4.50–4.46 (m, 4H; $NCH_2C\underline{H}_2$), 4.19 (d, 4H, $^2J_{HH}$ = 12.6 Hz; $ArCH_2Ar$), 4.00 (d, 4H, $^2J_{HH}$ = 13.0 Hz; $ArCH_2Ar$), 3.59–3.55 (m, 4H; $OC\underline{H}_2CH_2CH_3$), 3.26 (d, 4H, $^2J_{HH}$ = 13.0 Hz; $ArCH_2Ar$), 3.02 (d, 4H, $^2J_{HH}$ = 12.6 Hz; $ArCH_2Ar$), 1.55–1.49 (m, 4H; $C\underline{H}_2CH_3$), 1.32 (s, 18H; $C(CH_3)_3$), 1.27 (s, 18H; $C(CH_3)_3$), 0.92 (s, 18H; $C(CH_3)_3$), 0.81 (t, 6H, $^3J_{HH}$ = 7.4 Hz; CH_3), 0.80 (s, 18H; $C(CH_3)_3$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 153.40, 152.43, 150.18, 149.58, 147.28, 145.70 (C_{Ar}), 145.05 ($C_{Ar\,Trz}$)*, 143.83, 141.67, 135.68, 131.94, 131.91, 127.46 (C_{Ar}), 125.68, 125.58, 125.10 (CH_{Ar}), 124.67 ($CH_{Ar\,Trz}$)*, 124.32 (CH_{Ar}), 77.12, 74.16, 66.42 (OCH_2), 50.05 (NCH_2), 34.03, 33.88, 33.79, 33.51 ($\underline{C}(CH_3)_3$), 31.70, 31.63 ($C(\underline{C}H_3)_3$), 31.47, 31.38 ($ArCH_2Ar$), 31.11, 30.90 ($C(\underline{C}H_3)_3$), 22.81 ($\underline{C}H_2CH_3$), 10.51 (CH_3) ppm. ESI-MS *m*/*z*: 1619.0187 $[M+Na]^+$ for $C_{104}H_{134}NaN_6O_8$ (1619.0189).

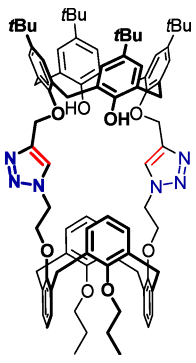


Calix[4]semitube ***BE*** was prepared according to *General procedure* from calixarene **B** (0.081 g, 0.10 mmol), calixarene **E** (0.087 g, 0.10 mmol), CuI (0.006 g, 0.03 mmol) and Et_3N (1 ml) in toluene (10 ml). The reaction mixture was stirred at 70 °C for 9 h. Column: gradient from dichloromethane/ethanol (40:1) to dichloromethane/ethanol (10:1). Yield 0.044 g (26%), white solid. M.p. >250 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.63 (s, 2H; ArH_{Trz}), 7.18 (s, 4H; ArH), 7.01 (s, 4H; ArH), 6.53 (s, 4H; ArH), 6.47 (s, 4H; ArH), 5.28 (s, 4H; OCH_2Trz), 5.05–4.99 (m, 4H; NCH_2), 4.53–4.47 (m, 4H; $NCH_2C\underline{H}_2$), 4.42 (d, 4H, $^2J_{HH}$ = 12.8 Hz; $ArCH_2Ar$), 4.36 (d, 4H, $^2J_{HH}$ = 12.8 Hz; $ArCH_2Ar$), 3.80–3.73 (m, 4H; $OC\underline{H}_2CH_2CH_3$), 3.71–3.65 (m, 4H; $OC\underline{H}_2CH_2CH_3$), 3.22 (d, 4H, $^2J_{HH}$ = 12.8 Hz; $ArCH_2Ar$), 3.15 (d, 4H, $^2J_{HH}$ = 12.8 Hz; $ArCH_2Ar$), 1.90–1.79 (m, 4H; $C\underline{H}_2CH_3$), 1.76–1.65 (m, 4H; $C\underline{H}_2CH_3$), 1.36 (s, 18H; $C(CH_3)_3$), 1.25

(s, 18H; $C(CH_3)_3$), 1.01 (t, 6H, $^3J_{HH}$ = 7.5 Hz; CH_3), 0.95 (t, 6H, $^3J_{HH}$ = 7.5 Hz; CH_3), 0.89 (s, 18H; $C(CH_3)_3$), 0.82 (s, 18H; $C(CH_3)_3$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 154.00, 152.41, 152.37, 151.72, 146.17, 146.04 (C_{Ar}), 144.97 ($C_{Ar\ Trz}$)*, 144.31, 144.11, 135.59, 134.94, 132.41, 131.69 (C_{Ar}), 125.89, 125.67, 124.51, 124.46 (CH_{Ar}), 123.37 ($CH_{Ar\ Trz}$)*, 77.67, 76.55, 71.44, 66.43 (OCH_2), 49.21 (NCH_2), 34.16, 33.95, 33.63, 33.59 ($\underline{C}(CH_3)_3$), 31.78 ($ArCH_2Ar$), 31.67, 31.59, 31.22, 31.09 ($C(\underline{C}H_3)_3$), 30.95 ($ArCH_2Ar$), 23.14, 22.88 ($\underline{C}H_2CH_3$), 10.57, 10.52 (CH_3) ppm. ESI-MS *m*/*z*: 1703.1123 $[M+Na]^+$ for $C_{110}H_{146}NaN_6O_8$ (1703.1128).

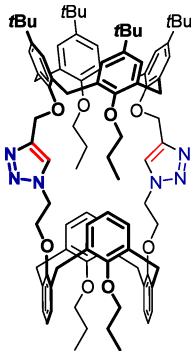


Tetrakis(calix[4]arene) ***B₂E₂*** was isolated as the less polar product during chromatographic purification of calix[4]semitube **BE**. Yield 0.034 g (20%), white solid. M.p. >250 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.46 (s, 2H; ArH_{Trz}), 7.11 (s, 4H; ArH), 6.72 (s, 4H; ArH), 6.71 (s, 4H; ArH), 6.49 (s, 4H; ArH), 5.29 (s, 4H; OCH_2Trz), 5.25–5.18 (m, 4H; NCH_2), 4.45–4.37 (m, 4H; $NCH_2C\underline{H}_2$), 4.30 (d, 4H, $^2J_{HH}$ = 12.8 Hz; $ArCH_2Ar$), 4.28 (d, 4H, $^2J_{HH}$ = 12.7 Hz; $ArCH_2Ar$), 3.82–3.76 (m, 4H; $OC\underline{H}_2CH_2CH_3$), 3.72–3.67 (m, 4H; $OC\underline{H}_2CH_2CH_3$), 3.17 (d, 4H, $^2J_{HH}$ = 12.8 Hz; $ArCH_2Ar$), 2.99 (d, 4H, $^2J_{HH}$ = 12.7 Hz; $ArCH_2Ar$), 2.05–1.94 (m, 4H; $C\underline{H}_2CH_3$), 1.91–1.80 (m, 4H; $C\underline{H}_2CH_3$), 1.34 (s, 18H; $C(CH_3)_3$), 1.05 (s, 18H; $C(CH_3)_3$), 1.01 (s, 18H; $C(CH_3)_3$), 1.00 (t, 6H, $^3J_{HH}$ = 7.5 Hz; CH_3), 0.94 (t, 6H, $^3J_{HH}$ = 7.5 Hz; CH_3), 0.84 (s, 18H; $C(CH_3)_3$) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 154.02, 153.43, 151.97, 151.67, 145.95 (C_{Ar}), 144.68 ($C_{Ar\ Trz}$)*, 144.41, 144.25, 144.03, 135.09, 134.57, 133.60, 131.76 (C_{Ar}), 125.67, 124.72, 124.71, 124.62 (CH_{Ar}), 123.62 ($CH_{Ar\ Trz}$)*, 77.84, 77.20, 71.56, 65.80 (OCH_2), 49.28 (NCH_2), 34.12, 33.73, 33.60 ($\underline{C}(CH_3)_3$), 31.67 ($C(\underline{C}H_3)_3$), 31.57 ($ArCH_2Ar$), 31.41, 31.35, 31.09 ($C(\underline{C}H_3)_3$), 30.90 ($ArCH_2Ar$), 23.54, 23.23 ($\underline{C}H_2CH_3$), 10.73, 10.57 (CH_3) ppm. ESI-MS *m*/*z*: 1703.1115 $[M+2Na]^{2+}$ for $C_{220}H_{292}Na_2N_{12}O_{16}$ (1703.1128).

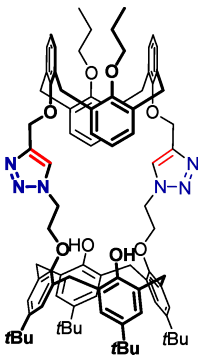


Calix[4]semitube ***AF*** was prepared according to *General procedure* from calixarene **A** (0.072 g, 0.10 mmol), calixarene **F** (0.065 g, 0.10 mmol), CuI (0.019 g, 0.10 mmol) and Et_3N (3 ml) in toluene (10 ml). The reaction mixture was stirred at room temperature for 48 h. Column: gradient from dichloromethane to dichloromethane/ethanol (100:1). Yield 0.026 g (19%), white solid. M.p. >250 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.83 (s, 2H; ArH_{Trz}), 7.08 (s, 4H; ArH), 7.04 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 7.02–6.97 (m, 6H; ArH), 6.91–

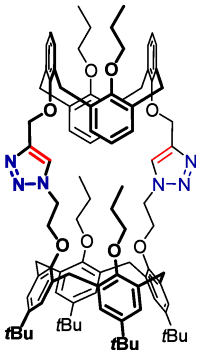
6.86 (m, 2H; ArH), 6.81 (s, 2H; OH), 6.76 (s, 4H; ArH), 5.18 (s, 4H; OCH_2Trz), 4.31 (d, 4H, $^2J_{HH}$ = 13.1 Hz; $ArCH_2Ar$), 4.01–3.96 (m, 4H; NCH_2), 3.94 (d, 4H, $^2J_{HH}$ = 16.7 Hz; $ArCH_2Ar$), 3.85 (d, 4H, $^2J_{HH}$ = 16.7 Hz; $ArCH_2Ar$), 3.62–3.56 (m, 4H; $NCH_2C\underline{H}_2$), 3.42–3.37 (m, 4H; $OC\underline{H}_2CH_2CH_3$), 3.37 (d, 4H, $^2J_{HH}$ = 13.1 Hz; $ArCH_2Ar$), 1.29 (s, 18H; $C(CH_3)_3$), 1.20–1.09 (m, 4H; $C\underline{H}_2CH_3$), 0.91 (s, 18H; $C(CH_3)_3$), 0.58 (t, 6H, $^3J_{HH}$ = 7.5 Hz; CH_3) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.73, 155.14, 150.31, 149.48, 147.41 (C_{Ar}), 144.62 ($C_{Ar\ Trz}$), 141.87, 134.18, 133.40, 132.22 (C_{Ar}), 129.33, 128.79 (CH_{Ar}), 127.80 (C_{Ar}), 125.60, 125.12, 123.20 (CH_{Ar}), 122.90 ($CH_{Ar\ Trz}$)*, 122.57 (CH_{Ar}), 71.68, 70.41, 66.74 (OCH_2), 48.71 (NCH_2), 38.03 ($ArCH_2Ar$), 33.90, 33.84 ($\underline{C}(CH_3)_3$), 31.67 ($C(\underline{C}H_3)_3$), 31.42 ($ArCH_2Ar$), 30.92 ($C(\underline{C}H_3)_3$), 22.66 ($\underline{C}H_2CH_3$), 10.18 (CH_3) ppm. ESI-MS *m/z*: 1371.7831 $[M+H]^+$ for $C_{88}H_{103}N_6O_8$ (1371.7832).



Calix[4]semitube ***BF*** was prepared according to *General procedure* from calixarene **B** (0.081 g, 0.10 mmol), calixarene **F** (0.065 g, 0.10 mmol), CuI (0.019 g, 0.10 mmol) and Et_3N (3 ml) in toluene (10 ml). The reaction mixture was stirred at 70 °C for 9 h. Column: gradient from dichloromethane to dichloromethane/ethanol (50:1). Yield 0.060 g (41%), white solid. M.p. >250 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.53 (s, 2H; ArH_{Trz}), 7.09 (s, 4H; ArH), 7.03 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.80 (t, 2H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.71–6.64 (m, 6H; ArH), 6.42 (s, 4H; ArH), 5.39 (s, 4H; OCH_2Trz), 4.23 (d, 4H, $^2J_{HH}$ = 12.7 Hz; $ArCH_2Ar$), 4.16–4.10 (m, 4H; NCH_2), 4.05–4.00 (m, 4H; $NCH_2C\underline{H}_2$), 3.77 (d, 4H, $^2J_{HH}$ = 15.5 Hz; $ArCH_2Ar$), 3.70–3.64 (m, 4H; $OC\underline{H}_2CH_2CH_3$), 3.63 (d, 4H, $^2J_{HH}$ = 15.5 Hz; $ArCH_2Ar$), 3.52–3.46 (m, 4H; $OC\underline{H}_2CH_2CH_3$), 3.09 (d, 4H, $^2J_{HH}$ = 12.7 Hz; $ArCH_2Ar$), 1.81–1.69 (m, 4H; $C\underline{H}_2CH_3$), 1.47–1.36 (m, 4H; $C\underline{H}_2CH_3$), 1.32 (s, 18H; $C(CH_3)_3$), 1.03 (t, 6H, $^3J_{HH}$ = 7.5 Hz; CH_3), 0.81 (s, 18H; $C(CH_3)_3$), 0.75 (t, 6H, $^3J_{HH}$ = 7.5 Hz; CH_3) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.42, 155.29, 153.51, 152.49, 145.16 (C_{Ar}), 145.12 ($C_{Ar\ Trz}$)*, 143.98, 135.60, 133.92, 133.06, 131.73 (C_{Ar}), 130.21, 129.15, 125.78 (CH_{Ar}), 125.25 ($CH_{Ar\ Trz}$)*, 124.34, 122.64, 121.42 (CH_{Ar}), 77.02, 72.58, 68.80, 65.64 (OCH_2), 49.75 (NCH_2), 37.22 ($ArCH_2Ar$), 34.02, 33.51 ($\underline{C}(CH_3)_3$), 31.71 ($ArCH_2Ar$), 31.67, 31.09 ($C(\underline{C}H_3)_3$), 23.21, 23.06 ($\underline{C}H_2CH_3$), 10.64, 10.21 (CH_3) ppm. ESI-MS *m/z*: 1478.8627 $[M+Na]^+$ for $C_{94}H_{114}NaN_6O_8$ (1478.8624).

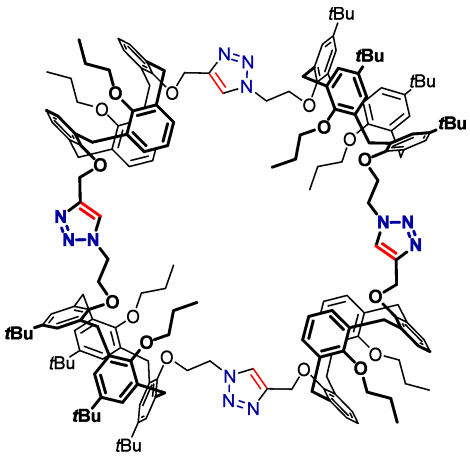


Calix[4]semitube ***CD*** was prepared according to *General procedure* from calixarene **C** (0.115 g, 0.20 mmol), calixarene **D** (0.157 g, 0.20 mmol), CuI (0.012 g, 0.06 mmol) and Et_3N (0.170 ml, 1.20 mmol) in toluene (15 ml). The reaction mixture was stirred at room temperature for 48 h. Column: gradient from dichloromethane to dichloromethane/ethanol (100:1), the product separated from the column was additionally washed with hexane. Yield 0.124 g (46%), white solid. M.p. 244–246 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.08 (s, 4H; ArH), 7.04 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 7.04 (s, 2H; OH), 6.86 (t, 2H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.77 (s, 4H; ArH), 6.70 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.46 (s, 2H; ArH_{Trz}), 6.26 (t, 2H, $^3J_{HH}$ = 7.5 Hz; ArH), 5.00–4.92 (m, 4H; NCH_2), 4.85 (c, 4H; OCH_2Trz), 4.41–4.34 (m, 4H; $NCH_2C\underline{H}_2$), 4.00 (d, 4H, $^2J_{HH}$ = 13.2 Hz; $ArCH_2Ar$), 3.76 (d, 4H, $^2J_{HH}$ = 15.9 Hz; $ArCH_2Ar$), 3.60 (d, 4H, $^2J_{HH}$ = 15.9 Hz; $ArCH_2Ar$), 3.38 (d, 4H, $^2J_{HH}$ = 13.2 Hz; $ArCH_2Ar$), 3.29–3.24 (m, 4H; $OC\underline{H}_2CH_2CH_3$), 1.30 (s, 18H; $C(CH_3)_3$), 1.30–1.22 (m, 4H; $C\underline{H}_2CH_3$), 0.90 (s, 18H; $C(CH_3)_3$), 0.66 (t, 6H, $^3J_{HH}$ = 7.5 Hz; CH_3) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 156.95, 155.53, 150.01, 148.64, 147.76 (C_{Ar}), 144.77 ($C_{Ar\,Trz}$), 142.07, 134.47, 134.06, 131.92 (C_{Ar}), 129.78, 128.94 (CH_{Ar}), 127.24 (C_{Ar}), 125.80 (CH_{Ar}), 125.54 ($CH_{Ar\,Trz}$)*, 125.14, 122.98, 121.56 (CH_{Ar}), 73.59, 71.58, 63.68 (OCH_2), 49.16 (NCH_2), 38.08 ($ArCH_2Ar$), 33.89, 33.86 ($\underline{C}(CH_3)_3$), 31.65 ($C(\underline{C}H_3)_3$), 31.48 ($ArCH_2Ar$), 30.83 ($C(\underline{C}H_3)_3$), 22.79 ($\underline{C}H_2CH_3$), 10.03 (CH_3) ppm. ESI-MS *m/z*: 1393.7649 $[M+Na]^+$ for $C_{88}H_{102}NaN_6O_8$ (1393.7651).

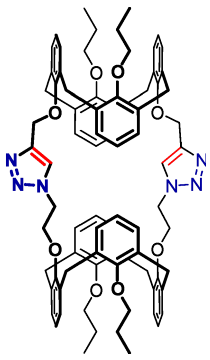


Calix[4]semitube ***CE*** was prepared according to *General procedure* from calixarene **C** (0.199 g, 0.34 mmol), calixarene **E** (0.296 g, 0.34 mmol), CuI (0.019 g, 0.10 mmol) and Et_3N (5 ml) in toluene (25 ml). The reaction mixture was stirred at 60 °C for 9 h. Column: gradient from dichloromethane to dichloromethane/ethanol (20:1). Yield 0.065 g (13%), white solid. M.p. >250 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.20 (bs, 6H; ArH + ArH_{Trz}), 7.08 (d, 4H, $^3J_{HH}$ = 7.6 Hz; ArH), 6.82 (t, 2H, $^3J_{HH}$ = 7.6 Hz; ArH), 6.78 (d, 4H, $^3J_{HH}$ = 7.4 Hz; ArH), 6.55 (s, 4H; ArH), 6.35 (t, 2H, $^3J_{HH}$ = 7.4 Hz; ArH), 5.24–5.19 (m, 4H; $OC\underline{H}_2CH_2$), 4.85 (s, 4H; OCH_2Trz), 4.55–4.49 (m, 4H; $OC\underline{H}_2CH_2$), 4.43 (d, 4H, $^2J_{HH}$ = 12.6 Hz; $ArCH_2Ar$), 3.81–3.77 (m, 4H; NCH_2), 3.75 (d, 4H, $^2J_{HH}$ = 15.8 Hz; $ArCH_2Ar$), 3.72 (d, 4H, $^2J_{HH}$ = 15.8 Hz; $ArCH_2Ar$), 3.56–3.51 (m, 4H; $OC\underline{H}_2CH_2$), 3.28 (d, 4H, $^2J_{HH}$ = 12.6 Hz; $ArCH_2Ar$), 2.15–2.06 (m, 4H; $C\underline{H}_2CH_3$), 1.71–1.62 (m, 4H; $C\underline{H}_2CH_3$), 1.38 (s, 18H; $C(CH_3)_3$), 1.10 (t, 6H,

$^3J_{HH}$ = 7.2 Hz; CH_3), 0.88 (t, 6H, $^3J_{HH}$ = 7.4 Hz; CH_3), 0.85 (s, 18H; $C(CH_3)_3$) ppm. ESI-MS *m/z*: 1456.8804 $[M+H]^+$ for $C_{94}H_{115}N_6O_8$ (1456.8804).



Tetrakis(calix[4]arene) ***C$_2$E$_2$*** was isolated as the more polar product during chromatographic purification of calix[4]semitube **CE**. Yield 0.054 g (11%), white solid. M.p. 243–245 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.10 (s, 4H; ArH), 7.08 (s, 2H; ArH_{Trz}), 6.99 (d, 4H, $^3J_{HH}$ = 7.4 Hz; ArH), 6.74 (t, 2H, $^3J_{HH}$ = 7.4 Hz; ArH), 6.62 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.51 (s, 4H; ArH), 6.02 (t, 2H, $^3J_{HH}$ = 7.5 Hz; ArH), 5.28–5.22 (m, 4H; $OC\underline{H}_2CH_2$), 4.71 (s, 4H; OCH_2Trz), 4.68–4.62 (m, 4H; $OC\underline{H}_2CH_2$), 4.47 (d, 4H, $^2J_{HH}$ = 12.7 Hz; $ArCH_2Ar$), 3.81–3.75 (m, 4H; NCH_2), 3.60 (d, 4H, $^2J_{HH}$ = 14.8 Hz; $ArCH_2Ar$), 3.50 (d, 4H, $^2J_{HH}$ = 14.8 Hz; $ArCH_2Ar$), 3.38–3.33 (m, 4H; $OC\underline{H}_2CH_2$), 3.20 (d, 4H, $^2J_{HH}$ = 12.7 Hz; $ArCH_2Ar$), 1.96–1.87 (m, 4H; $C\underline{H}_2CH_3$), 1.51–1.43 (m, 4H; $C\underline{H}_2CH_3$), 1.30 (s, 18H; $C(CH_3)_3$), 0.86 (t, 6H, $^3J_{HH}$ = 7.4 Hz; CH_3), 0.85 (s, 18H; $C(CH_3)_3$), 0.78 (t, 6H, $^3J_{HH}$ = 7.3 Hz; CH_3) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 156.34, 155.54, 153.88, 152.18, 145.72, 144.33 (C_{Ar}), 144.21 ($C_{Ar\ Trz}$), 135.03, 134.18, 133.36, 131.91 (C_{Ar}), 129.73, 129.69, 125.70, 124.66 (CH_{Ar}), 123.10 ($CH_{Ar\ Trz}$), 122.36, 121.58 (CH_{Ar}), 77.88, 72.96, 72.47, 64.88 (OCH_2), 49.91 (NCH_2), 36.74 ($ArCH_2Ar$), 34.09, 33.60 ($\underline{C}(CH_3)_3$), 31.66 ($C(\underline{C}H_3)_3$), 31.78 ($ArCH_2Ar$), 31.12 ($C(\underline{C}H_3)_3$), 23.45, 23.32 ($\underline{C}H_2CH_3$), 10.44, 10.29 (CH_3) ppm. ESI-MS *m/z*: 1456.8808 $[M+2H]^{2+}$ for $C_{188}H_{230}N_{12}O_{16}$ (1456.8804).



Calix[4]semitube ***CF*** was prepared according to *General procedure* from calixarene **C** (0.199 g, 0.34 mmol), calixarene **F** (0.220 g, 0.34 mmol), $CuSO_4 \cdot 5H_2O$ (0.054 g, 0.34 mmol) and sodium ascorbate (0.134 g, 0.68 mmol) in THF (40 ml) and H_2O (8 ml). The reaction mixture was stirred at 60 °C for 24 h. Column: gradient from dichloromethane to dichloromethane/ethanol (50:1). Yield 0.166 g (40%), white solid. M.p. >250 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.08 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 7.05 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.98 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.90 (t, 2H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.87 (t, 2H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.80 (d, 4H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.71 (t, 2H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.37 (t, 2H, $^3J_{HH}$ = 7.5 Hz; ArH), 6.26 (s, 2H; ArH_{Trz}), 4.81 (s, 4H; OCH_2Trz), 4.30–4.23 (m, 4H; NCH_2), 4.09–4.03 (m, 4H;

$NCH_2C\underline{H}_2$), 3.92 (d, 4H, $^2J_{HH}$ = 16.4 Hz; $ArCH_2Ar$), 3.48 (d, 4H, $^2J_{HH}$ = 16.4 Hz; $ArCH_2Ar$), 3.78 (d, 4H, $^2J_{HH}$ = 15.7 Hz; $ArCH_2Ar$), 3.61 (d, 4H, $^2J_{HH}$ = 15.7 Hz; $ArCH_2Ar$), 3.42–3.33 (m, 8H; $OC\underline{H}_2CH_2CH_3$), 1.44–1.31 (m, 4H; $C\underline{H}_2CH_3$), 1.21–1.09 (m, 4H; $C\underline{H}_2CH_3$), 0.71 (t, 6H, $^3J_{HH}$ = 7.5 Hz; CH_3), 0.68 (t, 6H, $^3J_{HH}$ = 7.5 Hz; CH_3) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.22, 156.93, 155.62, 154.92 (C_{Ar}), 144.39 ($C_{Ar\ Trz}$), 134.38, 134.37, 134.05, 133.38 (C_{Ar}), 129.90, 129.87, 129.29, 128.46 (CH_{Ar}), 124.12 ($CH_{Ar\ Trz}$)*, 123.24, 123.01, 122.42, 121.13 (CH_{Ar}), 71.94, 71.47, 68.35, 63.57 (OCH_2), 48.69 (NCH_2), 38.34, 37.97 ($ArCH_2Ar$), 22.98, 22.21 ($\underline{C}H_2CH_3$), 10.10, 9.92 (CH_3) ppm. ESI-MS *m*/*z*: 1231.6269 $[M+H]^+$ for $C_{78}H_{83}N_6O_8$ (1231.6267).

Tuning the conditions for the preparation of calix[4]semitubes

Table S1 Different catalytic systems used in the CuAAC reactions between calixarenes **A** and **D**

Entry	Catalyst (equiv per bis(azlkyne)/bis(azide))	External ligand (equiv per Cu)	Solvent	Temp., °C	Time, h	Reaction outcome			
						A or **D**	**AD**	Polymer	Other products
1	CuI·P(OEt)$_3$ (0.3)	–	toluene	110	1	+	+	+	–
2	CuI·P(OEt)$_3$ (3.0)	–	toluene	110	1	–	+	+	–
3	CuI (0.3)	–	toluene	110	2	+	–	–	–
4	CuI (0.3)	*i*Pr$_2$EtN (20)	toluene	110	1	+	+	+	–
5	CuI (0.3)	TBTA (2.0)	toluene	110	2	–	+	+	–
6	CuI (1.0)	TBTA (2.0)	toluene	110	2	–	+	+	–
7	CuI (2.0)	TBTA (2.0)	toluene	110	2	–	+	+	–
8	CuSO$_4$·5H$_2$O (0.3)/sodium ascorbate	–	THF/H$_2$O	65	7	–	+	+	–
9	CuI (0.3)	*i*Pr$_2$EtN (20)	toluene	rt	48	+	+	+	–
10	CuI (0.3)	Et$_3$N (20)	toluene	rt	48	–	+	+	–
11	CuI (0.3)	Et$_3$N (20)	CH$_2$Cl$_2$	rt	48	–	+	+	–
12	CuI (0.3)	Et$_3$N (20)	benzene	rt	48	–	+	+	–
13	CuI (0.3)	Et$_3$N (20)	CH$_3$CN	rt	48	–	–	+	+
14	CuI (0.3)	Et$_3$N (20)	DMF	rt	48	–	–	+	+
15	CuI (0.3)	–	DMF	rt	48	–	–	+	–
16	CuI (0.3)	TBTA (2.0)	toluene	rt	48	–	–	+	–
17	CuI (1.0)	TBTA (2.0)	toluene	rt	48	–	–	+	–
18	CuI (2.0)	TBTA (2.0)	toluene	rt	48	–	–	+	–
19	CuI (0.05)	Et$_3$N (20)	toluene	rt	72	+	+	+	–
20	CuCl (0.05)	Et$_3$N (20)	toluene	rt	72	–	+	+	+
21	Cu(OAc)$_2$ (0.3)	Et$_3$N (20)	toluene	rt	48	–	+	+	–
22	Cu(OAc)$_2$ (0.3)	Et$_3$N (20)	CH$_2$Cl$_2$	rt	48	–	+	+	–
23	Cu(OAc)$_2$ (0.3)	–	CH$_2$Cl$_2$	rt	48	+	–	–	–
24	[Cu(CH$_3$CN)$_4$]PF$_6$ (0.3)	–	toluene	rt	48	+	–	–	–
25	[Cu(CH$_3$CN)$_4$]PF$_6$ (0.3)	–	CH$_3$CN	rt	48	+	–	–	–
26	[Cu(CH$_3$CN)$_4$]PF$_6$ (0.3)	Et$_3$N (20)	toluene	rt	48	+	–	–	–
27	[Cu(CH$_3$CN)$_4$]PF$_6$ (0.3)	Et$_3$N (20)	CH$_3$CN	rt	48	–	–	+	+
28	[Cu(CH$_3$CN)$_4$]PF$_6$ (0.3)	Et$_3$N (20)	toluene	100	2	+	–	–	–
29	[Cu(CH$_3$CN)$_4$]PF$_6$ (1.0)	Et$_3$N (20)	toluene	100	2	+	–	–	–
30	[(*i*Pr)CuCl] (0.3)	–	CH$_2$Cl$_2$	rt	48	+	–	–	–
31	[(*i*Pr)CuCl] (0.3)	Et$_3$N (20)	CH$_2$Cl$_2$	rt	48	+	–	–	–

Table S2 Tuning the CuI/Et_3N/toluene catalytic system for the preparation of the calix[4]semitube **AD**

Entry	Catalyst loading, equiv per bis(azlkyne)/bis(azide)	Et_3N/Cu molar ratio	Temp., °C	Time, h	Reaction outcome			
					A or **D**	**AD**	Polymer	Other products
1	0.01	20	100	2	–	+	+	–
2	0.05	20	100	2	–	+	+	–
3	0.30	20	100	2	–	+	+	–
4	1.00	20	100	2	–	+	+	–
5	0.0005	20	rt	48	+	–	–	–
6	0.001	20	rt	48	+	–	–	–
7	0.005	20	rt	48	+	–	–	–
8	0.01	20	rt	48	+	–	–	–
9	0.30	20	rt	48	–	+	+	–
10	0.30	330	rt	48	–	+	+	–
11	1.00	20	rt	48	–	+	+	–
12	1.00	330	rt	48	–	+	+	–
13	2.00	20	rt	48	–	+	+	–
14	2.00	330	rt	48	–	+	+	+

Table S3 Tuning the CuI/Et_3N/toluene catalytic system in the CuAAC between calixarenes **C** and **E**

Entry	Catalyst (equiv per bis(azlkyne)/bis(azide))	External ligand (equiv per Cu)	Solvent	Temp., °C	Time, h	Reaction outcome			
						C or **E**	**CD**	Polymer	Other products
1	CuI (0.3)	Et_3N (20)	toluene	rt	48	+	+	+	–
2	CuI (0.3)	Et_3N (400)	toluene	60	9	–	+	+	+
3	CuI (1.0)	Et_3N (20)	toluene/1,2-dichloroethane	rt	48	–	+	++	+
4	CuI (1.0)	Et_3N (20)	toluene/1,2-dichloroethane	60	9	–	+	++	–
5	CuI (1.0)	Et_3N (20)	toluene	60	9	+	+	+	+
6	CuI (1.0)	Et_3N (20)	1,2-dichloroethane	60	9	+	+	+	–
7	CuI (1.0)	Et_3N (20)	DMF	60	9	+	–	+	+

Table S4 Different catalytic systems tested in the CuAAC reactions between calixarenes **C** and **F**

Entry	Catalyst (equiv per bis(azlkyne)/bis(azide))	External ligand (equiv per Cu)	Solvent	Temp., °C	Time, h	Reaction outcome			
						C or **F**	**CF**	Polymer	Other products
1	CuI (0.3)	Et_3N (20)	toluene/1,2-dichloroethane	rt	48	+	+	+	+
2	CuI (1.0)	Et_3N (20)	toluene/1,2-dichloroethane	rt	48	–	+	+	+
3	CuI (0.3)	Et_3N (20)	toluene/1,2-dichloroethane	60	24	–	+	+	+
4	CuI (1.0)	Et_3N (20)	toluene/1,2-dichloroethane	60	24	–	+	+	+
5	CuI (1.0)*	Et_3N (20)	toluene/1,2-dichloroethane	60	24	–	+	+	+
6	CuI (0.3)	TBTA (2)	toluene/1,2-dichloroethane	60	24	–	+	++	+
7	CuI (1.0)	TBTA (2)	toluene/1,2-dichloroethane	60	24	–	–	++	+
8	CuCl (1.0)	–	toluene/1,2-dichloroethane	60	24	–	+	++	+
9	CuCl (1.0)	Et_3N (20)	toluene/1,2-dichloroethane	rt	48	+	–	+	–
10	CuCl (1.0)	Et_3N (20)	toluene/1,2-dichloroethane	60	24	–	–	+	+
11	CuI·$P(OEt)_3$ (0.3)	–	toluene/1,2-dichloroethane	60	24	–	+	+	+
12	CuI·$P(OEt)_3$ (1.0)	–	toluene/1,2-dichloroethane	60	24	–	+	+	+
13	$CuSO_4$/Na asc. (0.3)	–	THF/H_2O (5:1)	60	24	–	+	+	+
14	$CuSO_4$/Na asc. (1.0)	–	THF/H_2O (5:1)	rt	48	+	++	+	–
15	$CuSO_4$/Na asc. (1.0)	–	THF/H_2O (5:1)	60	6	+	++	+	–
16	$CuSO_4$/Na asc. (1.0)	–	THF/H_2O (5:1)	60	24	–	++	+	–
17	$CuSO_4$/Na asc. (1.0)	–	THF/H_2O (5:1)**	60	24	+	–	–	+
18	$CuSO_4$/Na asc. (1.0)	TBTA (2)	THF/H_2O (5:1)	60	24	–	–	+	+
19	$CuSO_4$/Na asc. (2.0)	–	THF/H_2O (5:1)	60	24	–	+	+	+

* – the bis(alkyne) **C** was pre-reacted with the copper catalyst for 12 h at rt;
** – the reaction was conducted in a diluted solution (5 volumes of the solvent were used).

Table S5 Testing the catalytic system $CuSO_4 \cdot 5H_2O$ (1.0 equiv)/Na asc., THF/H_2O (5:1), 60 °C, 24 h for the preparation of bis(calixarenes) **AE**, **AF**, **BD**, **BE**, **BF**, **CD** and **CE**

Entry	Starting calixarenes	Reaction outcome			
		Starting material	Bis(calixarene)	Polymer	Other products
1	**A** + **E**	–	+	+	–
2	**A** + **F**	–	+	+	–
3	**B** + **D**	+	–	–	+
4	**B** + **E**	+	–	–	–
5	**B** + **F**	+	+	+	–
6	**C** + **D**	–	+	++	–
7	**C** + **E**	–	+	++	+

NMR spectra of novel compounds

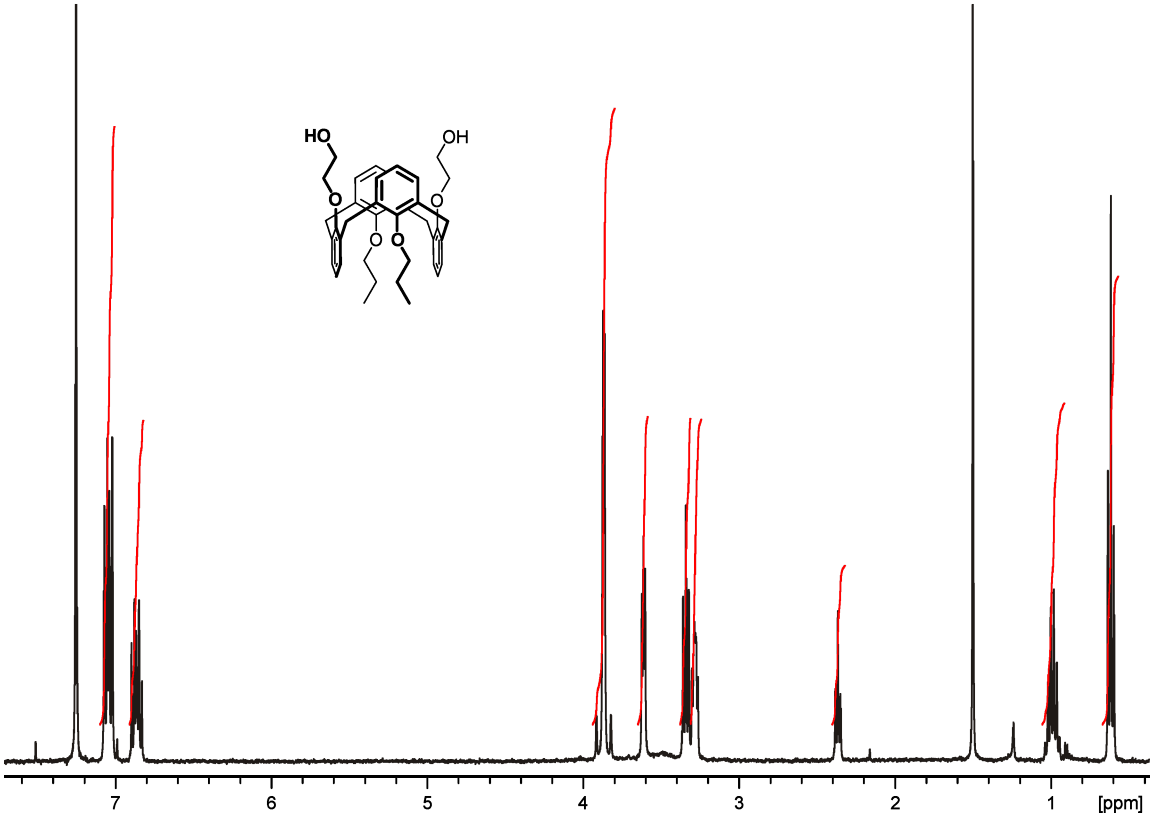


Figure S1. ^{1}H NMR spectrum of calixarene **4** (400 MHz, $CDCl_3$).

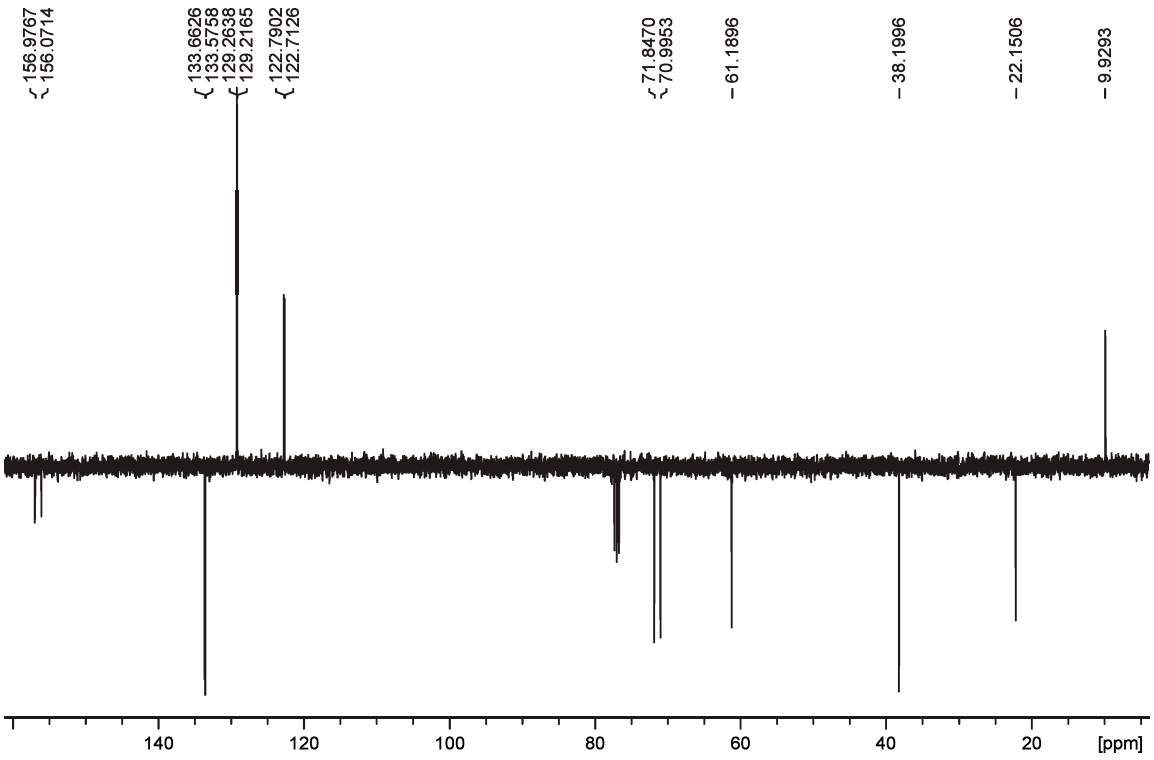


Figure S2. ^{13}C NMR spectrum (APT) of calixarene **4** (100 MHz, $CDCl_3$).

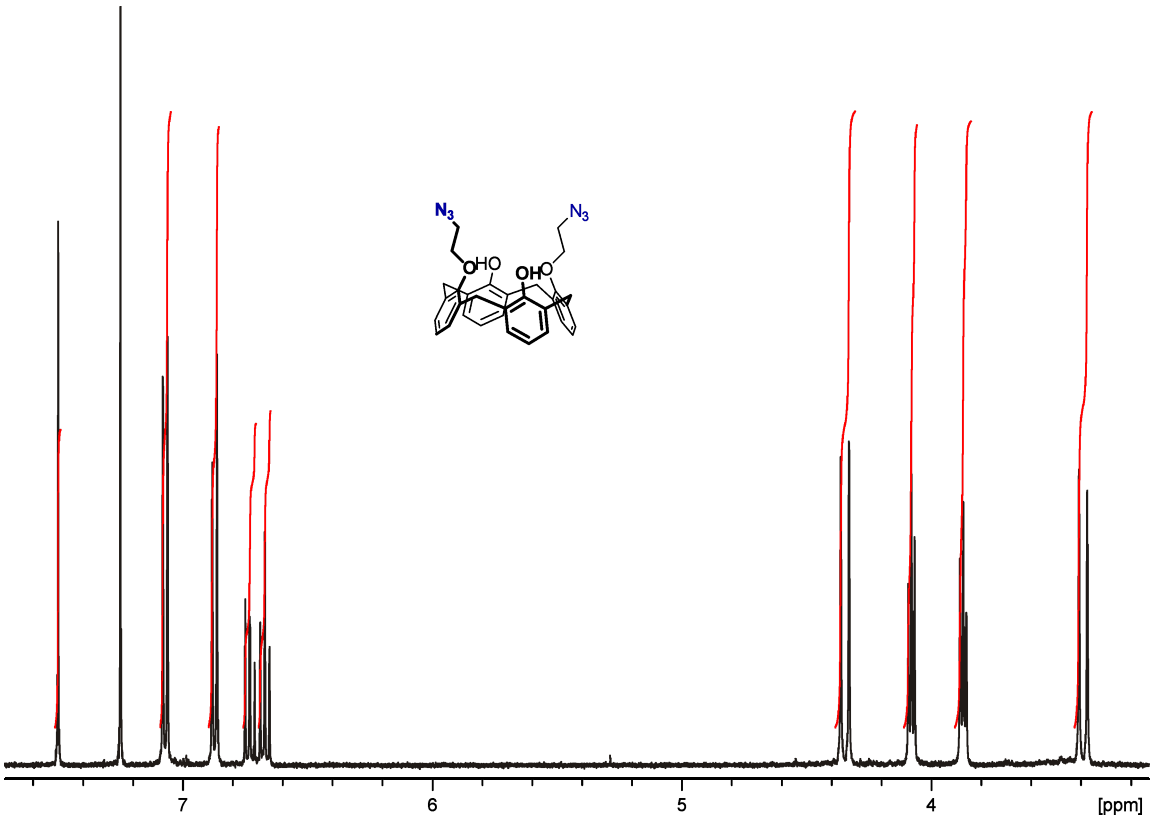


Figure S3. ^{1}H NMR spectrum of calixarene **6** (400 MHz, $CDCl_3$).

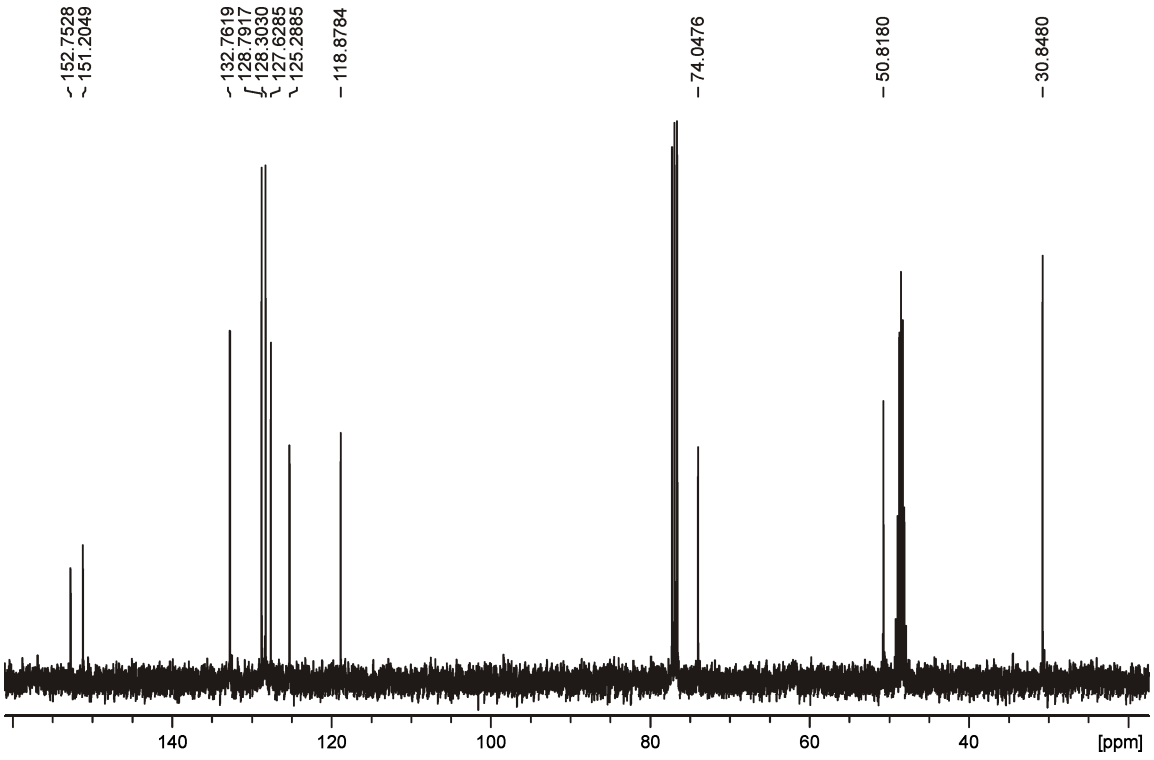


Figure S4. ^{13}C NMR spectrum of calixarene **6** (100 MHz, $CDCl_3$+CD_3OD).

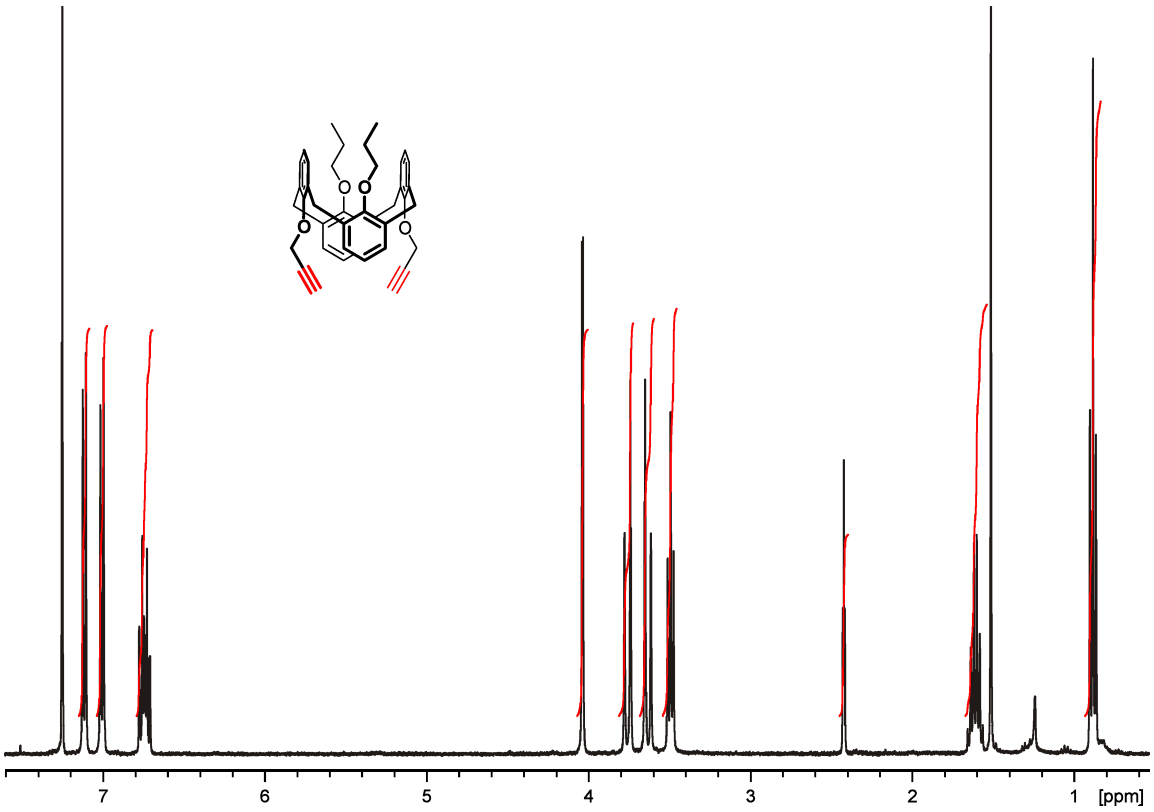


Figure S5. ^{1}H NMR spectrum of calixarene **C** (400 MHz, $CDCl_3$).

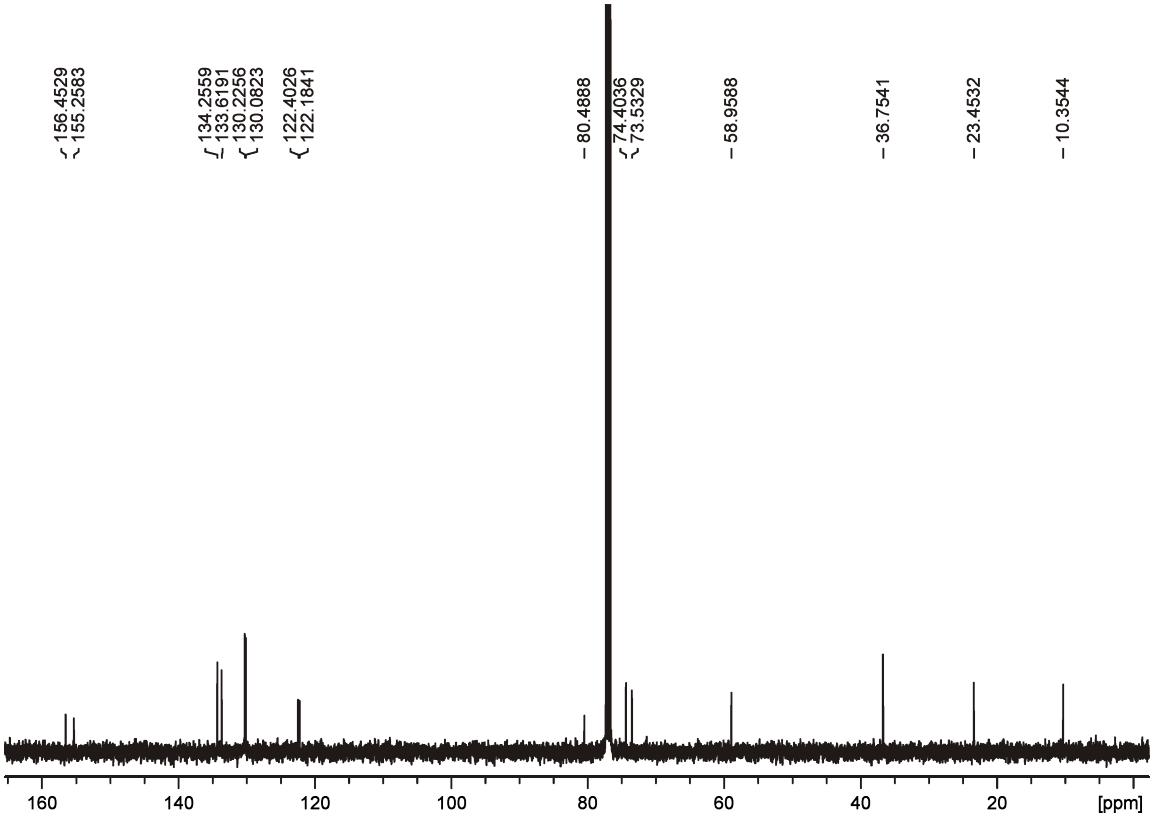


Figure S6. ^{13}C NMR spectrum of calixarene **C** (100 MHz, $CDCl_3$).

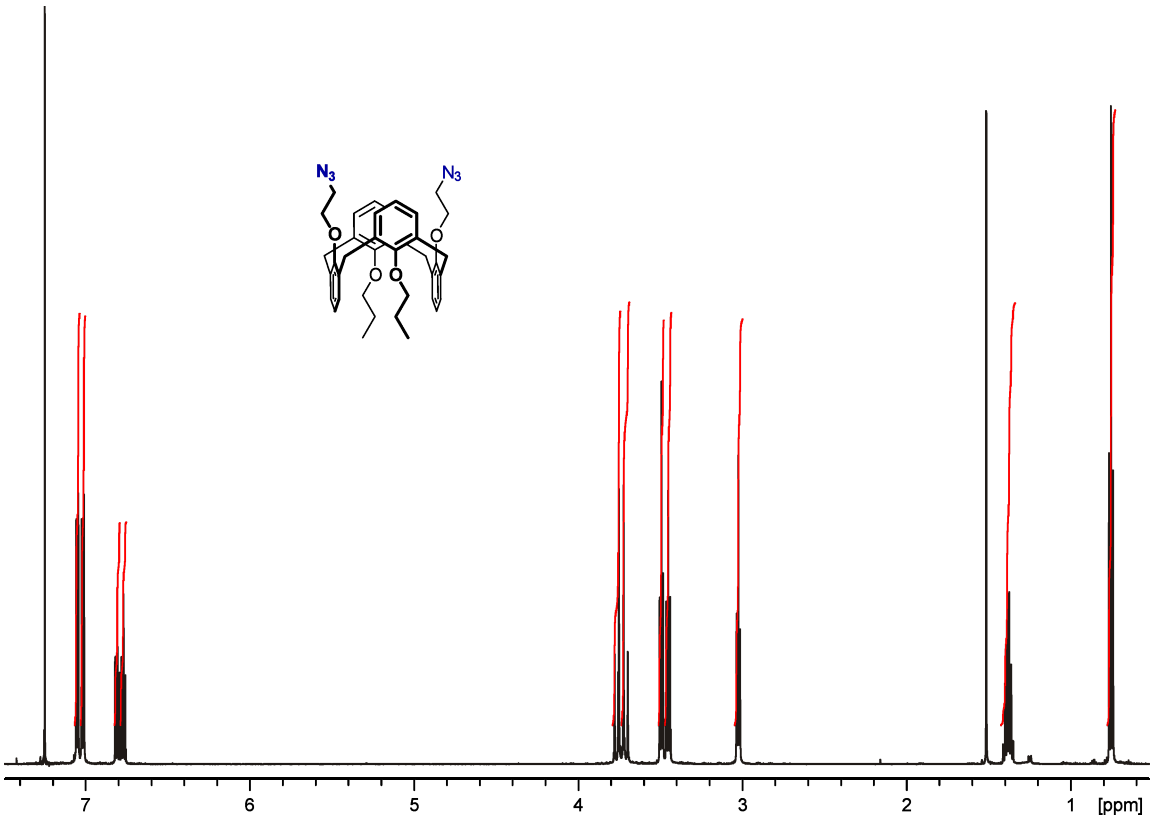


Figure S7. ^{1}H NMR spectrum of calixarene **F** (600 MHz, $CDCl_3$).

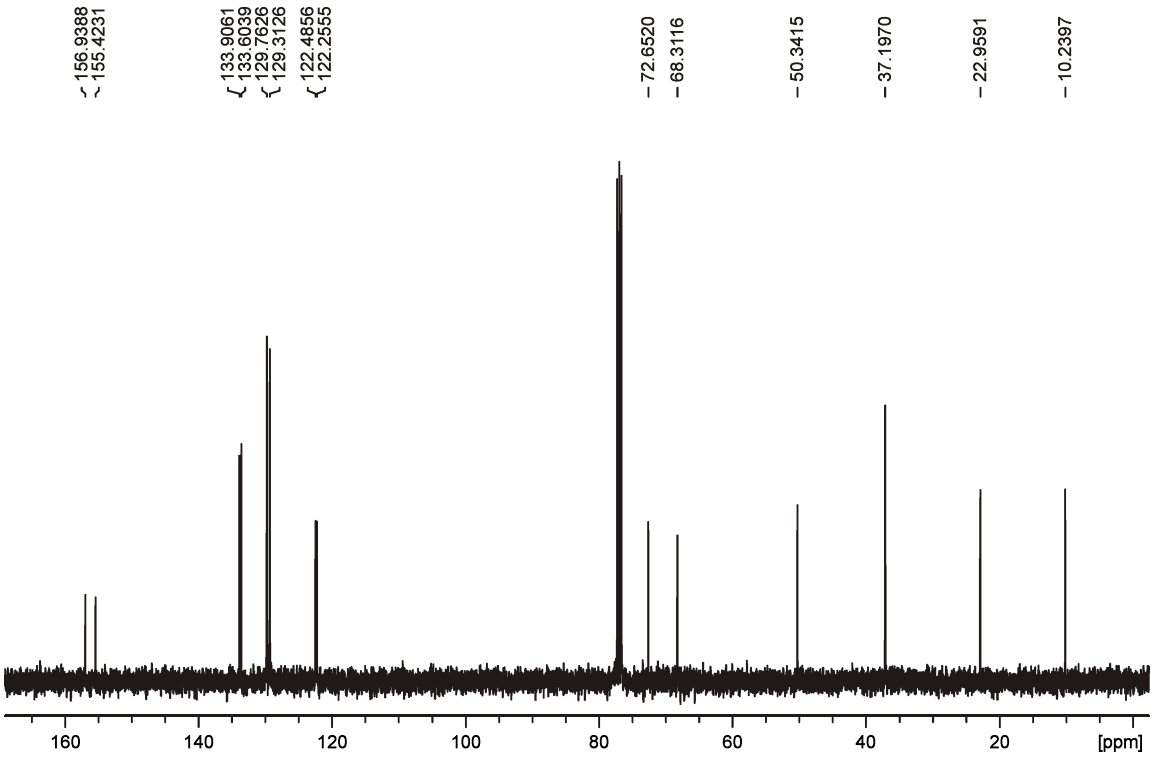


Figure S8. ^{13}C NMR spectrum of calixarene **F** (100 MHz, $CDCl_3$).

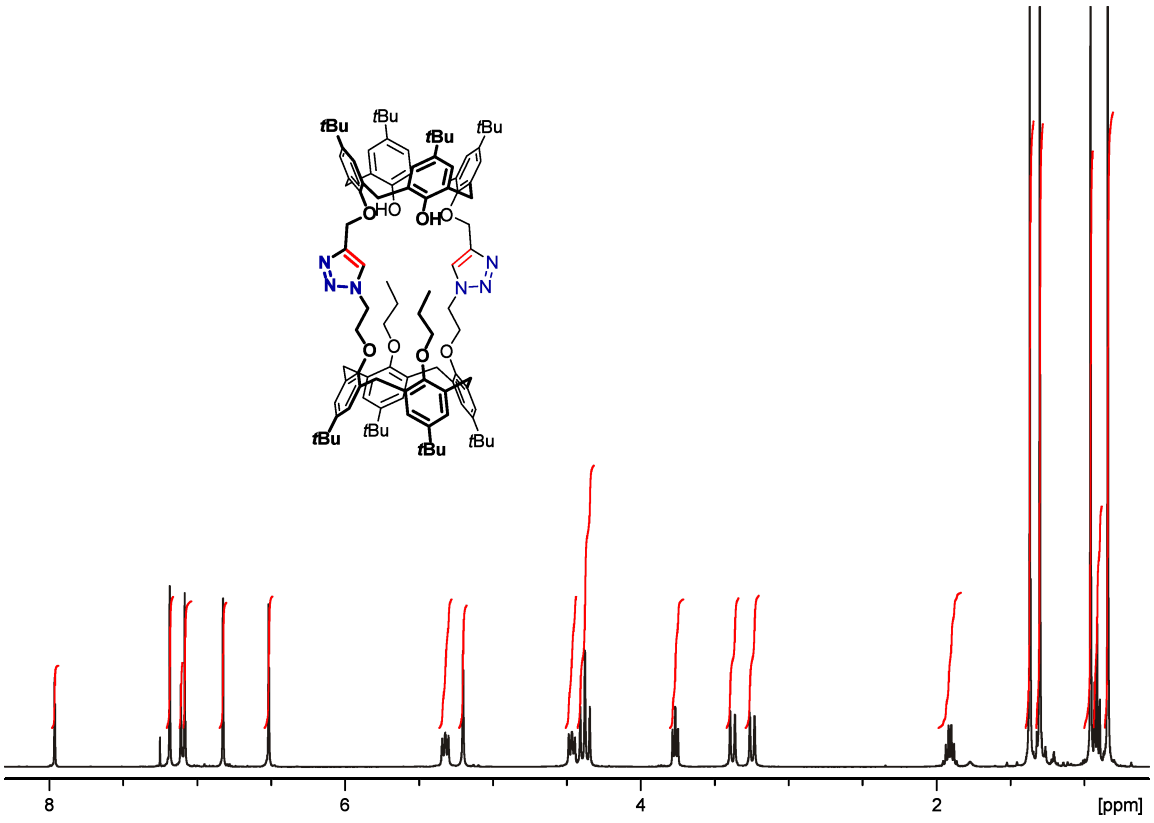


Figure S9. ^{1}H NMR spectrum of calix[4]semitube **AE** (400 MHz, $CDCl_3$).

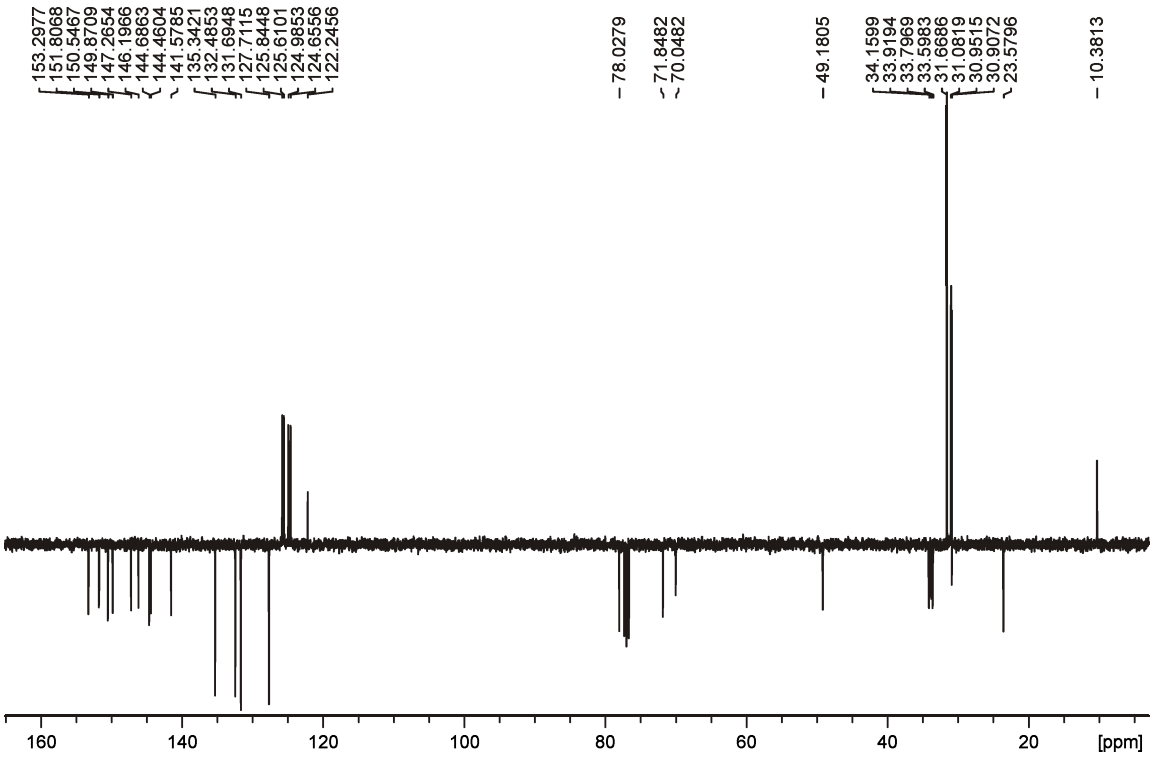


Figure S10. ^{13}C NMR spectrum (APT) of calix[4]semitube **AE** (100 MHz, $CDCl_3$).

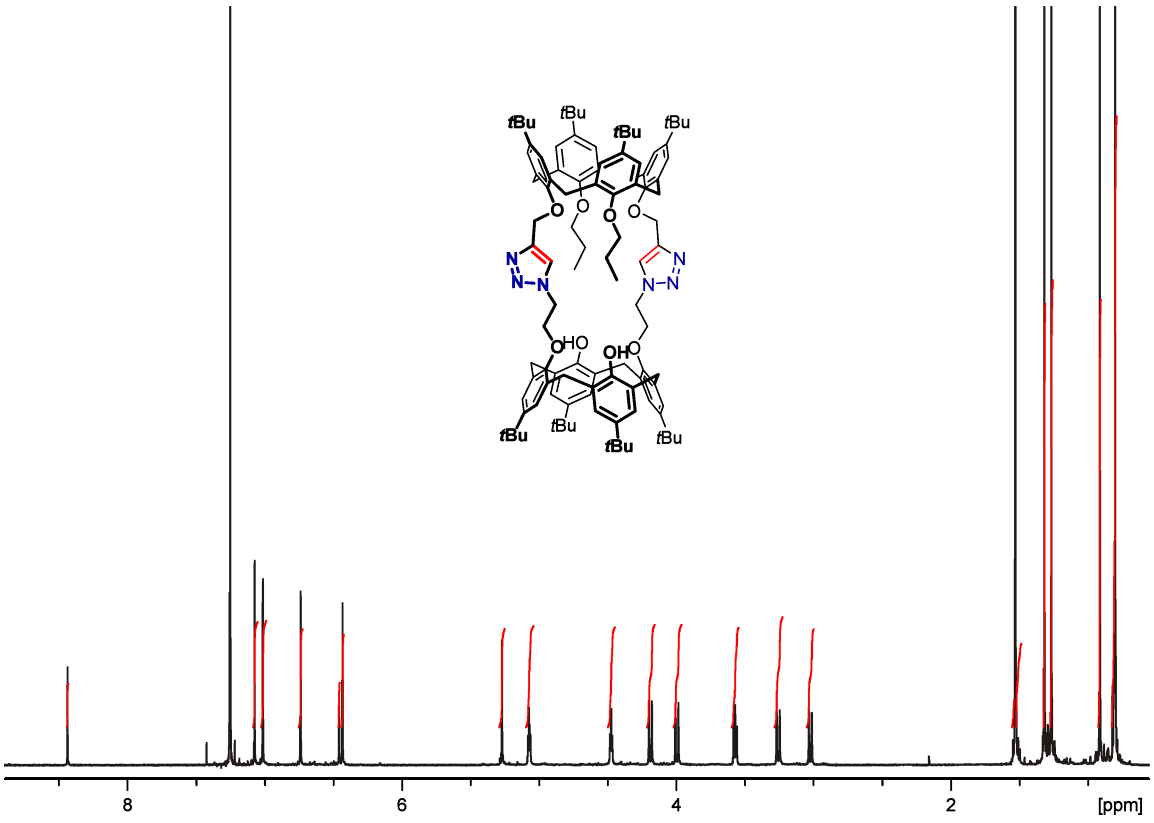


Figure S11. ^{1}H NMR spectrum of calix[4]semitube **BD** (600 MHz, $CDCl_3$).

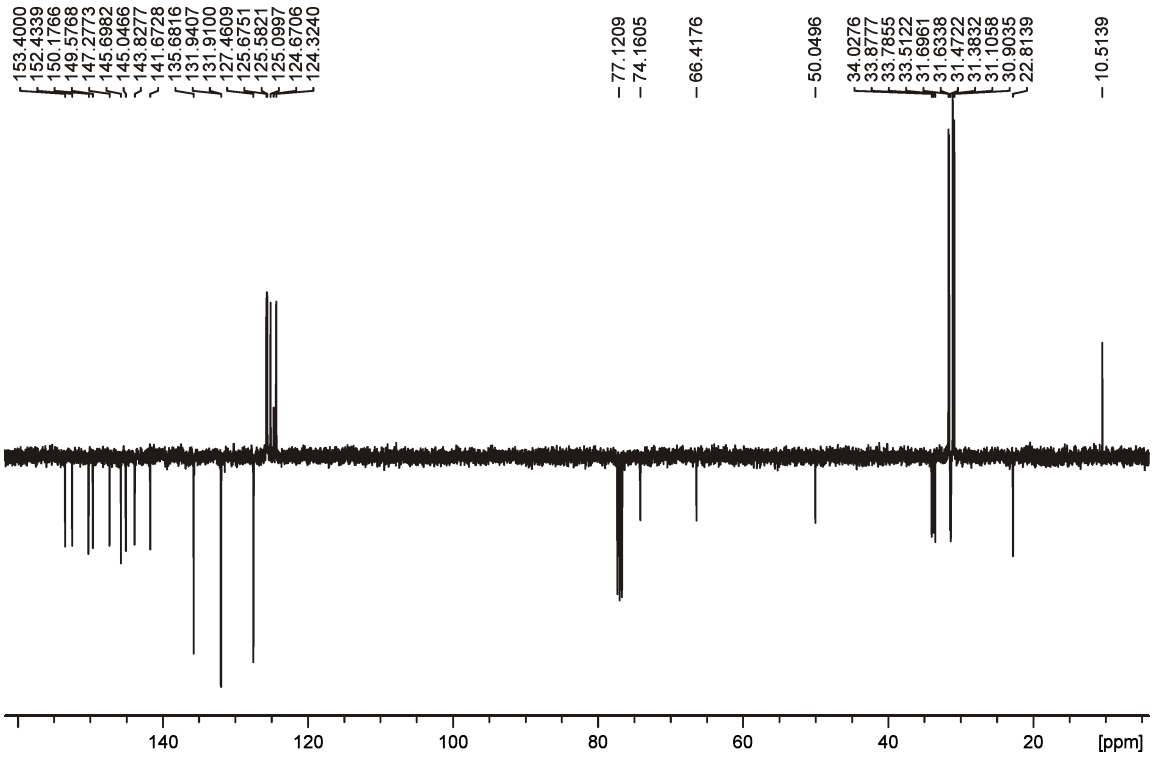


Figure S12. ^{13}C NMR spectrum (APT) of calix[4]semitube **BD** (100 MHz, $CDCl_3$).

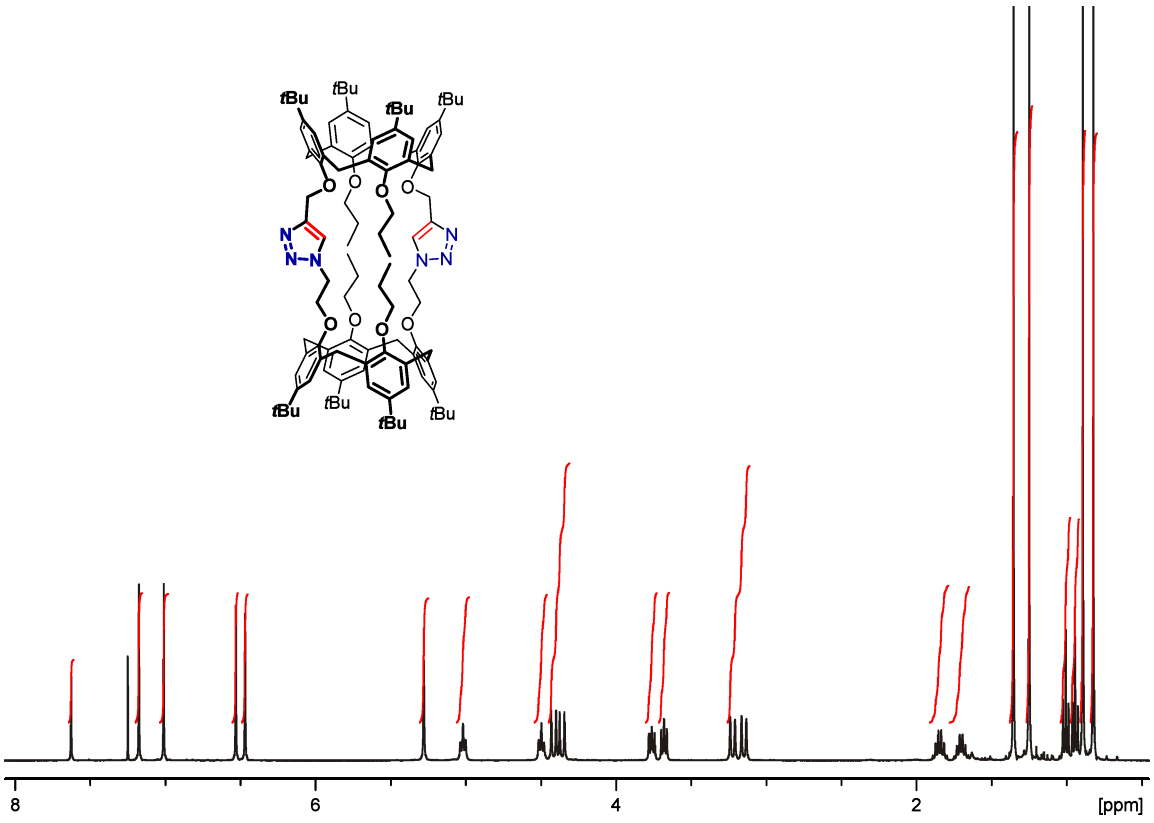


Figure S13. ^{1}H NMR spectrum of calix[4]semitube **BE** (400 MHz, $CDCl_3$).

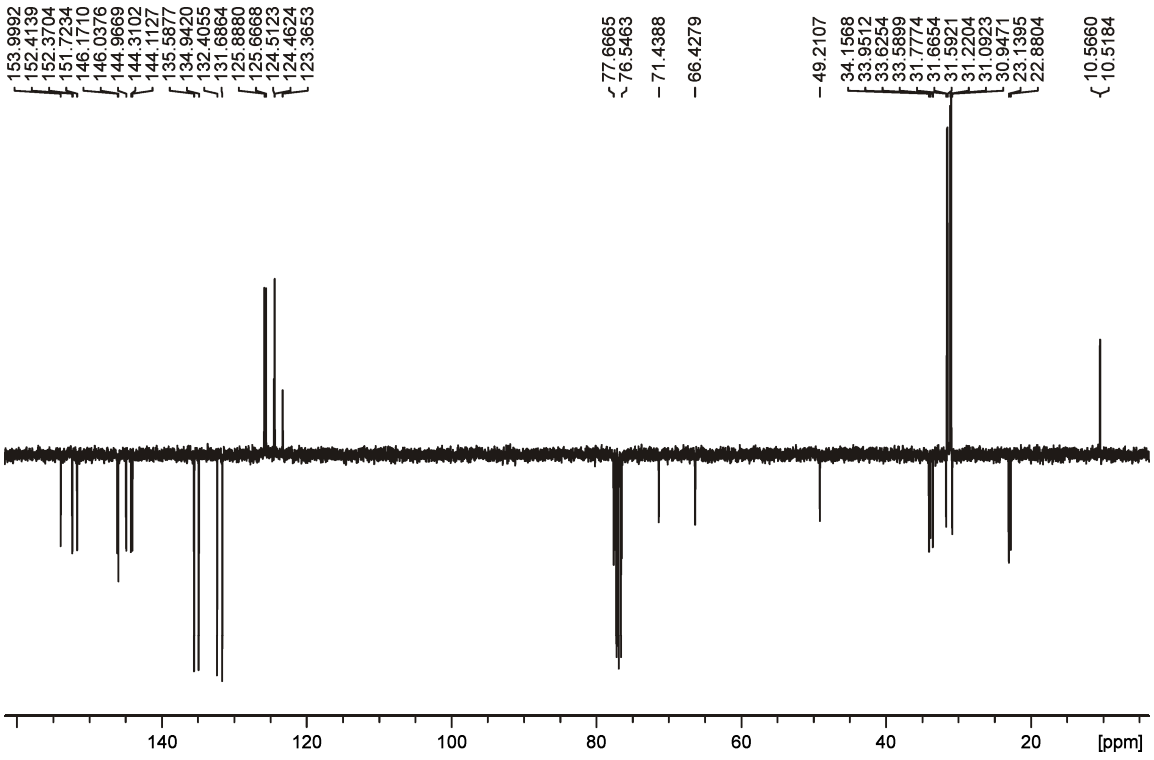


Figure S14. ^{13}C NMR spectrum (APT) of calix[4]semitube **BE** (100 MHz, $CDCl_3$).

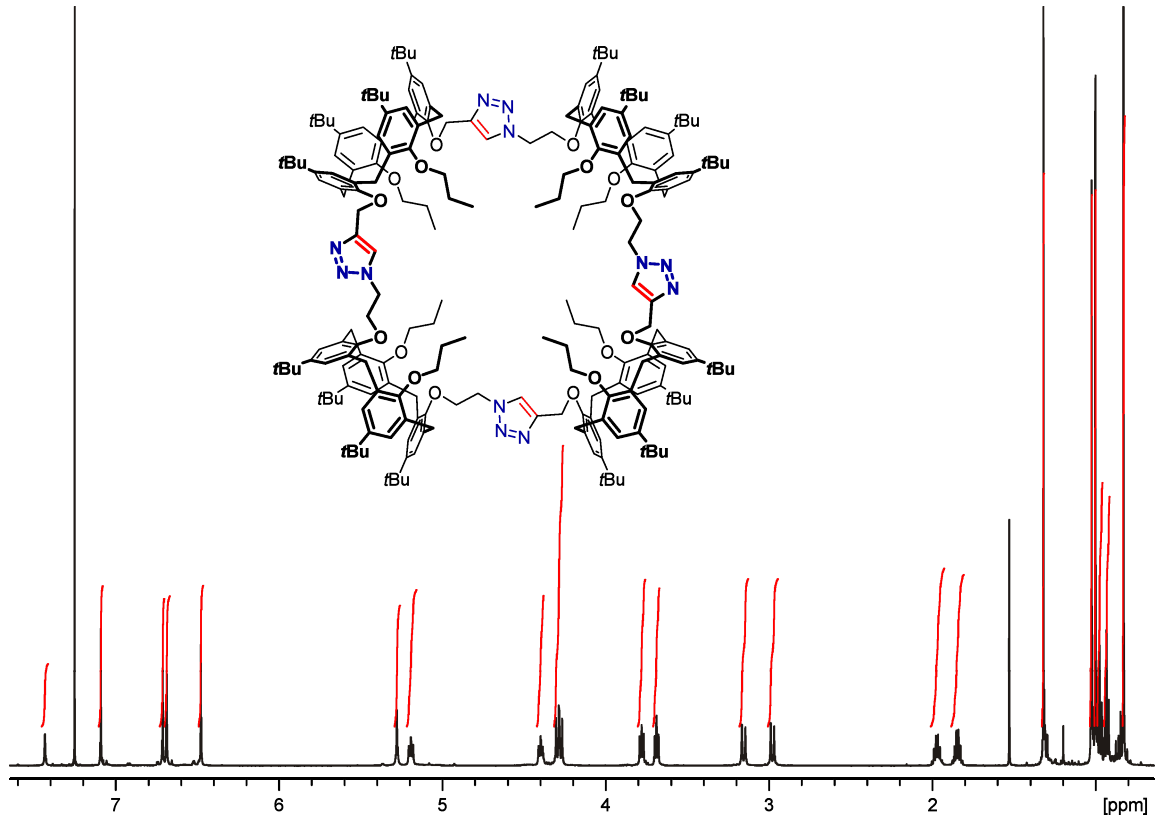


Figure S15. ^{1}H NMR spectrum of tetrakis(calix[4]arene) $\mathbf{B_2E_2}$ (600 MHz, $CDCl_3$).

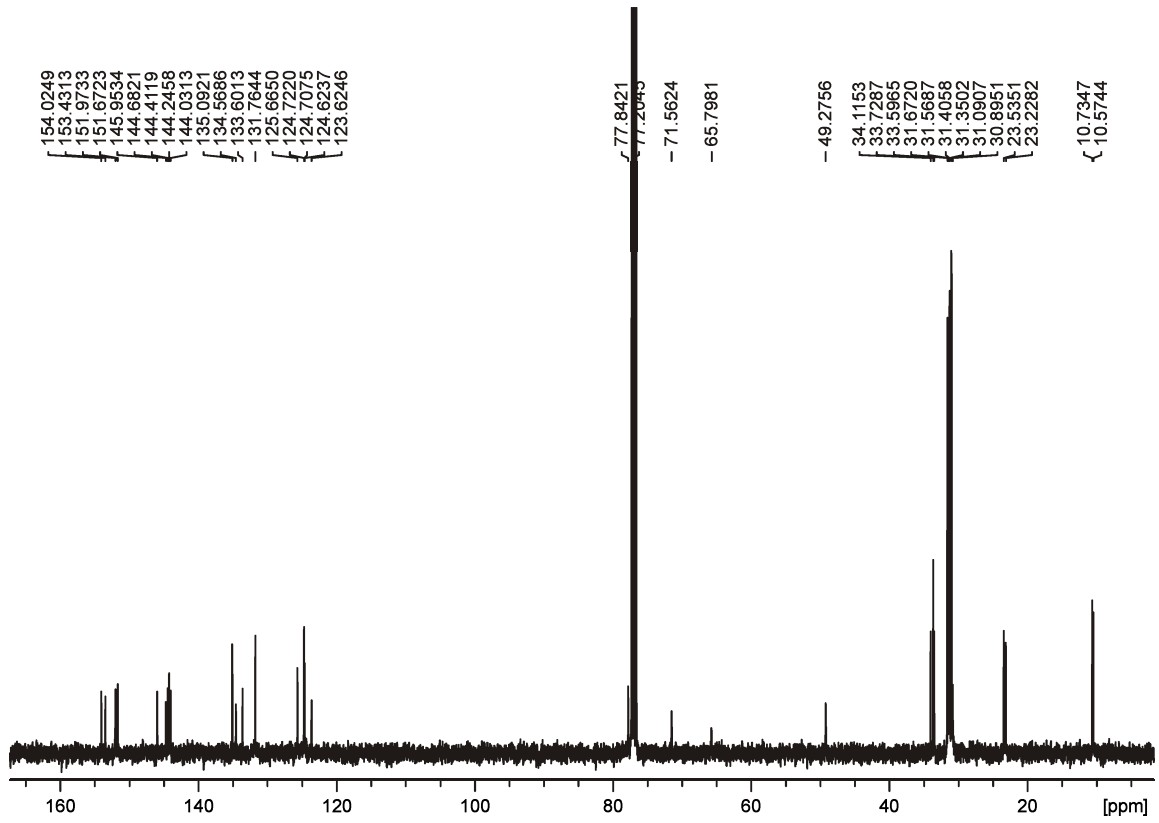


Figure S16. ^{13}C NMR spectrum of tetrakis(calix[4]arene) $\mathbf{B_2E_2}$ (100 MHz, $CDCl_3$).

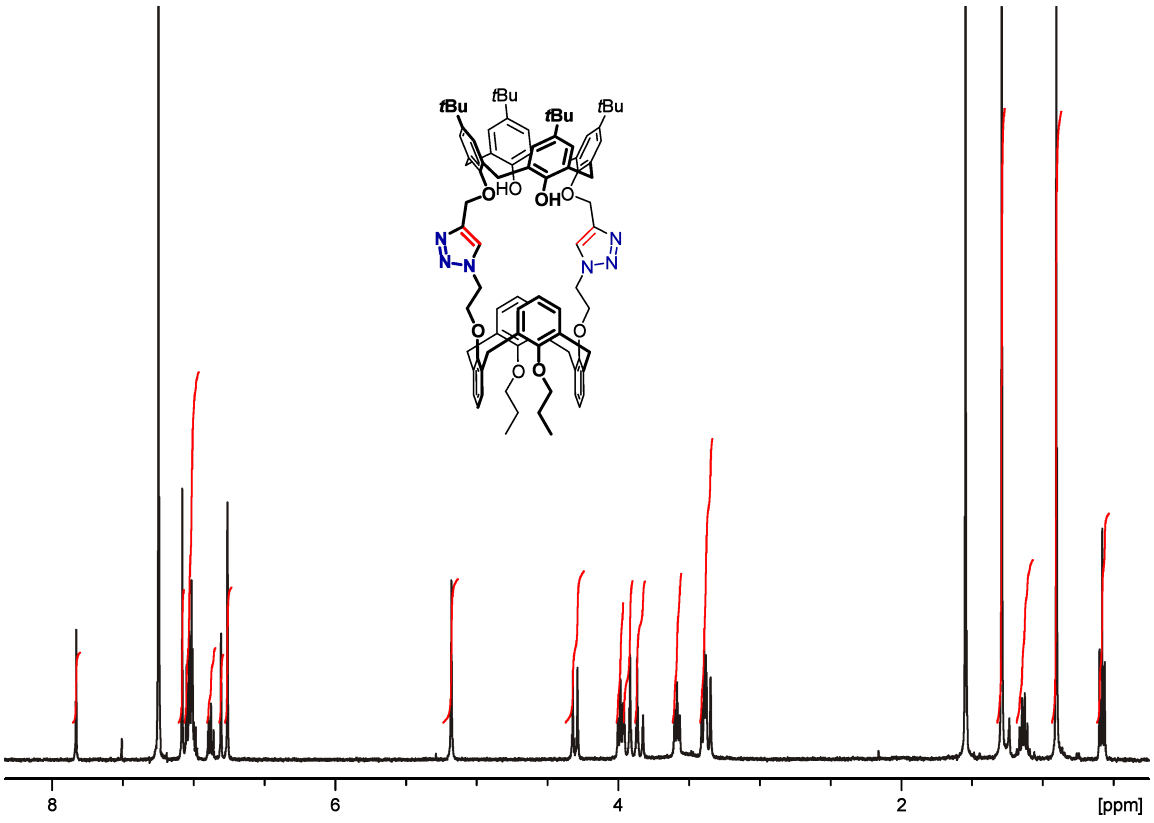


Figure S17. ^{1}H NMR spectrum of calix[4]semitube **AF** (400 MHz, $CDCl_3$).

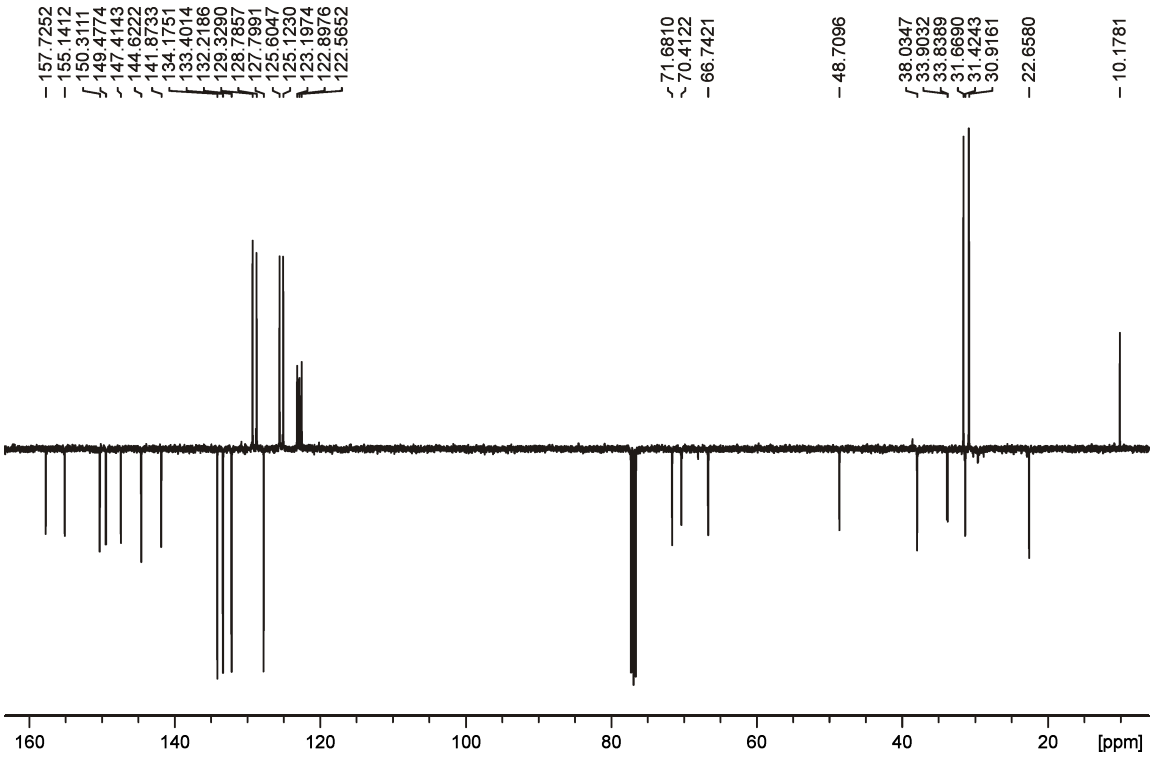


Figure S18. ^{13}C NMR spectrum (APT) of calix[4]semitube **AF** (100 MHz, $CDCl_3$).

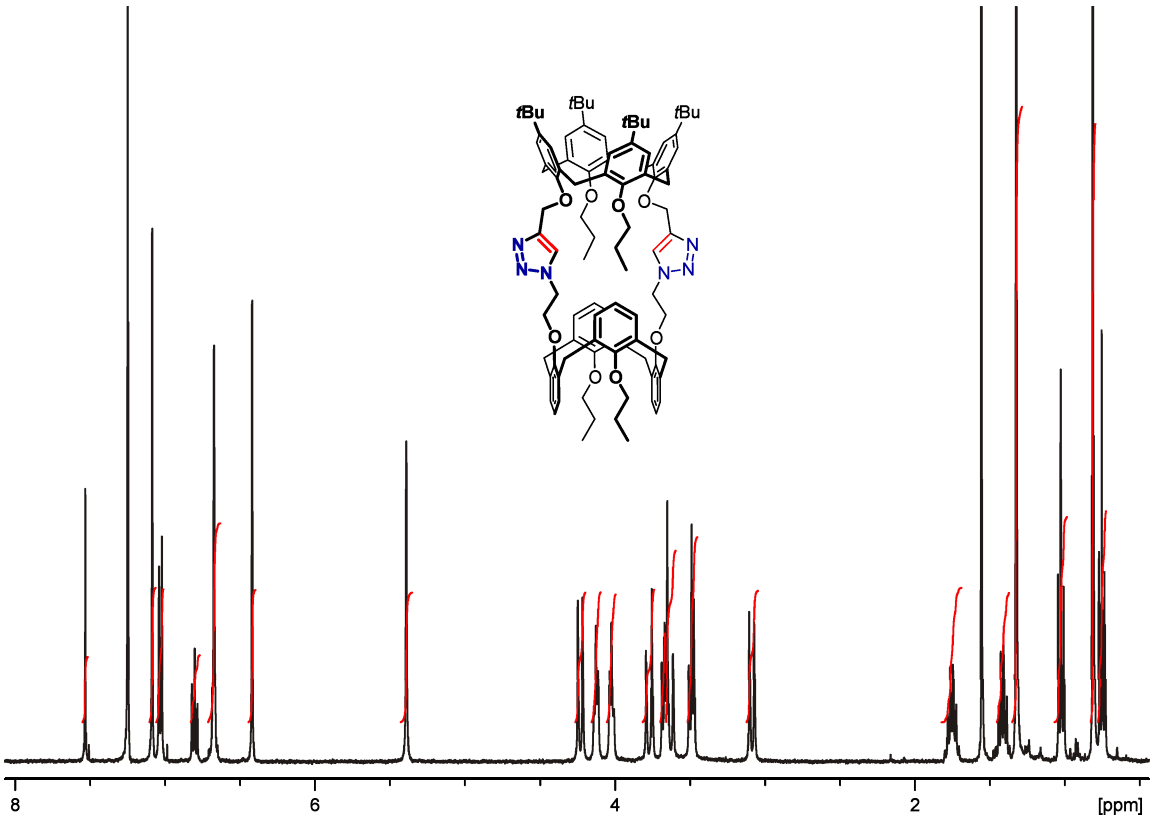


Figure S19. ^{1}H NMR spectrum of calix[4]semitube **BF** (400 MHz, $CDCl_3$).

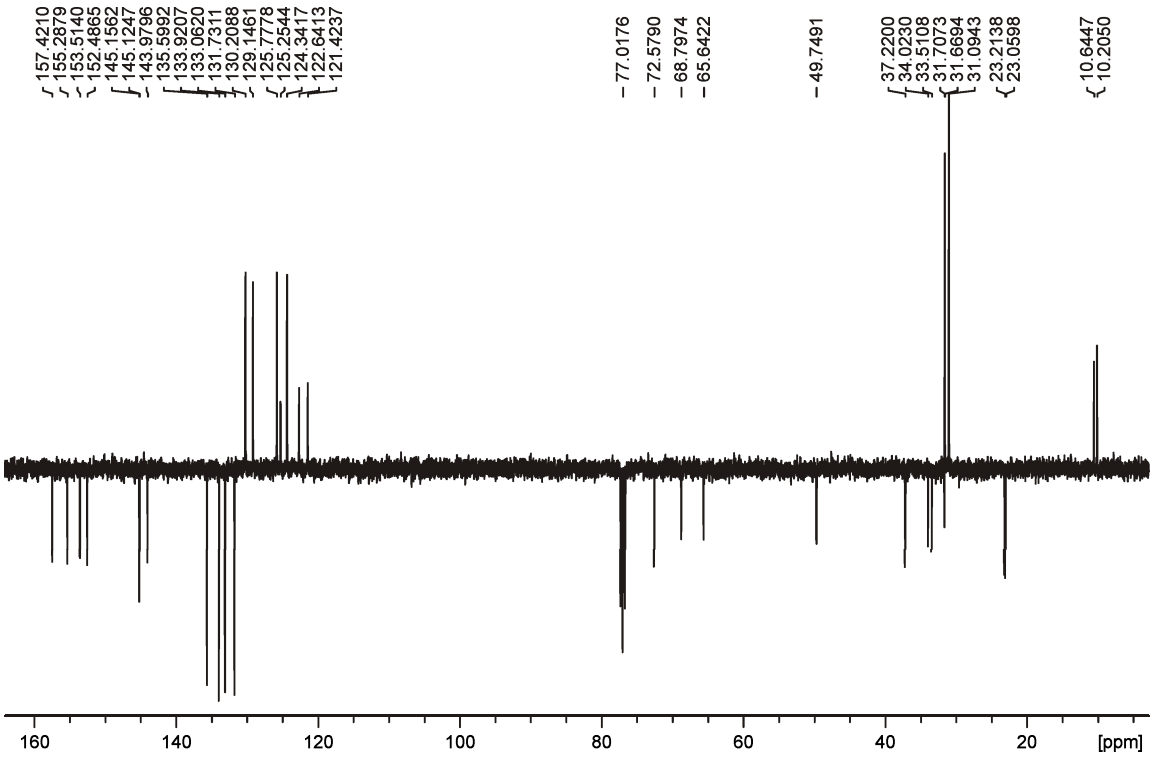


Figure S20. ^{13}C NMR spectrum (APT) of calix[4]semitube **BF** (100 MHz, $CDCl_3$).

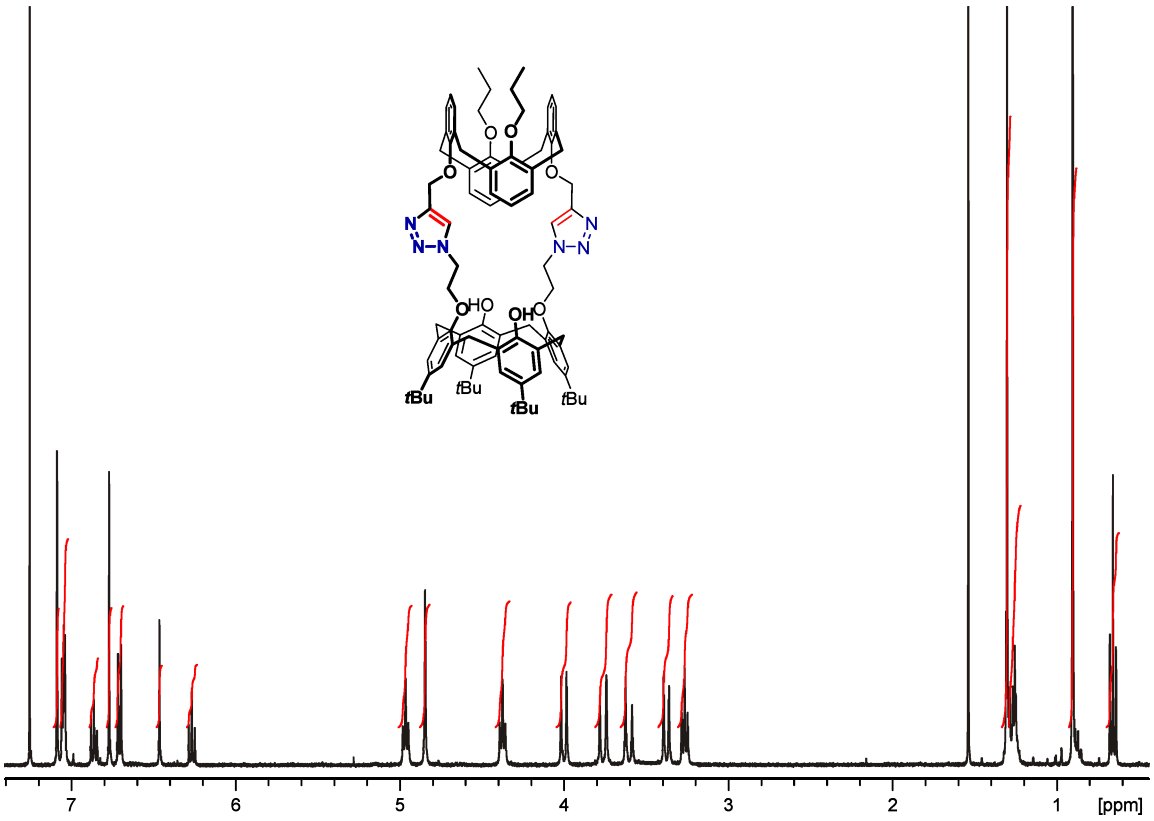


Figure S21. ^{1}H NMR spectrum of calix[4]semitube **CD** (400 MHz, $CDCl_3$).

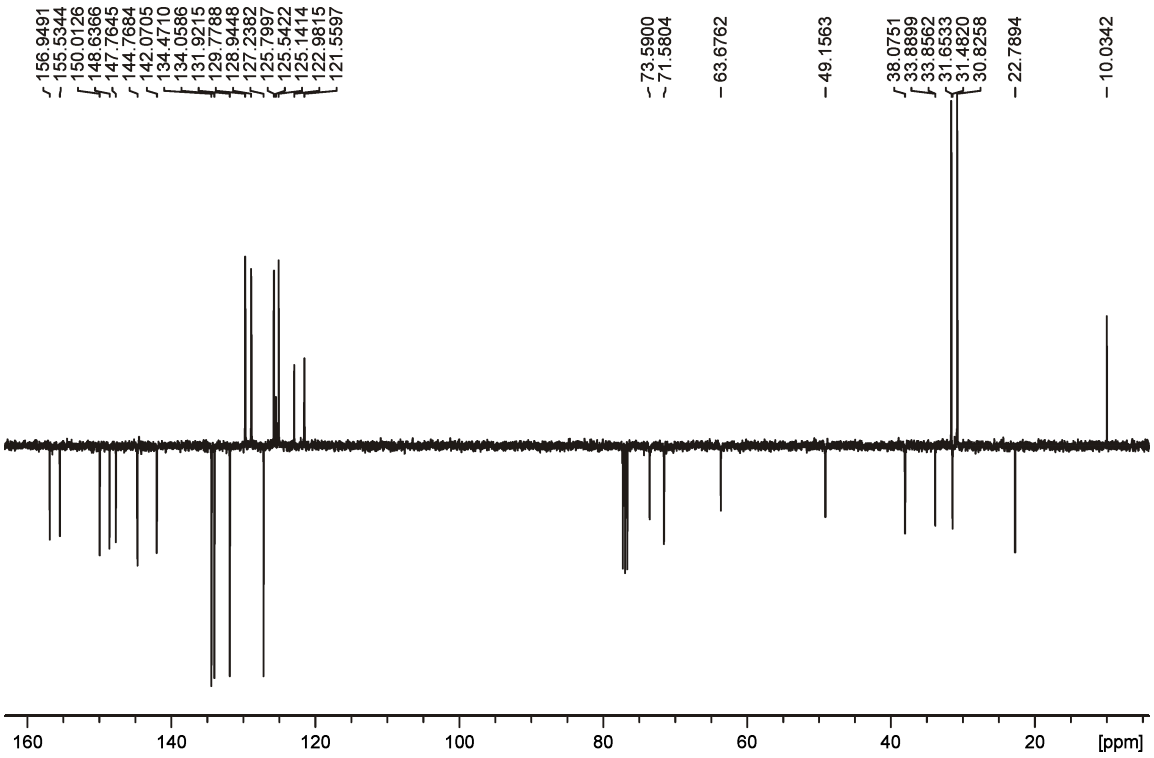


Figure S22. ^{13}C NMR spectrum (APT) of calix[4]semitube **CD** (100 MHz, $CDCl_3$).

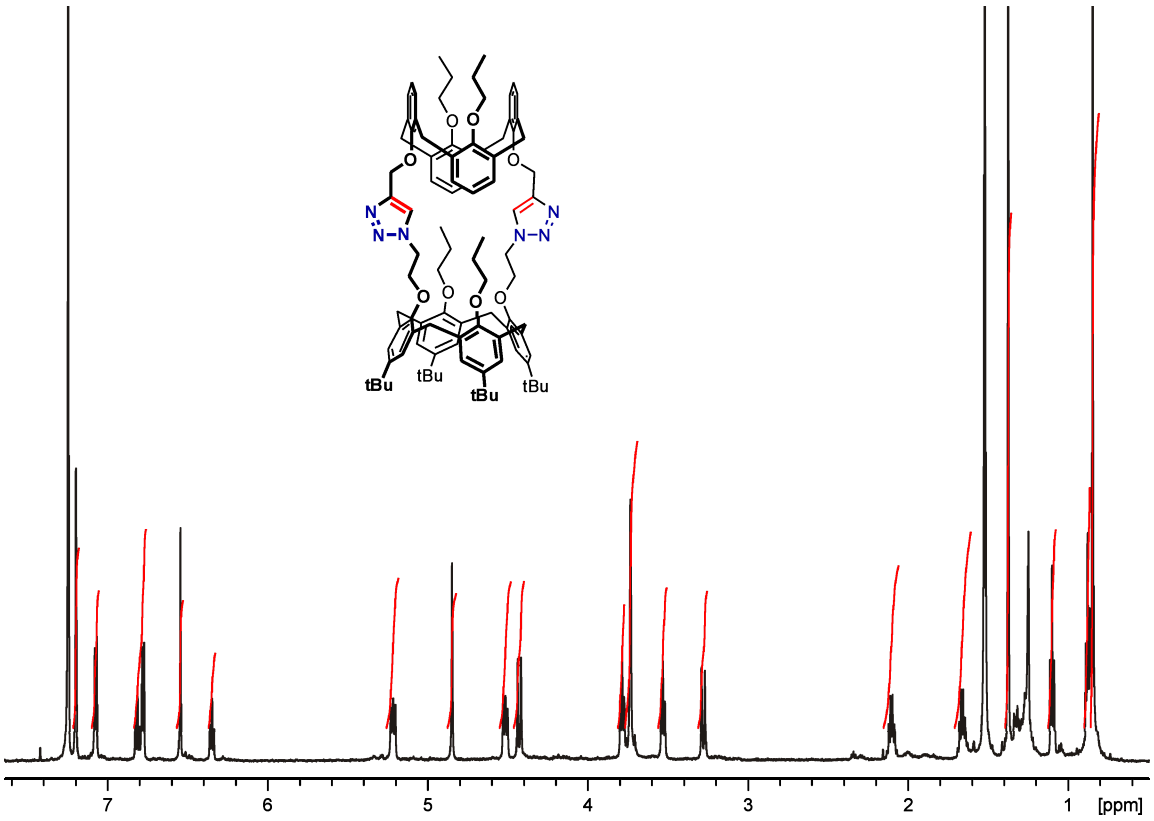


Figure S23. ^{1}H NMR spectrum of calix[4]semitube **CE** (600 MHz, $CDCl_3$).

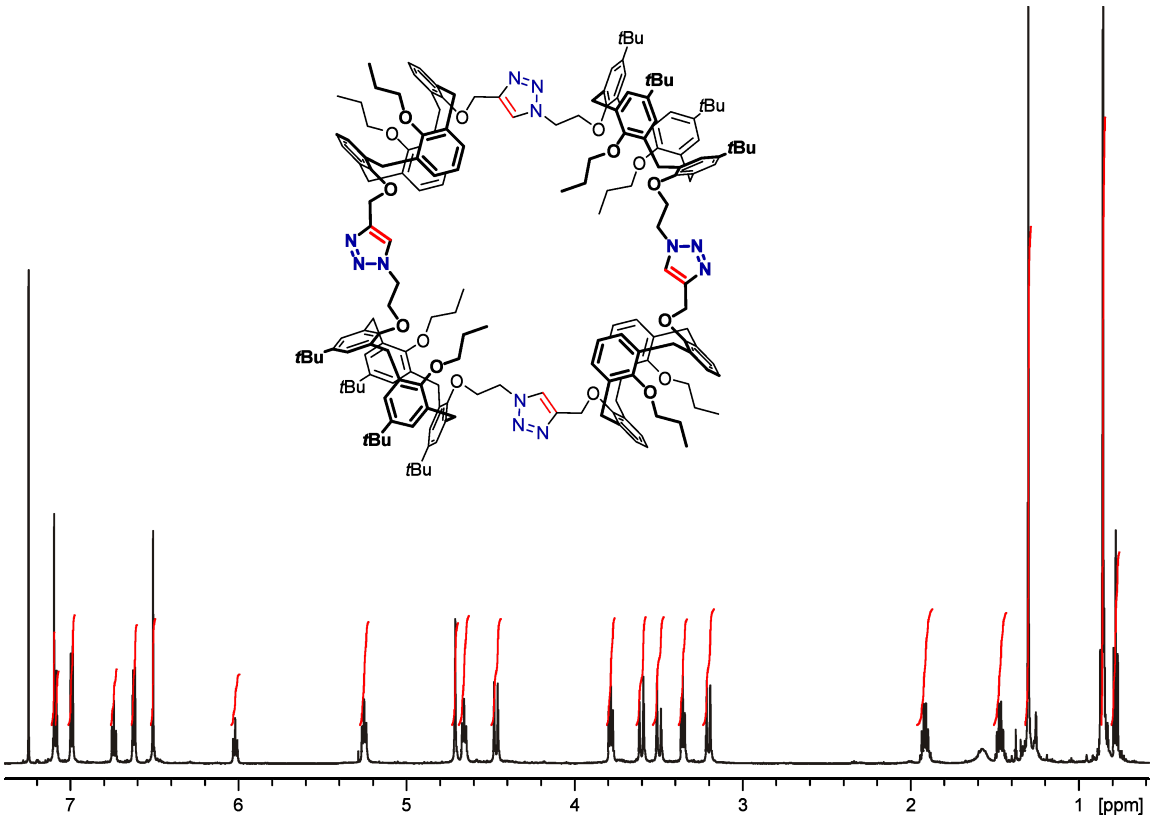


Figure S24. ^{1}H NMR spectrum of tetrakis(calix[4]arene) $\mathbf{C_2E_2}$ (600 MHz, $CDCl_3$).

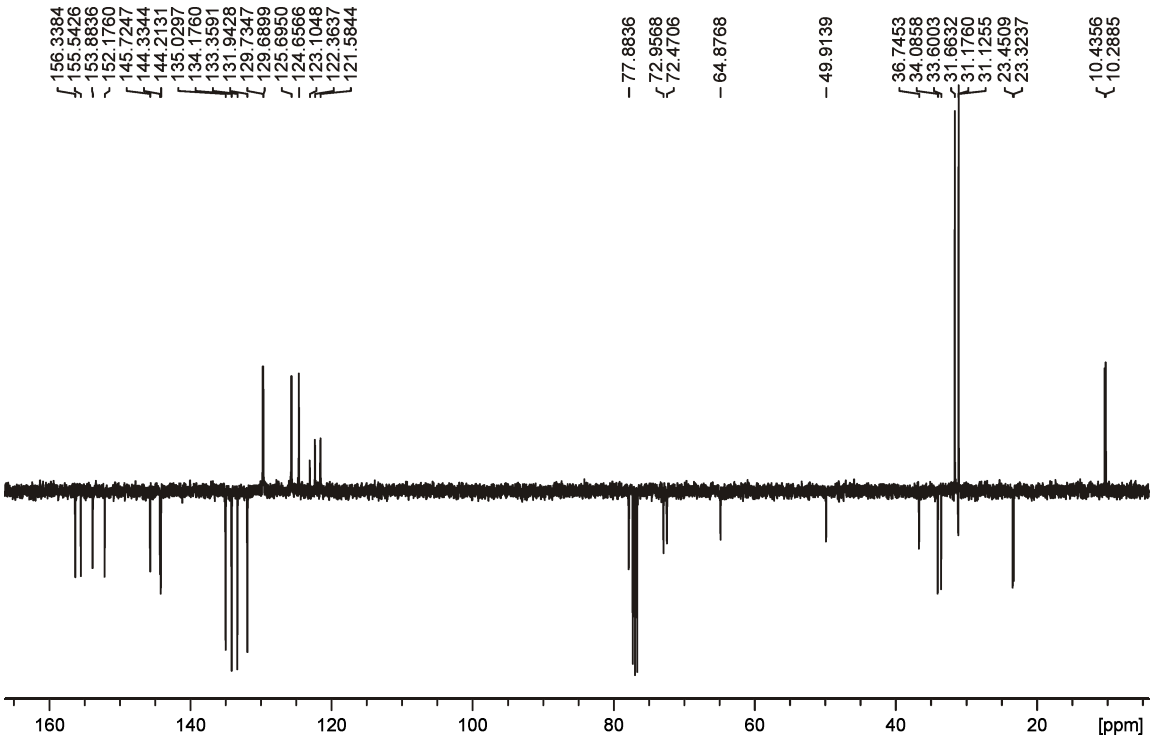


Figure S25. ^{13}C NMR spectrum (APT) of tetrakis(calix[4]arene) $\mathbf{C_2E_2}$ (100 MHz, $CDCl_3$).

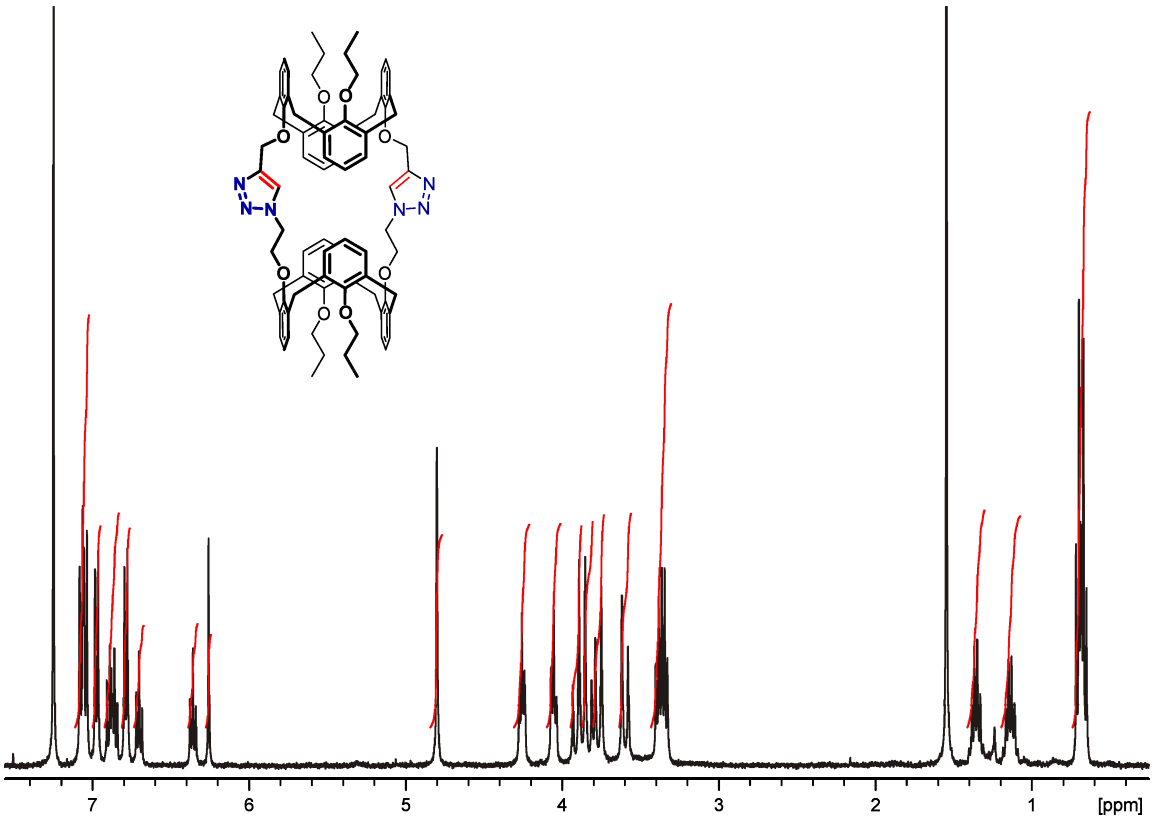


Figure S26. ^{1}H NMR spectrum of calix[4]semitube **CF** (400 MHz, $CDCl_3$).

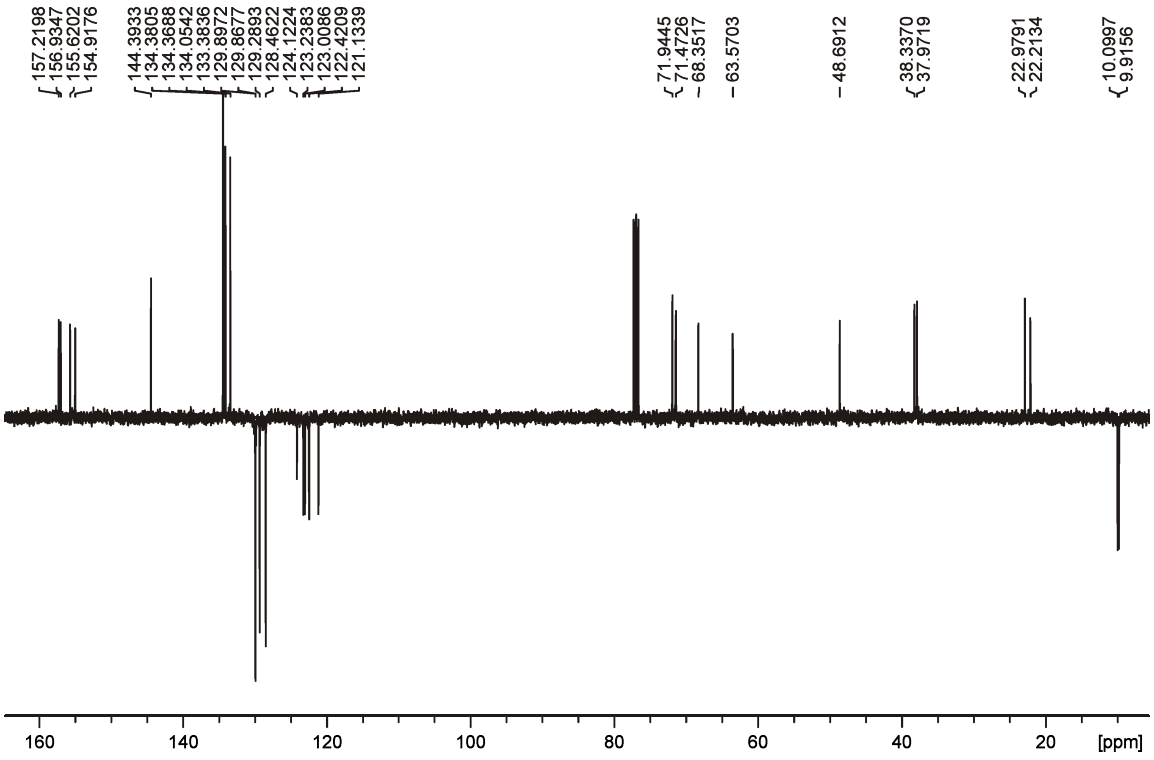


Figure S27. ^{13}C NMR spectrum (APT) of calix[4]semitube **CF** (100 MHz, $CDCl_3$).

Details of X-ray diffraction measurements

Crystallographic data were collected at 100 and 150 K on Bruker D8 Venture and Bruker SMART APEX II diffractometers using graphite monochromatized Mo–Kα radiation (λ = 0.71073 Å) using a ω-scan mode. Absorption correction based on measurements of equivalent reflections was applied.[S11] The structures were solved by direct methods and refined by full matrix least-squares on F^2 with anisotropic thermal parameters for all non-hydrogen atoms. Hydrogen atoms were placed in calculated positions and refined using a riding model. In structures of **6**, **AE**, **BD**, **BE**, **B_2E_2**, **CE** solvent dichloromethane and methanol molecules were not located and their contribution was suppressed by the SQUEEZE procedure.[S12] Crystallographic details are presented in Tables S6–S8.

Table S6 Details of the X-ray crystal data collection and structure refinement for compounds **6**, **C**, **AE**

Compound	**6**	**C**	**AE**
CCDC number	2064439	2064446	2064443
Empirical formula	$C_{32}H_{30}N_6O_4$	$C_{40}H_{40}O_4$	$C_{104}H_{134}N_6O_8{\cdot}CH_2Cl_2$
M_w	562.62	584.72	1681.09
Temperature (K)	150(2)	150(2)	100(2)
Size (mm)	0.25 x 0.22 x 0.16	0.30 x 0.22 x 0.15	0.22 x 0.16 x 0.13
Cryst. system	trigonal	monoclinic	monoclinic
Space group	R-3	C2/c	C2/c
a (Å)	35.3864(8)	25.2023(14)	23.9917(12)
b (Å)	35.3864(8)	7.6250(4)	33.8220(15)
c (Å)	11.7374(2)	19.8425(17)	24.4169(11)
α (deg)	90	90	90
β (deg)	90	126.177(2)	90.909(2)
γ (deg)	120	90	90
V (Å^3)	12728.4(6)	3077.9(4)	19810.5(16)
Z	18	4	8
ρ_{cald} (g·cm^{-3})	1.321	1.262	1.127
Abs coeff (mm^{-1})	0.090	0.080	0.122
F(000)	5328	1248	7248
θ range (deg)	2.30 < *θ* < 25.05	2.54 < *θ* < 25.05	1.70 < *θ* < 25.09
no. of collected/unique rflns	39404 / 5010	9144 / 2707	96317 / 17589
Completeness to *θ* (%)	99.9	99.0	99.8
no. of data/restraints/params	5010/3/401	2707/0/200	17589/62/1103
Goodness of fit on F^2	1.046	1.078	1.029
Final *R* indices ($I > 2\sigma(I)$)	R1 = 0.0451, wR2 = 0.1103	R1 = 0.0571, wR2 = 0.1086	R1 = 0.0881, wR2 = 0.2430
R indices (all data)	R1 = 0.0567, wR2 = 0.1169	R1 = 0.0770, wR2 = 0.1154	R1 = 0.1292, wR2 = 0.2792
Largest diff peak/hole (e/Å^3)	0.23 / –0.26	0.24 / –0.24	0.89 / –0.88

Table S7 Details of the X-ray crystal data collection and structure refinement for compounds **AF**, **BD**, **BE**

Compound	**AF**	**BD**	**BE**
CCDC number	2064441	2064442	2064444
Empirical formula	$C_{88}H_{102}N_6O_8 \cdot 3CH_2Cl_2 \cdot CH_3OH$	$C_{104}H_{134}N_6O_8 \cdot 1.25CH_2Cl_2 \cdot CH_3OH$	$C_{110}H_{146}N_6O_8 \cdot CH_2Cl_2$
M_w	1658.57	1733.35	1765.25
Temperature (K)	100(2)	100(2)	100(2)
Size (mm)	0.32 x 0.26 x 0.20	0.15 x 0.13 x 0.02	0.25 x 0.21 x 0.16
Cryst. system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	$P2_1/c$
a (Å)	12.1055(11)	13.9064(5)	12.5392(4)
b (Å)	16.3679(16)	19.3357(7)	36.1127(17)
c (Å)	23.864(2)	21.9559(8)	25.3044(13)
α (deg)	102.046(3)	64.9250(10)	90
β (deg)	103.504(3)	81.1730(10)	94.7740(10)
γ (deg)	96.551(3)	82.5030(10)	90
V (Å^3)	4430.0(7)	5269.8(3)	11418.7(9)
Z	2	2	4
ρ_{cald} (g·cm^{-3})	1.243	1.092	1.027
Abs coeff (mm^{-1})	0.253	0.130	0.109
F(000)	1760	1866	3816
θ range (deg)	$2.00 < \theta < 26.36$	$1.75 < \theta < 25.05$	$1.61 < \theta < 26.38$
no. of collected/unique rflns	91488 / 18060	45764 / 18538	120847 / 23255
Completeness to θ (%)	99.8	99.3	99.5
no. of data/restraints/params	18060/4/1074	18538/84/1136	23255/68/1240
Goodness of fit on F^2	1.035	1.033	1.019
Final *R* indices ($I > 2\sigma(I)$)	R1 = 0.0585, wR2 = 0.1477	R1 = 0.0983, wR2 = 0.2579	R1 = 0.0776, wR2 = 0.2110
R indices (all data)	R1 = 0.0659, wR2 = 0.1529	R1 = 0.1201, wR2 = 0.2758	R1 = 0.1031, wR2 = 0.2305
Largest diff peak/hole (e/Å^3)	1.36 / –0.98	1.18 / –0.85	0.82 / –1.29

Table S8 Details of the X-ray crystal data collection and structure refinement for compounds **B_2E_2**, **CE**, **CF**

Compound	**B_2E_2**	**CE**	**CF**
CCDC number	2064445	2064440	2064838
Empirical formula	$C_{220}H_{292}N_{12}O_{16}\cdot 6CH_2Cl_2 \cdot 2CH_3OH$	$C_{94}H_{114}N_6O_8\cdot CH_2Cl_2$	$C_{78}H_{82}N_6O_8$
M_w	3934.28	1540.83	1231.49
Temperature (K)	100(2)	100(2)	150(2)
Size (mm)	0.40 x 0.27 x 0.22	0.25 x 0.21 x 0.16	0.22 x 0.18 x 0.01
Cryst. system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	$P2_1/c$
a (Å)	18.6271(18)	11.4467(13)	11.1105(7)
b (Å)	19.3721(18)	20.509(2)	33.701(2)
c (Å)	20.3105(19)	20.597(2)	17.9090(12)
α (deg)	66.725(3)	98.909(4)	90
β (deg)	86.028(3)	98.788(4)	101.548(2)
γ (deg)	67.569(3)	101.578(4)	90
V ($Å^3$)	6194.4(10)	4594.5(9)	6570.1(8)
Z	1	2	4
ρ_{cald} ($g\cdot cm^{-3}$)	1.055	1.114	1.245
Abs coeff (mm^{-1})	0.190	0.126	0.081
F(000)	2112	1652	2624
θ range (deg)	$1.95 < \theta < 25.70$	$1.85 < \theta < 26.44$	$1.87 < \theta < 25.05$
no. of collected/unique rflns	88173 / 23558	74441 / 18774	64876 / 11639
Completeness to θ (%)	99.9	99.0	99.9
no. of data/restraints/params	23558/33/1271	18774/2/1037	11639/1/842
Goodness of fit on F^2	1.029	1.021	0.987
Final *R* indices ($I > 2\sigma(I)$)	R1 = 0.0937, wR2 = 0.2659	R1 = 0.0647, wR2 = 0.1496	R1 = 0.0696, wR2 = 0.1227
R indices (all data)	R1 = 0.1138, wR2 = 0.2860	R1 = 0.0835, wR2 = 0.1598	R1 = 0.1822, wR2 = 0.1595
Largest diff peak/hole ($e/Å^3$)	1.55 / –1.43	1.44 / –0.99	0.46 / –0.22

Changes in NMR spectra of calix[4]semitubes upon addition of Zn^{2+} and Ag^{+}

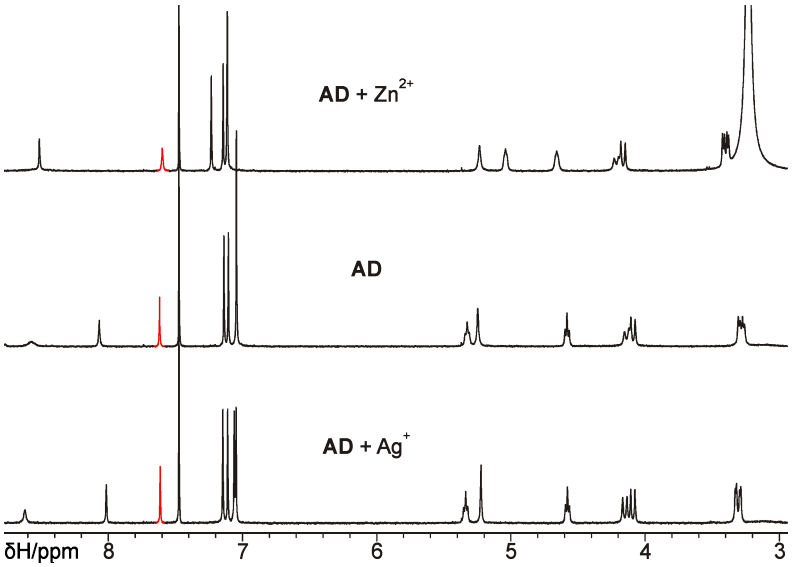


Figure S28. Parts of ^{1}H NMR spectra of calix[4]semitube **AD** (middle) and its equilibrated mixtures with 10 equiv of $Zn(ClO_4)_2 \cdot 6H_2O$ (top) and $AgClO_4 \cdot H_2O$ (bottom); $CD_3CN/CDCl_3$ (1:1), 400 MHz, 20 °C; signals of the triazole protons are marked red.

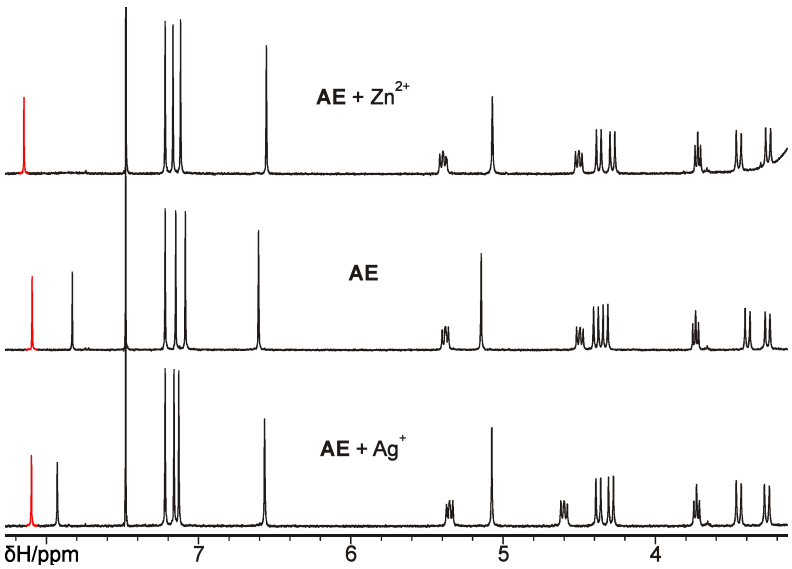


Figure S29. Parts of ^{1}H NMR spectra of calix[4]semitube **AE** (middle) and its equilibrated mixtures with 10 equiv of $Zn(ClO_4)_2 \cdot 6H_2O$ (top) and $AgClO_4 \cdot H_2O$ (bottom); $CD_3CN/CDCl_3$ (1:1), 400 MHz, 20 °C; signals of the triazole protons are marked red.

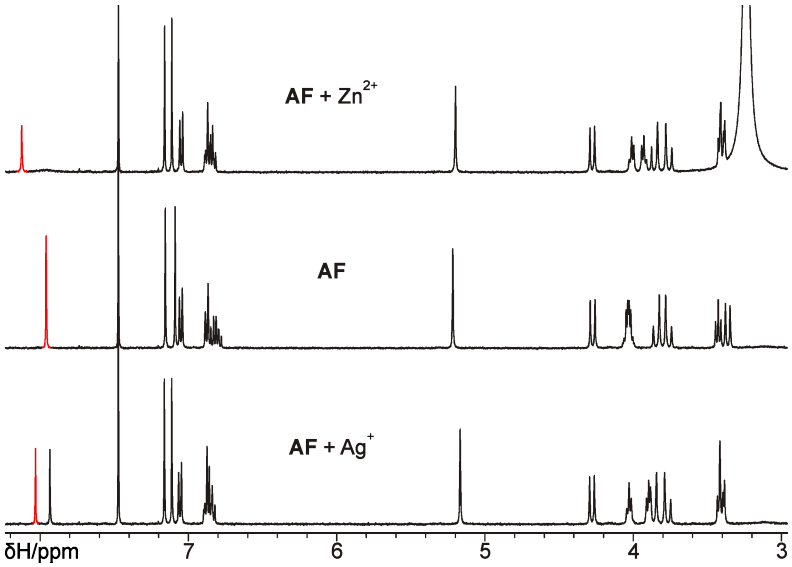


Figure S30. Parts of ^{1}H NMR spectra of calix[4]semitube **AF** (middle) and its equilibrated mixtures with 10 equiv of $Zn(ClO_4)_2 \cdot 6H_2O$ (top) and $AgClO_4 \cdot H_2O$ (bottom); $CD_3CN/CDCl_3$ (1:1), 400 MHz, 20 °C; signals of the triazole protons are marked red.

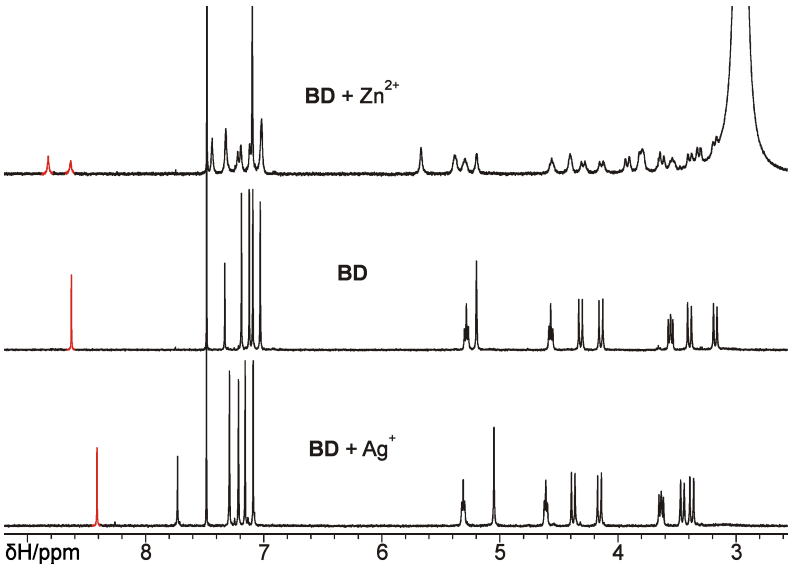


Figure S31. Parts of ^{1}H NMR spectra of calix[4]semitube **BD** (middle) and its equilibrated mixtures with 10 equiv of $Zn(ClO_4)_2 \cdot 6H_2O$ (top) and $AgClO_4 \cdot H_2O$ (bottom); $CD_3CN/CDCl_3$ (1:1), 400 MHz, 20 °C; signals of the triazole protons are marked red.

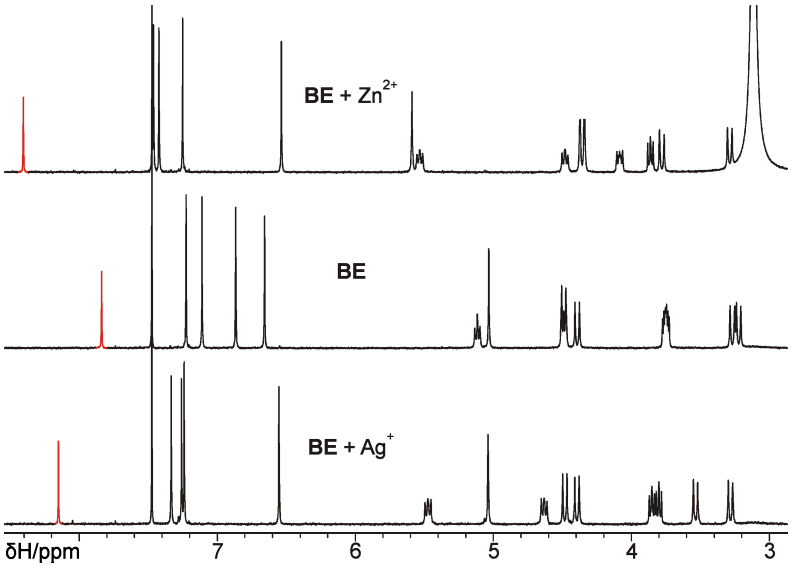


Figure S32. Parts of ^{1}H NMR spectra of calix[4]semitube **BE** (middle) and its equilibrated mixtures with 10 equiv of $Zn(ClO_4)_2 \cdot 6H_2O$ (top) and $AgClO_4 \cdot H_2O$ (bottom); $CD_3CN/CDCl_3$ (1:1), 400 MHz, 20 °C; signals of the triazole protons are marked red.

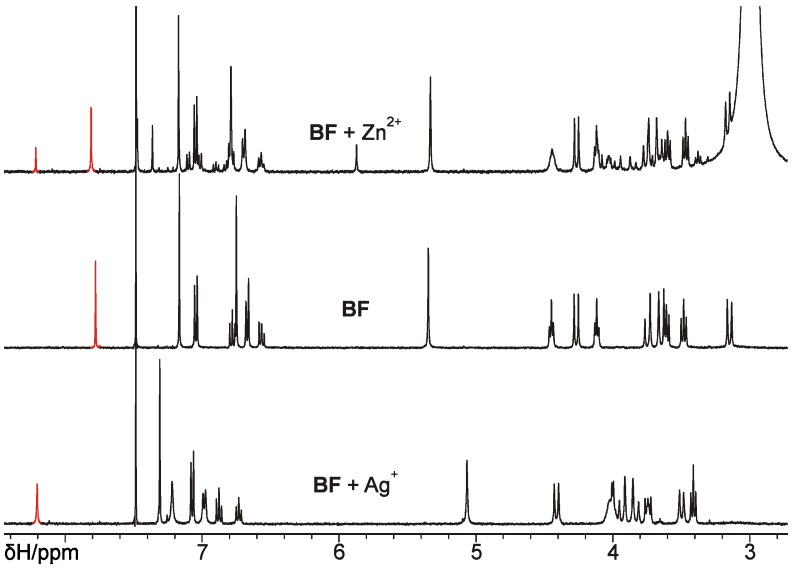


Figure S33. Parts of ^{1}H NMR spectra of calix[4]semitube **BF** (middle) and its equilibrated mixtures with 10 equiv of $Zn(ClO_4)_2 \cdot 6H_2O$ (top) and $AgClO_4 \cdot H_2O$ (bottom); $CD_3CN/CDCl_3$ (1:1), 400 MHz, 20 °C; signals of the triazole protons are marked red.

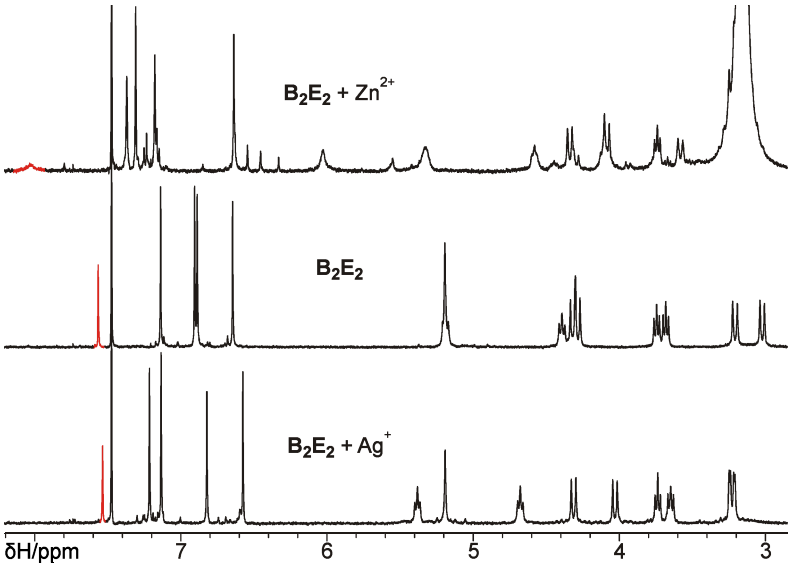


Figure S34. Parts of ^{1}H NMR spectra of tetrakis(calixarene) **B_2E_2** (middle) and its equilibrated mixtures with 10 equiv of $Zn(ClO_4)_2 \cdot 6H_2O$ (top) and $AgClO_4 \cdot H_2O$ (bottom); $CD_3CN/CDCl_3$ (1:1), 400 MHz, 20 °C; signals of the triazole protons are marked red.

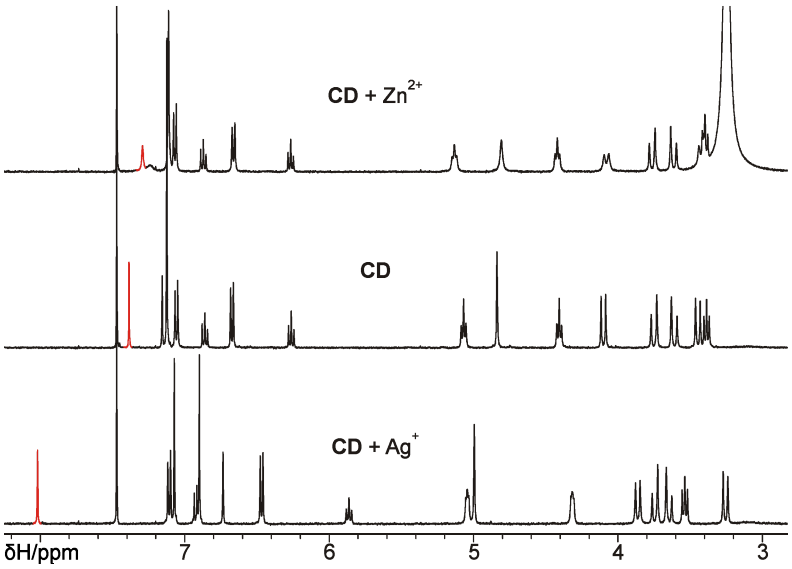


Figure S35. Parts of ^{1}H NMR spectra of calix[4]semitube **CD** (middle) and its equilibrated mixtures with 10 equiv of $Zn(ClO_4)_2 \cdot 6H_2O$ (top) and $AgClO_4 \cdot H_2O$ (bottom); $CD_3CN/CDCl_3$ (1:1), 400 MHz, 20 °C; signals of the triazole protons are marked red.

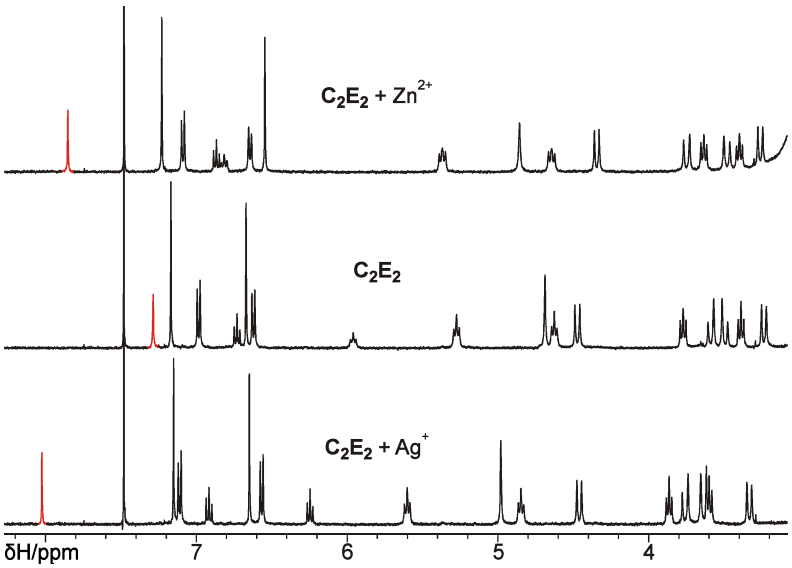


Figure S36. Parts of ^{1}H NMR spectra of tetrakis(calixarene) **C_2E_2** (middle) and its equilibrated mixtures with 10 equiv of $Zn(ClO_4)_2 \cdot 6H_2O$ (top) and $AgClO_4 \cdot H_2O$ (bottom); $CD_3CN/CDCl_3$ (1:1), 400 MHz, 20 °C; signals of the triazole protons are marked red.

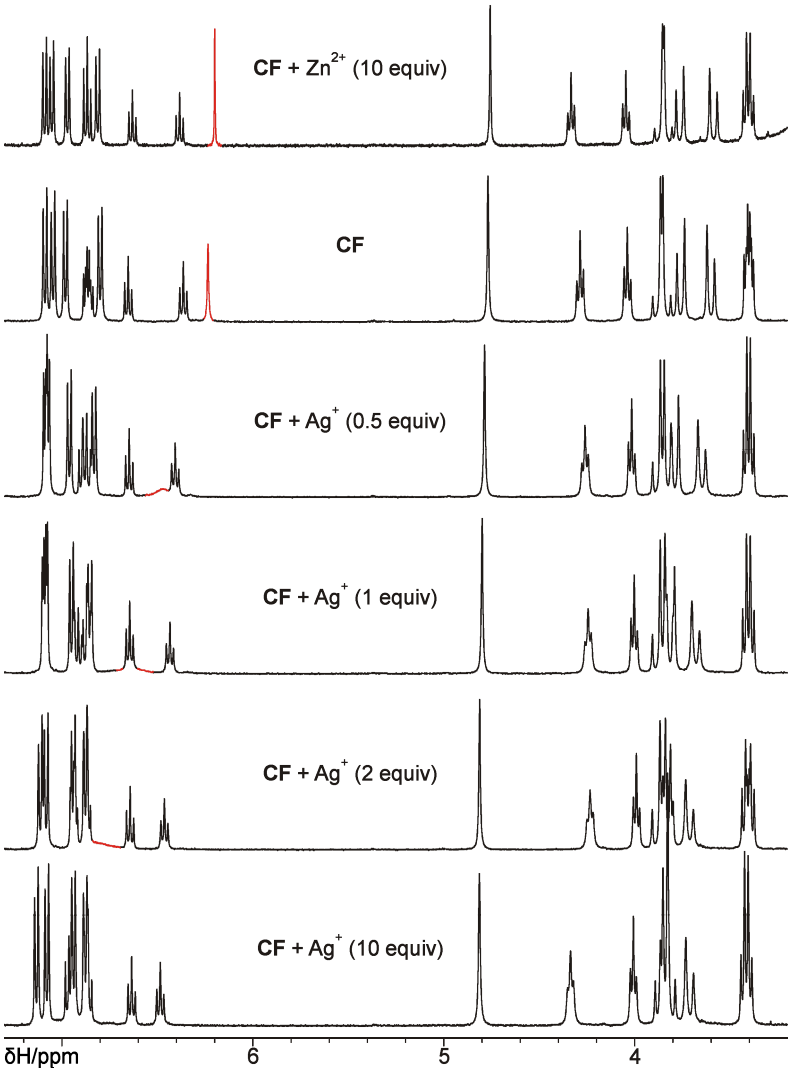


Figure S37. Parts of ^{1}H NMR spectra of calix[4]semitube **CF** and its equilibrated mixtures with 10 equiv of $Zn(ClO_4)_2 \cdot 6H_2O$ different amount of $AgClO_4 \cdot H_2O$; $CD_3CN/CDCl_3$ (1:1), 400 MHz, 20 °C; signals of the triazole protons are marked red.

Atomic coordinates of the calculated structures

Complex **BE**·Zn^{2+}, E = –6981.462674 E_h

Zn	-2.136123	1.842592	-0.835067	H	1.858907	-3.473562	-1.303855
O	2.069382	-3.921207	0.713289	H	2.203013	-2.077773	-0.221929
O	3.289497	-1.080953	1.554234	C	5.018357	-2.501189	4.483443
O	-4.094090	1.865390	-0.986835	H	5.008657	-2.394527	5.569266
O	0.421903	-1.972527	3.820733	C	0.179439	-2.796965	-0.090063
O	-0.822394	-4.881215	2.339932	H	-0.410667	-3.701801	-0.285807
O	0.709789	3.036408	-3.483711	H	0.019402	-2.497570	0.953063
O	-1.180493	3.683447	-0.507556	C	-6.753924	6.121484	-3.803437
O	-2.094435	1.359067	-3.738255	C	-4.691860	2.925515	-1.711256
N	-0.331906	-1.714604	-0.938217	C	-4.985891	0.906126	-0.315543
N	-0.913747	0.947574	3.020253	H	-4.334109	0.059812	-0.049101
C	2.957406	-4.922871	0.362817	H	-5.708514	0.564195	-1.071691
C	2.473327	-6.240810	0.344849	C	-3.036462	6.853188	0.038016
C	3.349801	-7.257844	-0.065802	H	-3.980464	7.171571	0.480890
H	2.959872	-8.275566	-0.108344	C	0.963287	-6.503477	5.122668
C	-2.758375	1.665903	-4.940892	H	0.982571	-6.437005	6.210836
C	-0.670320	5.974237	-1.160519	C	5.920577	-3.406899	3.900244
C	0.935181	-6.569614	2.329551	C	-3.985570	4.525647	0.178790
N	-0.794731	-0.621459	-0.383166	H	-3.654106	3.605765	0.677113
C	-4.155096	1.526854	-4.974149	H	-4.681417	5.018449	0.874394
N	-1.173859	0.169911	-1.364216	C	2.219172	-1.744314	5.422140
C	5.840660	-3.568242	2.514516	C	1.689278	-7.515377	4.477686
H	6.465928	-4.308822	2.014985	C	-0.898237	0.106534	4.234283
C	-2.768381	2.236275	-7.280670	H	-1.813391	0.355781	4.792669
H	-2.209978	2.549769	-8.166251	H	-0.036963	0.416732	4.841483
C	-0.550155	6.434068	-4.185273	C	3.040705	-0.899782	4.458073
H	-0.590067	7.402264	-3.687738	H	3.531775	-0.081523	5.011948
C	-0.479138	3.918755	-5.395571	H	2.382995	-0.460646	3.700061
C	-5.396578	5.207206	-1.833323	C	-2.093461	7.814507	-0.349032
H	-5.444485	6.202015	-1.385847	C	-4.882265	2.209077	-8.729622
N	-1.658424	1.675823	1.189114	C	0.494290	-3.452010	5.761672
C	4.298834	-4.618411	0.056327	C	-0.569343	2.431306	1.473684
C	4.678402	-7.005319	-0.431939	C	-0.404186	-1.655773	-2.297162
C	1.058237	-6.563045	0.808235	H	-0.068603	-2.463866	-2.942824
H	0.778156	-7.551628	0.409791	C	-7.277862	5.692070	-5.188064
H	0.348531	-5.833630	0.397931	H	-7.811036	6.533286	-5.656416
C	0.489141	5.544029	-2.043615	H	-7.989697	4.853837	-5.123511
H	0.931951	4.607120	-1.691787	H	-6.459948	5.403290	-5.867200
H	1.279210	6.310700	-1.995475	C	-1.659490	7.499166	-6.260839
C	0.091568	4.103485	-4.121983	C	-0.958253	-0.416518	-2.569513
C	4.952899	-2.832205	1.717175	C	-0.517475	-4.440240	5.185448
C	-1.045929	5.022573	-6.044133	H	-1.221590	-3.949295	4.506642
H	-1.491842	4.859281	-7.026288	H	-1.102763	-4.870350	6.013921
C	-0.067821	1.959891	2.674718	C	5.637769	-8.124253	-0.890927
H	0.779196	2.251244	3.289469	C	-5.691649	1.471288	0.904073
C	-2.049240	2.089426	-6.084564	H	-6.273985	2.361331	0.612541
C	0.115037	-5.655111	3.021534	H	-4.941424	1.794231	1.644245
C	-0.940414	7.338011	-0.994415	C	1.036667	-3.697907	7.028965
H	-0.212048	8.048058	-1.390422	H	0.597179	-4.506409	7.617555
C	-4.153397	2.023003	-7.383006	C	2.712870	-2.028848	6.709430
C	4.100830	-1.749031	3.739462	H	3.596329	-1.482370	7.042913
C	5.127922	-5.673201	-0.349424	C	-2.092424	8.639947	-5.319159
H	6.164864	-5.439837	-0.604816	H	-2.809834	8.295190	-4.556843
C	-5.990776	4.986197	-3.089842	H	-2.576587	9.439505	-5.900986
C	4.127766	-1.872167	2.332933	H	-1.233606	9.097025	-4.803214
C	1.037092	-2.385367	5.007227	C	-0.107237	3.431328	0.446665
C	-1.080033	6.303905	-5.477051	H	0.200003	4.382024	0.903215
C	-0.595095	2.548574	-6.052584	H	0.747816	3.021412	-0.117954
H	-0.235065	2.610662	-7.090935	C	4.968001	-9.511781	-0.884674
H	0.066470	1.838065	-5.544385	H	4.644151	-9.810881	0.125160
C	-4.726741	4.202244	-1.124966	H	5.688036	-10.268027	-1.235028
C	1.692352	-7.483193	3.073862	H	4.095790	-9.556558	-1.555198
H	2.303117	-8.201821	2.522637	C	-2.890937	7.067013	-7.090787
N	-1.873719	0.789617	2.125148	H	-2.630457	6.368785	-7.899492
C	-4.822453	1.690231	-6.198599	H	-3.355634	7.945528	-7.564900
H	-5.903501	1.544391	-6.208221	H	-3.649394	6.577249	-6.459404
C	-4.959362	1.323654	-3.702111	C	-0.571468	8.036175	-7.220244
H	-4.437906	0.628029	-3.033756	H	0.308155	8.394150	-6.661273
H	-5.930179	0.870245	-3.957494	H	-0.963613	8.877751	-7.814549
C	-1.580594	5.059629	-0.601514	H	-0.231917	7.256043	-7.919702
C	0.023280	5.359887	-3.490277	C	-4.219075	1.332077	-9.815626
C	-5.187493	2.660998	-2.993772	H	-3.158521	1.586574	-9.968555
C	4.857694	-3.207576	0.240724	H	-4.733483	1.472469	-10.779735
H	5.862379	-3.178630	-0.209140	H	-4.276762	0.262932	-9.554142
H	4.255056	-2.468233	-0.303772	C	2.141163	3.048055	-3.569139
C	0.188310	-5.563443	4.424495	H	2.546486	3.908279	-3.003549
C	-2.821481	5.469505	-0.090921	H	2.450364	3.188277	-4.621414
C	-0.865464	-1.414460	3.969719	C	-5.816778	7.334591	-4.007130
H	-1.394169	-1.877523	4.817466	H	-4.957688	7.066480	-4.641402
H	-1.438145	-1.639900	3.055811	H	-5.425586	7.734122	-3.058911
C	-5.839066	3.712538	-3.655514	H	-6.359615	8.151548	-4.508764
H	-6.222195	3.519754	-4.656438	C	-7.961530	6.542897	-2.931966
C	1.670190	-3.038854	-0.304678	H	-8.530562	7.339734	-3.437023

H	-7.646223	6.933288	-1.951236
H	-8.645551	5.697279	-2.756863
C	2.439801	-8.631034	5.239699
C	-1.164962	0.288948	-3.871016
H	-0.182175	0.680579	-4.178398
H	-1.505593	-0.428962	-4.635181
C	2.125672	-2.979736	7.552795
C	6.893954	-4.217162	4.780001
C	-4.798237	3.697174	-9.147036
H	-5.242989	4.350913	-8.379311
H	-5.348149	3.861262	-10.087808
H	-3.759658	4.025033	-9.310456
C	6.856020	-8.172207	0.064044
H	7.426812	-7.231112	0.048288
H	7.542945	-8.983799	-0.224559
H	6.532446	-8.349660	1.103506
C	6.115436	-7.834495	-2.332733
H	5.267875	-7.851236	-3.037275
H	6.839718	-8.599035	-2.656450
H	6.612684	-6.855127	-2.419359
C	-6.370065	1.818532	-8.641112
H	-6.503259	0.767088	-8.340328
H	-6.843961	1.941890	-9.626906
H	-6.930046	2.451862	-7.935330
C	1.733717	-9.985378	4.986687
H	1.726540	-10.248802	3.917242
H	0.689849	-9.963990	5.338306
H	2.255580	-10.792910	5.525914
C	-6.619900	0.423377	1.524902
H	-7.388987	0.085045	0.811275
H	-7.143048	0.841349	2.397816
H	-6.058061	-0.463238	1.863015
C	3.903412	-8.741909	4.751911
H	4.433951	-9.514941	5.329381
H	4.445046	-7.792598	4.886214
H	3.972235	-9.027502	3.689785
C	2.693355	1.749130	-3.000064
H	2.190365	1.551166	-2.033340
H	2.415972	0.914456	-3.667629
C	2.459607	-8.375015	6.757539
H	1.447458	-8.374821	7.192198
H	2.941471	-7.416182	7.007163
H	3.029048	-9.168429	7.264605
C	3.859659	0.097269	0.987121
H	3.261900	0.310188	0.081140
H	4.897213	-0.097406	0.657558
C	-2.317830	9.324635	-0.150338
C	6.069662	-5.106198	5.741030
H	6.734431	-5.701295	6.389925
H	5.430851	-5.800162	5.171714
H	5.412688	-4.507090	6.389621
C	4.208785	1.800202	-2.798860
H	4.736403	2.043256	-3.735628
H	4.598544	0.836722	-2.436562
H	4.485634	2.566706	-2.056899
C	2.667367	-3.314508	8.958216
C	3.808660	1.312002	1.916805
H	2.796930	1.349542	2.354072
H	4.502511	1.164479	2.760409
C	-3.448083	9.603927	0.857595
H	-3.255182	9.125895	1.831708
H	-4.429337	9.262872	0.490442
H	-3.532227	10.687598	1.030407
C	4.100027	2.638964	1.213670
H	3.402149	2.809383	0.373400
H	5.120079	2.676355	0.798893
H	3.998861	3.487024	1.910528
C	7.784365	-3.251788	5.595110
H	7.188938	-2.585946	6.240345
H	8.395129	-2.617449	4.931012
H	8.468686	-3.820960	6.246110
C	-1.022434	9.986194	0.380940
H	-1.198445	11.054026	0.584532
H	-0.193622	9.927056	-0.341495
H	-0.688958	9.516926	1.320320
C	7.812455	-5.131956	3.946424
H	8.483738	-5.692928	4.616801
H	8.444549	-4.554442	3.253122
H	7.243400	-5.870726	3.357199
C	-2.701481	9.951337	-1.513494
H	-3.611693	9.483685	-1.922931
H	-1.898265	9.832741	-2.257757
H	-2.899069	11.029873	-1.401052
C	3.211857	-4.763467	8.953817
H	2.428839	-5.495596	8.701409
H	3.608149	-5.028477	9.947575
H	4.027634	-4.881631	8.224166
C	-3.304666	-3.819751	0.719785
H	-4.222916	-3.211897	0.654307
H	-3.296522	-4.504023	-0.145682
H	-2.451406	-3.131946	0.618710
C	1.531332	-3.205357	10.000953
H	1.131284	-2.179689	10.053825
H	1.909670	-3.475448	11.000326
H	0.692076	-3.880631	9.776091
C	3.806278	-2.371518	9.389307
H	4.675449	-2.429258	8.715534
H	4.159207	-2.652486	10.393935
H	3.473264	-1.322244	9.436636
C	-2.080508	-5.562868	2.199600
H	-2.253487	-6.182496	3.096245
H	-2.029668	-6.255423	1.335587
C	-3.249131	-4.597005	2.037008
H	-4.165734	-5.205564	2.135134
H	-3.258321	-3.896375	2.890351

Complex **BE**·Ag^+, E = –5349.545981 E_h

Ag	-2.924312	-0.023089	-0.944349	H	-1.041324	-5.633129	-2.776913
O	0.941752	-4.790287	-0.238209	H	-1.414195	-5.240565	-1.082547
O	1.756328	-2.236390	1.736324	C	-6.100284	6.421968	-3.918783
O	-4.765487	1.409121	-1.520065	C	-4.831497	2.656352	-2.145957
O	-0.107473	-1.765932	4.090149	C	-6.063323	0.796848	-1.312356
O	-0.856519	-4.975148	2.857239	H	-5.922943	-0.287991	-1.454902
O	1.152643	2.580080	-2.454626	H	-6.743940	1.149589	-2.104489
O	-1.482467	3.095409	-0.591334	C	-3.151006	6.092519	0.694879
O	-2.111946	0.571098	-3.962136	H	-4.150451	6.375155	1.033054
N	-1.258278	-3.615961	-2.350212	C	0.550926	-6.640343	5.811880
N	-1.689541	0.496345	3.126828	H	0.611273	-6.456547	6.884622
C	2.080374	-5.367451	0.336595	C	5.786437	-1.100661	1.924483
C	1.947787	-6.561836	1.080053	C	-4.161127	3.851557	0.037166
C	3.117036	-7.201643	1.513964	H	-3.879785	2.829549	0.316268
H	3.007049	-8.140376	2.057971	H	-4.956542	4.169061	0.730839
C	-2.389685	1.479393	-4.996755	C	2.143577	-1.577146	4.864422
C	-0.617902	5.327170	-0.224652	C	1.028452	-7.846974	5.285626
C	0.433215	-7.013573	3.041880	C	-1.732748	-0.004044	4.499261
N	-2.037404	-2.899255	-1.544865	H	-2.745703	0.167132	4.897583
C	-3.732180	1.715089	-5.371169	H	-1.029231	0.606629	5.081889
N	-2.380500	-1.815005	-2.191799	C	2.473956	-0.533509	3.807505
C	5.334754	-1.958294	0.905830	H	2.886521	0.362014	4.299837
H	6.036093	-2.331985	0.156722	H	1.550943	-0.241841	3.289725
C	-1.641927	2.714014	-6.925740	C	-2.097944	7.018249	0.782158
H	-0.813056	3.126938	-7.501232	C	-3.270503	3.447168	-8.794467
C	0.237234	6.081498	-3.129957	C	0.714808	-3.339949	5.779222
H	0.181073	7.021026	-2.579169	C	-1.205097	1.520416	1.273865
C	0.257690	3.604616	-4.451226	C	-1.097686	-2.982163	-3.546460
C	-5.063487	5.044934	-2.020603	H	-0.505382	-3.396049	-4.358621
H	-4.986399	5.963416	-1.434322	C	-6.446943	6.308034	-5.416245
N	-2.198286	0.609506	1.073733	H	-6.845272	7.268111	-5.780551
C	3.342537	-4.752729	0.214433	H	-7.217939	5.545902	-5.610109
C	4.404701	-6.686425	1.294505	H	-5.561573	6.063930	-6.023306
C	0.589895	-7.116565	1.523446	C	-0.254126	7.341193	-5.327608
H	0.505008	-8.173202	1.220594	C	-1.823174	-1.806321	-3.434940
H	-0.204519	-6.556422	1.019273	C	-0.455759	-4.321445	5.649591
C	0.719740	5.026032	-0.899917	H	-1.267484	-3.896812	5.050602
H	1.182204	4.113167	-0.512171	H	-0.862777	-4.530918	6.652246
H	1.413355	5.844930	-0.653770	C	5.654862	-7.465726	1.750554
C	0.673281	3.702675	-3.105770	C	-6.651989	1.090975	0.062945
C	3.992630	-2.375083	0.806457	H	-6.609089	2.177233	0.243741
C	-0.052182	4.796815	-5.121662	H	-6.023561	0.616346	0.835668
H	-0.354955	4.735741	-6.166487	C	1.728532	-3.620685	6.717576
C	-0.868700	1.444846	2.612048	H	1.555793	-4.443948	7.412213
H	-0.136750	1.977799	3.211995	C	3.131264	-1.937459	5.783062
C	-1.336558	2.094110	-5.698764	H	4.087582	-1.412613	5.730440
C	-0.146291	-5.868439	3.632212	C	-0.355954	8.598929	-4.444681
C	-0.854659	6.614882	0.275168	H	-1.184851	8.526676	-3.720880
H	-0.020780	7.318360	0.266097	H	-0.546898	9.478449	-5.080678
C	-2.943808	2.816670	-7.426066	H	0.573810	8.793095	-3.885905
C	3.489985	-1.027556	2.789903	C	-0.571162	2.330562	0.184088
C	4.475630	-5.434009	0.680994	H	0.190847	2.966672	0.654820
H	5.439085	-4.939764	0.560960	H	-0.059711	1.675342	-0.527923
C	-5.527675	5.106545	-3.345575	C	5.478087	-7.929888	3.212070
C	3.076327	-1.892345	1.758890	H	5.284573	-7.072126	3.875260
C	0.895427	-2.234917	4.920991	H	6.387170	-8.442750	3.566477
C	-0.029041	6.057736	-4.502295	H	4.644306	-8.634417	3.328408
C	0.066685	2.233532	-5.123976	C	-1.559648	7.239656	-6.144897
H	0.806227	2.106336	-5.933275	H	-1.566731	6.371043	-6.819597
H	0.258046	1.453547	-4.378145	H	-1.698655	8.140645	-6.765090
C	-4.705285	3.842619	-1.394837	H	-2.429989	7.150463	-5.475699
C	0.982732	-7.989152	3.887145	C	0.951848	7.513786	-6.280769
H	1.383692	-8.898421	3.430546	H	1.892379	7.577393	-5.708529
N	-2.490845	-0.002012	2.191810	H	0.852745	8.437475	-6.874716
C	-3.975444	2.348522	-6.594992	H	1.040720	6.669638	-6.983177
H	-5.015752	2.483869	-6.901052	C	-2.002968	3.890314	-9.548231
C	-4.894327	1.458248	-4.415783	H	-1.433590	4.647476	-8.986968
H	-4.705282	0.581194	-3.786136	H	-2.281686	4.341596	-10.513291
H	-5.805512	1.258288	-5.002152	H	-1.331112	3.043907	-9.760593
C	-1.681451	4.401712	-0.189264	C	2.573595	2.514463	-2.264480
C	0.571642	4.925785	-2.413396	H	2.726490	1.828530	-1.415099
C	-5.093204	2.693369	-3.527009	H	2.960692	3.502910	-1.958718
C	3.546648	-3.333678	-0.299317	C	-5.089364	7.575951	-3.752619
H	4.320696	-3.341503	-1.083605	H	-4.157982	7.368662	-4.301549
H	2.625208	-2.973298	-0.771210	H	-4.826384	7.754876	-2.699178
C	-0.029296	-5.641770	5.015877	H	-5.514521	8.511484	-4.151832
C	-2.975001	4.790625	0.204156	C	-7.398961	6.771154	-3.151750
C	-1.384323	-1.489245	4.619975	H	-7.849614	7.689232	-3.563674
H	-1.452571	-1.744979	5.690535	H	-7.210065	6.942398	-2.079808
H	-2.133387	-2.084124	4.071929	H	-8.141443	5.961360	-3.239803
C	-5.468562	3.921058	-4.091338	C	1.567416	-8.982556	6.182908
H	-5.724537	3.937913	-5.148516	C	-2.093259	-0.760213	-4.480495
C	0.689883	-5.132608	-1.589258	H	-1.329807	-0.852739	-5.274550
H	0.932484	-6.197563	-1.760640	H	-3.068898	-0.979431	-4.957280
H	1.324808	-4.544559	-2.281761	C	2.936446	-2.914619	6.770405
C	4.833160	-0.654544	2.856068	C	7.255178	-0.652662	2.080583
H	5.137463	0.026716	3.653275	C	-4.168027	4.690946	-8.592656
C	-0.796382	-4.956080	-1.944271	H	-5.119918	4.439565	-8.100394

H	-4.413574	5.152642	-9.563008
H	-3.661092	5.448835	-7.972161
C	6.939393	-6.618676	1.673511
H	7.177037	-6.317005	0.641362
H	7.791891	-7.209483	2.046059
H	6.871266	-5.708367	2.287643
C	5.833610	-8.697364	0.833258
H	4.934524	-9.333781	0.828046
H	6.684297	-9.314491	1.168636
H	6.030340	-8.384621	-0.205574
C	-4.014340	2.405763	-9.662307
H	-3.382723	1.521661	-9.840632
H	-4.283749	2.835889	-10.640579
H	-4.944765	2.061915	-9.184444
C	0.578588	-10.170624	6.126018
H	0.447185	-10.543217	5.097863
H	-0.413126	-9.873548	6.503902
H	0.942223	-11.008259	6.743915
C	-8.101865	0.611037	0.178294
H	-8.756420	1.144095	-0.530153
H	-8.498294	0.792037	1.189512
H	-8.198447	-0.468105	-0.031519
C	2.959167	-9.448578	5.699936
H	3.343520	-10.244568	6.358498
H	3.681678	-8.616904	5.715048
H	2.935962	-9.862981	4.680121
C	3.337370	2.007009	-3.486249
H	2.872517	1.066622	-3.830511
H	3.227060	2.731574	-4.311630
C	1.713114	-8.547323	7.654722
H	0.743288	-8.297091	8.112165
H	2.375243	-7.673726	7.760364
H	2.151207	-9.366888	8.246150
C	0.892710	-1.751280	0.701187
H	-0.025440	-1.421299	1.213534
H	0.615490	-2.607088	0.073931
C	-2.327319	8.449532	1.308310
C	7.794724	-1.103648	3.457305
H	8.859412	-0.836503	3.562303
H	7.694611	-2.193058	3.589980
H	7.256835	-0.607688	4.277478
C	4.817580	1.770673	-3.171976
H	5.310961	2.691202	-2.817322
H	5.365332	1.421490	-4.061235
H	4.947789	1.006882	-2.386105
C	4.045630	-3.177988	7.810697
C	1.455201	-0.630676	-0.171397
H	1.410058	0.329960	0.366272
H	2.522038	-0.797417	-0.373362
C	-3.348952	8.454123	2.464867
H	-3.034226	7.784341	3.280883
H	-4.353587	8.145442	2.137727
H	-3.445496	9.470001	2.879299
C	0.716721	-0.549958	-1.501742
H	-0.364216	-0.410387	-1.355532
H	0.851159	-1.477343	-2.080913
H	1.059714	0.286252	-2.119491
C	7.329478	0.890715	2.013404
H	6.707938	1.364508	2.786703
H	6.987964	1.267127	1.034748
H	8.364598	1.235896	2.172950
C	-1.018782	9.078030	1.834180
H	-1.223741	10.070440	2.265970
H	-0.271112	9.222855	1.040204
H	-0.562366	8.456592	2.621649
C	8.161050	-1.233873	0.982011
H	9.191972	-0.871087	1.117543
H	7.833791	-0.920951	-0.022111
H	8.191898	-2.336245	1.006489
C	-2.882418	9.312961	0.150024
H	-3.814283	8.880329	-0.245966
H	-2.164118	9.380142	-0.683278
H	-3.104390	10.337055	0.492888
C	5.308262	-3.728763	7.107724
H	5.097113	-4.678495	6.589286
H	6.109696	-3.909951	7.843458
H	5.697092	-3.024372	6.360480
C	-4.355173	-4.725480	1.432571
H	-4.900968	-3.892381	0.962378
H	-4.953299	-5.069602	2.293571
H	-4.329454	-5.554782	0.704896
C	3.598197	-4.187332	8.880358
H	2.704206	-3.833141	9.417508
H	4.398794	-4.337464	9.622727
H	3.366866	-5.169573	8.439910
C	4.402623	-1.848121	8.521976
H	4.810851	-1.103681	7.821359
H	5.165519	-2.020175	9.299542
H	3.516677	-1.407062	9.006686
C	-2.194394	-5.397264	2.583995
H	-2.704723	-5.661169	3.531950
H	-2.184323	-6.320894	1.971775
C	-2.946063	-4.294123	1.855349
H	-3.001263	-3.403249	2.503397
H	-2.360484	-3.984882	0.974844

Complex **BF**·Ag^+, E = –4721.484507 E_h

Ag	0.900447	-0.399167	-0.686299	H	-2.682937	-0.336984	3.041963
O	-5.076421	1.957173	-5.204359	C	4.886626	-2.863568	5.570968
O	1.640881	1.776008	1.759130	C	-2.318299	-3.309386	-1.074514
O	-0.742277	-1.587325	1.751905	H	-3.233233	-3.850558	-0.848081
O	-2.508025	-2.480411	-4.779164	C	1.279672	-3.648557	2.050488
O	-0.228078	3.133871	-4.887420	H	1.563612	-4.712796	2.011347
O	-1.563697	1.803790	2.930318	H	1.024130	-3.335121	1.030892
O	-0.530873	-0.160019	-8.632833	C	0.483030	0.215542	8.076007
O	2.731675	-1.605511	0.471532	C	-3.107878	3.818005	-7.092005
N	-1.605584	-3.501557	-2.220513	H	-4.132231	4.189751	-7.026492
N	1.559909	3.348314	-2.493117	C	0.429350	4.329860	-4.525529
N	-0.523783	-2.729693	-2.244651	H	-0.223935	4.970848	-3.901045
N	-0.532000	-2.028492	-1.147854	H	0.703159	4.920874	-5.419132
N	1.359559	1.686398	-1.197280	C	-1.747928	-2.131043	3.879100
N	1.575283	2.023246	-2.439776	C	-6.329118	2.408782	-4.678346
C	-4.087443	0.302003	-3.750496	H	-6.153887	3.227199	-3.953790
C	-4.353975	-1.235981	-5.745450	H	-6.821016	1.588621	-4.117998
C	1.221346	2.793142	-0.415984	C	0.821480	0.637823	-6.799381
C	2.516570	2.208137	2.738418	C	-0.506169	2.765709	-7.248603
C	-3.216906	2.599242	-3.815530	C	5.474204	3.755369	5.572817
C	3.826832	1.693477	2.715433	C	1.728604	4.029220	-3.778316
C	-0.808971	-2.413606	2.865006	H	2.376286	3.385972	-4.388420
C	-1.470977	0.203559	4.737585	H	2.259654	4.973348	-3.586508
C	2.106218	3.084924	3.769892	C	-3.262814	-1.706874	-8.293217
C	0.069970	-3.504778	2.972904	H	-2.825123	-1.864091	-9.280663
C	-1.015063	1.393551	4.136077	C	-1.125487	-2.654953	-7.311287
C	-1.613583	-2.342709	-0.381715	H	-0.983459	-3.594610	-6.755575
C	0.434390	1.783230	6.029995	H	-0.944544	-2.883348	-8.372901
H	1.202629	2.395993	6.501839	C	0.582049	-1.895446	-5.600988
C	-0.995620	-0.125671	6.011953	H	0.463208	-2.861474	-5.108302
H	-1.360190	-1.045295	6.468022	C	0.894821	2.753480	1.049819
C	-0.057993	0.656544	6.700196	H	1.079125	3.760712	1.451680
C	2.467874	-2.819871	2.553834	H	-0.173247	2.515516	1.189490
C	4.764132	2.211455	3.624263	C	-1.287090	2.935645	-8.401074
H	5.785423	1.835185	3.560601	H	-0.878801	2.625670	-9.364529
C	-3.155654	-1.963374	-5.900031	C	1.486557	0.338026	-5.603108
C	-2.364697	3.677724	-5.912097	H	2.063630	1.116415	-5.103489
C	-1.938942	-3.087564	4.879912	C	-1.517613	-5.302794	6.052754
H	-2.705237	-2.889233	5.633057	C	-2.564716	3.487865	-8.332689
C	-3.190596	0.024280	-2.710813	H	-3.152574	3.631529	-9.242403
H	-3.143079	-0.991276	-2.318606	C	0.843942	2.065251	-7.340287
C	3.881506	-0.817439	2.446813	H	1.167118	2.083342	-8.392626
C	-1.181068	-4.266471	4.960614	H	1.604492	2.623031	-6.773683
C	0.636426	3.372220	4.082817	C	-4.493739	-1.063897	-8.170619
H	0.053049	3.648723	3.197590	H	-5.030346	-0.729646	-9.061604
H	0.593378	4.236830	4.763235	C	-7.223440	2.886001	-5.814149
C	3.003060	-1.733554	1.834140	C	-8.598644	3.349727	-5.322767
C	4.438459	3.182196	4.581228	C	5.138961	3.269318	7.004537
C	4.209559	0.537273	1.802515	H	4.122827	3.565182	7.311787
H	3.674902	0.619075	0.849039	H	5.843434	3.700637	7.733873
H	5.289029	0.599282	1.586116	H	5.206216	2.171704	7.076634
C	3.041031	-3.113829	3.799172	C	5.584777	-1.716835	6.327896
H	2.670654	-3.991931	4.328496	H	6.129265	-2.123434	7.194636
C	-3.045479	3.910896	-4.566331	H	4.856917	-0.980388	6.699734
H	-4.016868	4.390826	-4.753022	H	6.323817	-1.189758	5.705488
H	-2.467070	4.605658	-3.937020	C	-1.888518	-1.620862	0.904976
C	-4.141106	1.621352	-4.248444	H	-2.163298	-0.575666	0.680487
C	-1.038107	3.206711	-6.019750	H	-2.744459	-2.095204	1.407555
C	-0.018685	2.169037	4.760329	C	0.293205	-0.356956	-9.783495
C	4.423900	-1.166567	3.690918	H	0.728006	-1.375183	-9.766379
H	5.145369	-0.485777	4.144245	H	1.145855	0.349487	-9.770941
C	-0.150528	-4.422509	4.019958	C	1.397210	-0.925396	-5.021440
H	0.500818	-5.296450	4.067808	H	1.920384	-1.138531	-4.088403
C	-2.353956	2.281122	-2.760170	C	5.969967	-3.836700	5.041995
H	-1.653630	3.039104	-2.402915	H	6.649322	-3.326734	4.339962
C	4.089581	-2.360246	4.349768	H	5.514831	-4.687615	4.510254
C	-2.358874	1.012052	-2.185609	H	6.573776	-4.235693	5.874197
H	-1.673010	0.779654	-1.367890	C	-0.653801	-0.328594	8.967013
C	-4.891629	-0.829878	-4.377996	H	-1.134858	-1.221896	8.538148
H	-5.944965	-0.535996	-4.497967	H	-1.434504	0.431289	9.128547
H	-4.882682	-1.684039	-3.683257	H	-0.254145	-0.622566	9.950597
C	-2.553830	-2.140259	-7.164084	C	3.983951	-3.603788	6.578415
C	3.090656	3.574842	4.642775	H	4.581210	-3.943870	7.439204
H	2.771312	4.277765	5.417257	H	3.510402	-4.496444	6.143589
C	-1.924064	-4.338055	-3.377822	H	3.188198	-2.942210	6.955319
H	-2.282845	-5.311592	-3.011232	C	5.449011	5.299389	5.540987
H	-0.975479	-4.488497	-3.909618	H	5.708546	5.682691	4.540731
C	-0.110896	-1.641997	-6.790814	H	6.182453	5.704675	6.255962
C	0.076214	-0.389657	-7.418317	H	4.466288	5.710051	5.819172
C	1.348270	3.883072	-1.257787	C	-0.547454	-0.148430	-11.034500
H	1.314990	4.954064	-1.073014	H	-1.074567	0.815985	-10.940041
C	-2.967446	-3.731178	-4.314734	H	-1.335204	-0.920907	-11.068342
H	-3.121492	-4.442112	-5.148268	C	6.909348	3.300782	5.240468
H	-3.939484	-3.636266	-3.790218	H	7.039705	2.213127	5.359392
C	-5.010690	-0.796574	-6.903732	H	7.621542	3.786782	5.924430
H	-5.936111	-0.226771	-6.799115	H	7.199861	3.574083	4.213468
C	-2.408271	-0.764998	4.011894	C	1.521710	-0.909061	7.837326
H	-3.339844	-0.882846	4.589935	H	1.917695	-1.289285	8.794755

H	2.366559	-0.535750	7.237247
H	1.082033	-1.757345	7.287812
C	1.173080	1.370948	8.828977
H	0.483789	2.212629	9.002803
H	2.052285	1.756178	8.290120
H	1.529526	1.016262	9.808923
C	-2.926452	-5.881930	5.771251
H	-3.702202	-5.101803	5.830419
H	-3.177094	-6.658690	6.511439
H	-2.980212	-6.339292	4.769988
C	0.278818	-0.179157	-12.321041
H	0.804250	-1.140833	-12.447740
H	1.043776	0.615765	-12.333345
H	-0.363724	-0.033150	-13.203089
C	-0.502046	-6.457741	6.081699
H	-0.486167	-7.020113	5.134834
H	-0.763021	-7.168729	6.880810
H	0.517550	-6.090015	6.284390
C	-1.527527	-4.639398	7.450340
H	-0.531719	-4.253075	7.720140
H	-1.822819	-5.376821	8.214771
H	-2.240965	-3.802791	7.517367
H	-8.515925	4.179619	-4.600997
H	-9.147352	2.532420	-4.824478
H	-9.220575	3.703297	-6.159778
H	-7.336951	2.067505	-6.545254
H	-6.711155	3.704976	-6.347683
C	3.852088	-2.003701	-0.346101
C	-2.776016	2.552153	3.072083
H	4.098553	-3.057837	-0.123977
H	4.733303	-1.397466	-0.071907
C	3.526753	-1.817717	-1.817193
H	-2.582732	3.463936	3.670084
H	-3.516080	1.954483	3.638041
C	-3.326547	2.915169	1.701556
H	3.189906	-0.776929	-1.975128
H	2.684441	-2.474787	-2.092231
C	4.729038	-2.094555	-2.720519
H	-3.459835	1.992993	1.109778
H	-2.579929	3.523237	1.160694
C	-4.652429	3.675173	1.798590
H	5.103301	-3.124830	-2.598297
H	5.562717	-1.409398	-2.497443
H	4.458854	-1.958852	-3.779096
H	-4.540841	4.612136	2.369058
H	-5.424958	3.072483	2.304376
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C	0.586990	-3.005661	-2.488942	C	3.670986	5.902266	-3.796805
C	0.931626	-4.327059	-2.804458	C	3.577983	7.059637	4.194356
C	1.945451	-4.950400	-2.048173	C	2.835895	7.118847	-4.261324
C	2.517311	-4.313161	-0.924607	C	4.034994	5.035076	-5.027071
C	2.131737	-2.996283	-0.641636	C	4.981974	6.424175	-3.176577
C	1.191867	-2.330483	-1.427744	C	2.874932	7.635486	5.438571
C	3.528649	-5.005056	-0.023504	C	3.705461	8.184171	3.141010
C	3.110584	-6.341324	0.570397	C	4.991406	6.588089	4.622676
C	3.881230	-7.484948	0.323597	O	0.662099	2.407676	-0.406022
C	3.522484	-8.723671	0.853906	C	-1.378870	-6.594138	-2.702803
C	2.352340	-8.840709	1.602233	C	-1.879527	-6.546489	2.547694
C	1.539247	-7.728726	1.866066	C	-1.044387	-7.507732	1.951090
C	0.245978	-7.912776	2.649734	C	-1.452263	-8.089410	0.730100
O	2.347945	-6.212877	-2.407676	C	-2.615149	-7.634469	0.054531
N	-0.203259	-2.996643	2.455823	C	-3.431134	-6.697611	0.697287
N	-0.440426	-1.722736	2.586260	C	-3.086649	-6.156357	1.944362
N	0.632906	-1.175093	3.149712	C	-2.983426	-8.081816	-1.353103
C	1.591886	-2.115039	3.380006	C	-1.931579	-7.863727	-2.433665
C	1.039718	-3.299133	2.923705	C	-1.508633	-8.943725	-3.220884
C	1.576405	-4.699098	2.915525	C	-0.558296	-8.773473	-4.228354
O	1.237755	-5.328462	1.684142	C	0.001477	-7.515174	-4.445231
C	0.634072	0.264967	3.405859	C	-0.384632	-6.403434	-3.682824
C	1.687311	1.049447	2.597518	C	0.244451	-5.042387	-3.960137
O	1.121036	2.284384	2.184451	O	-0.656161	-9.058419	0.191846
C	1.594331	4.544664	-3.176988	N	-2.512366	-3.084040	-0.605232
C	0.845268	3.705154	-2.350999	N	-2.378924	-1.794990	-0.478481
C	1.379477	3.323193	-1.098743	N	-2.642194	-1.246839	-1.659082
C	2.621574	3.834069	-0.668301	C	-2.944675	-2.203106	-2.578903
C	3.326115	4.687923	-1.535822	C	-2.852049	-3.397670	-1.887216
C	2.854568	5.047752	-2.804452	C	-2.965327	-4.818971	-2.345351
C	-0.501313	3.146387	-2.801809	O	-1.775757	-5.495657	-1.954512
C	3.272170	3.409106	0.651805	C	-2.357890	0.178890	-1.855128
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C	1.642059	3.499173	2.629302	O	-2.117945	2.184763	-0.502365
C	1.017667	4.176702	3.687729	C	-2.129224	5.476575	4.323533
C	1.643135	5.343384	4.160420	C	-1.556074	4.347145	3.721302
C	2.815716	5.859951	3.591992	C	-2.183042	3.783260	2.590414
C	3.308472	5.218456	2.440606	C	-3.338536	4.390326	2.045301

C	-3.859725	5.524020	2.679326
C	-3.296062	6.083568	3.837438
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O	-1.669059	2.622381	2.105683
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H	3.787776	-4.300796	0.784427
H	4.469047	-5.170601	-0.572762
H	4.776512	-7.394669	-0.297974
H	4.142924	-9.602513	0.662228
H	2.054227	-9.815650	1.994799
H	0.294351	-7.353650	3.597891
H	0.183551	-8.974598	2.937402
C	3.541959	-6.283581	-3.190555
H	2.550353	-1.882818	3.837276
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H	0.744846	0.430897	4.488051
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H	1.951985	0.475738	1.690722
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H	1.184807	4.795628	-4.158825
H	4.298351	5.048905	-1.198925
H	-0.533892	2.081148	-2.542752
H	-0.547052	3.219718	-3.899731
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H	4.928379	5.792312	5.382756
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H	0.845900	2.404032	0.558179
H	-1.614042	-6.148897	3.530776
H	-4.354955	-6.371259	0.212101
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H	-3.257464	-9.147953	-1.359967
H	-1.935219	-9.933485	-3.038271
H	-0.243107	-9.625269	-4.835822
H	0.760243	-7.384768	-5.221895
H	0.965247	-5.181610	-4.782471
H	-0.524507	-4.360097	-4.360212
C	-1.142891	-10.407057	0.180484
H	-3.179413	-1.972147	-3.614743
H	-3.106430	-4.851358	-3.438875
H	-3.847997	-5.296760	-1.882524
H	-2.733587	0.463435	-2.847230
H	-1.265425	0.303682	-1.842080
H	-2.921267	0.465356	0.203597
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H	-4.710125	5.888335	-0.756081
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H	4.396510	-5.879685	-2.615119
H	3.440196	-5.647754	-4.091035
C	3.810864	-7.729472	-3.575631
H	-2.005000	-10.501000	-0.502757
H	-1.502359	-10.681362	1.190859
C	-0.020703	-11.328673	-0.275257
H	0.917672	-1.298197	-1.194500
H	-3.777412	-5.489764	2.468015
H	3.005290	-8.084997	-4.238982
H	3.746288	-8.344875	-2.663153
C	5.175384	-7.898873	-4.247409
H	0.796962	-11.288504	0.463489
H	0.393732	-10.921856	-1.213237
C	-0.491029	-12.771785	-0.477909
H	5.995584	-7.611292	-3.567998
H	5.264705	-7.275817	-5.152435
H	5.346844	-8.943198	-4.550871
H	-1.277621	-12.839951	-1.248513
H	-0.902581	-13.204788	0.449749
H	0.340711	-13.415467	-0.802804
Ag	-1.573078	-4.251624	1.124644

Complex **CF**·Ag^+ (isomer 1) E = –4093.383850 E_h

Ag	-0.623702	1.635766	1.131875
O	-3.581811	1.204848	1.541677
O	-0.679591	4.585750	-0.249428
O	5.821037	-4.618800	0.895797
O	-3.383545	5.323247	2.853648
O	1.096354	-4.121161	1.698541
O	4.486148	-1.130899	-2.510638
O	1.648512	-5.426640	-2.925029
O	-4.658901	4.217340	-1.335377
N	2.714370	1.838165	-1.346260
N	-0.973702	-2.191291	2.901581
N	1.078432	2.346707	-0.096609
N	1.896516	1.377467	-0.413953
N	-1.283337	-0.338783	1.922585
C	4.688575	-2.500038	-2.564108
C	-4.726866	1.992951	1.664835
C	1.361724	3.461458	-0.824047
C	-1.467333	5.734185	-0.302905
C	-2.315654	4.514022	3.126825
C	-2.195419	5.980573	-1.484533
C	5.288840	-3.399567	1.229481
C	3.031494	-5.556374	1.786492
C	5.686524	-2.219340	0.556559
N	-0.359082	-1.130201	2.395995
C	3.941457	-3.306403	-3.455745
C	5.791916	-3.028384	-1.853444
C	1.412407	-3.018893	-3.177876
C	1.794122	-5.222337	1.197513
C	-4.919181	2.677606	2.882151
C	6.488577	-2.245917	-0.745798
H	7.486814	-2.683337	-0.588453
H	6.652029	-1.207002	-1.069265
C	-5.646446	2.097355	0.601183
C	-2.508646	3.227424	3.678482
C	1.086687	-4.238074	-2.536141
C	2.630591	-2.857344	-4.096803
H	2.494942	-3.418694	-5.034869
H	2.699831	-1.797920	-4.388409
C	4.290795	-3.370996	2.229774
C	-3.798360	3.239296	-1.767210
C	4.435052	-4.586833	-3.745389
H	3.912354	-5.196474	-4.482694
C	-1.371509	2.452413	3.951803
H	-1.502933	1.465419	4.401758
C	-2.929451	7.170707	-1.573713
H	-3.482225	7.388640	-2.491706
C	3.821341	-2.125426	2.665723
H	3.062469	-2.087970	3.451882
C	6.232523	-4.318984	-2.172811
H	7.111382	-4.719334	-1.664657
C	-1.026283	4.978216	2.778801
C	-2.595876	3.583716	-2.423844
C	-1.535237	6.600909	0.806009
C	-0.082786	2.916312	3.667075
H	0.788467	2.307454	3.920121
C	-2.519918	-0.866983	2.129576
C	2.425820	3.134180	-1.648405
H	2.979331	3.703286	-2.390991
C	0.671376	4.780074	-0.628344
H	1.209857	5.355865	0.150119
H	0.744794	5.370445	-1.559441
C	7.189898	-4.844811	1.242407
H	7.349816	-4.607579	2.311497
H	7.851698	-4.173834	0.666623
C	-4.130101	1.889927	-1.509066
C	-3.884508	2.654243	3.995086
H	-3.733249	1.618059	4.340000
H	-4.315592	3.188611	4.857051
C	-2.166326	5.024409	-2.664386
H	-1.147976	4.990649	-3.085885
H	-2.786664	5.466904	-3.461167
C	0.631018	-1.897493	-2.853552
H	0.804463	-0.963077	-3.395483
C	0.079364	4.171158	3.071799
H	1.083418	4.529940	2.829924
C	-2.326169	-2.080586	2.768856
H	-3.018223	-2.831396	3.141487
C	-6.121202	3.373976	3.066214
H	-6.298929	3.886504	4.015257
C	-5.413554	1.509088	-0.784678
H	-6.271001	1.813138	-1.407304
H	-5.463586	0.406889	-0.750919
C	-2.958206	8.079299	-0.517204
H	-3.522477	9.010202	-0.609982
C	-3.791991	-0.190889	1.693528
H	-4.135804	-0.636617	0.740809
H	-4.581895	-0.388206	2.439835
C	3.714098	-4.657102	2.810610
H	3.009348	-4.376789	3.608566
H	4.514512	-5.240661	3.291657
C	-1.787239	2.546257	-2.908362
H	-0.868784	2.800153	-3.445698
C	-7.093986	3.407218	2.069593
H	-8.036187	3.933194	2.241033
C	7.549172	-6.293279	0.940889
H	7.143642	-6.548992	-0.052575
H	7.037205	-6.954869	1.659479
C	0.188559	-4.275579	-1.445199
C	-6.841904	2.791386	0.844857
H	-7.586736	2.847832	0.046463
C	-2.280078	7.782135	0.663550
H	-2.323254	8.480969	1.503458
C	-0.329737	-1.936385	-1.842632
H	-0.899851	-1.042120	-1.589324
C	1.276035	-5.908344	-4.219210
H	1.763748	-5.309413	-5.008982
H	0.184684	-5.794169	-4.361571
C	3.475060	-0.502253	-1.745224
H	3.492384	-0.828660	-0.695765
H	2.471940	-0.705140	-2.138881
C	-3.906788	6.117496	3.921277
H	-3.085632	6.673389	4.413015
H	-4.366496	5.471052	4.693439
C	5.585142	-5.084523	-3.139622
H	5.966555	-6.071477	-3.411711
C	5.224185	-0.996101	1.064582
H	5.572621	-0.072432	0.592057
C	-0.507639	-3.109794	-1.112032
H	-1.208302	-3.131743	-0.273092
C	1.690329	-7.366213	-4.359602
H	1.093470	-7.982687	-3.666334
H	2.740407	-7.466132	-4.035516
C	0.163946	-4.456428	2.705132
H	0.588578	-5.210908	3.394655
H	-0.753194	-4.903245	2.272237
C	3.790280	0.989569	-1.868576
H	4.723876	1.231562	-1.336340
H	3.935441	1.239859	-2.929286
C	1.251455	-5.973970	0.134046
C	-3.286915	0.887696	-2.008356
H	-3.552164	-0.162883	-1.854284
C	-0.830195	6.338976	2.131437
H	0.256017	6.505431	2.020726
H	-1.168908	7.119023	2.832335
C	3.660466	-6.736220	1.365536
H	4.607340	-7.019177	1.827561
C	3.107022	-7.535566	0.367607
H	3.611310	-8.452394	0.052554
C	4.318863	-0.939368	2.125589
H	3.965726	0.023369	2.502590
C	1.928195	-7.137001	-0.259041
H	1.519568	-7.732716	-1.077170
C	-2.134775	1.208940	-2.727151
H	-1.511327	0.419089	-3.147044
C	0.003729	-5.543104	-0.626938
H	-0.290625	-6.372426	-1.288185
H	-0.837662	-5.380780	0.064387
C	9.058129	-6.536505	0.975690
H	9.294753	-7.596873	0.797535
H	9.495337	-6.255234	1.948975
H	9.578409	-5.949268	0.201280
C	-5.542628	4.763426	-2.316850
H	-6.105556	3.947664	-2.810204
H	-4.966311	5.277284	-3.109813
C	-0.192329	-3.243192	3.559396
H	-0.773102	-3.584812	4.428896
H	0.723027	-2.758928	3.923735
C	-4.941208	7.070100	3.344702
H	-5.695744	6.471003	2.809115
H	-4.449707	7.693871	2.580800
C	1.523237	-7.865500	-5.795337
H	2.167712	-7.305508	-6.492145
H	0.483012	-7.753370	-6.146099
H	1.792922	-8.929574	-5.882377
C	-6.485363	5.742986	-1.638007
H	-7.062833	5.201844	-0.870755
H	-5.874878	6.482949	-1.095227
C	-5.604258	7.944621	4.407475
H	-6.323042	8.640547	3.947233
H	-4.865854	8.550237	4.960797
H	-6.155678	7.340547	5.148060
C	-7.422074	6.439794	-2.624718
H	-8.042158	5.717968	-3.184084
H	-6.861867	7.035814	-3.365617
H	-8.106347	7.124627	-2.099380

Complex **CF**·Ag^+ (isomer 2) E = –4093.390853 E_h

C	1.728703	-7.149597	3.337028
C	1.552495	-5.899731	2.726956
C	0.253208	-5.354038	2.689386
C	-0.856518	-6.042215	3.218578
C	-0.629109	-7.291616	3.816279
C	0.649107	-7.843905	3.882697
C	-2.268410	-5.471013	3.248880
C	-2.823581	-4.749982	2.033178
C	-3.382793	-3.473611	2.182498
C	-3.946946	-2.802357	1.095778
C	-3.920502	-3.396588	-0.165815
C	-3.354569	-4.665898	-0.365755
C	-2.851100	-5.353079	0.756992
C	-3.336078	-5.262822	-1.765400
O	-2.333295	-6.615087	0.610952
O	0.061807	-4.152936	2.035611
N	-0.137377	-0.509125	2.317258
N	-1.262557	-0.029614	2.877442
N	-1.027595	1.179184	3.278635
C	0.264174	1.512690	2.986005
C	0.848509	0.418268	2.363127
C	0.807772	2.863073	3.291383
C	-0.111747	-1.848567	1.742284
C	0.095573	-2.953410	2.778523
O	0.612283	3.755142	2.151438
C	2.110285	7.063927	2.779406
C	2.015678	5.717294	2.401703
C	0.739560	5.124771	2.430506
C	-0.430160	5.851953	2.716468
C	-0.279849	7.195891	3.085758
C	0.978289	7.794372	3.139670
C	-1.812696	5.222107	2.664522
C	-2.284183	4.658060	1.328419
C	-2.796927	3.349322	1.282831
C	-3.293642	2.811214	0.093560
C	-3.226246	3.558138	-1.083044
C	-2.692205	4.854248	-1.091113
C	-2.276554	5.418040	0.136341
C	-2.574052	5.612215	-2.403144
O	-1.808843	6.707400	0.158745
C	-2.038716	-7.158065	-2.813109
C	-2.037908	-5.858800	-2.289015
C	-0.834584	-5.123389	-2.330939
C	0.363740	-5.689200	-2.813072
C	0.304264	-6.987973	-3.342206
C	-0.882330	-7.718777	-3.354446
C	1.703393	-4.965303	-2.818452
C	2.230190	-4.347345	-1.529474
C	2.801666	-3.065673	-1.574808
C	3.347853	-2.474885	-0.434951
C	3.304914	-3.160460	0.779856
C	2.747515	-4.444796	0.873937
C	2.243026	-5.044078	-0.301126
C	2.779394	-5.158784	2.216027
O	1.709256	-6.301939	-0.241988
O	-0.871056	-3.845341	-1.807099
N	-1.157671	-0.289593	-2.353876
N	-0.642942	0.224723	-1.245007
N	-0.295112	1.454577	-1.515551
C	-0.587306	1.758121	-2.808339
C	-1.148553	0.621036	-3.364475
C	-0.306271	3.104239	-3.414271
C	-1.652432	-1.666505	-2.334514
C	-0.565605	-2.723791	-2.607414
O	-0.122913	4.049733	-2.376262
C	-1.098531	7.496665	-3.207022
C	-1.205991	6.164738	-2.782168
C	-0.032976	5.383990	-2.774493
C	1.227614	5.914308	-3.110242
C	1.278505	7.250387	-3.533239
C	0.127685	8.034961	-3.595443
C	2.511002	5.094502	-3.082386
C	2.872529	4.348077	-1.806814
C	3.192043	2.983800	-1.867107
C	3.548593	2.271594	-0.720966
C	3.557339	2.918011	0.516443
C	3.246254	4.282593	0.626650
C	2.944842	4.998773	-0.554203
C	3.268191	4.958169	1.990566
O	2.662731	6.336684	-0.477188
H	2.732706	-7.581408	3.384662
H	-1.477373	-7.837790	4.238874
H	0.802900	-8.817072	4.355238
H	-2.344687	-4.776383	4.104323
H	-2.943208	-6.305290	3.504541
H	-3.384193	-3.000217	3.168369
H	-4.359298	-2.873583	-1.021297
H	-3.669147	-4.471881	-2.460397
H	-4.107016	-6.048945	-1.835934
C	-3.255132	-7.699710	0.729554
H	1.883484	2.819495	3.521695
H	0.275609	3.287043	4.155434
H	0.690063	-1.887444	0.993169
H	-1.070821	-2.012840	1.234447
H	-0.706212	-2.917174	3.538498
H	1.063371	-2.826801	3.301906
H	3.092651	7.543471	2.786640
H	-1.169938	7.777245	3.338259
H	1.074864	8.839316	3.443851
H	-2.533646	5.982515	3.006436
H	-1.875836	4.404669	3.400756
H	-2.803701	2.749462	2.196048
H	-3.580297	3.125274	-2.023429
H	-3.279879	6.458799	-2.412303
H	-2.929667	4.941038	-3.204155
C	-2.790690	7.736563	0.323965
H	-2.968895	-7.732932	-2.802466
H	1.219178	-7.436537	-3.739561
H	-0.902129	-8.727729	-3.773229
H	1.693796	-4.168563	-3.581910
H	2.450404	-5.689069	-3.185171
H	2.839764	-2.534844	-2.531129
H	3.726749	-2.700475	1.679031
H	3.612508	-5.882801	2.208823
H	3.072944	-4.409318	2.972111
C	2.606934	-7.402971	-0.397076
H	-1.144240	3.395772	-4.072815
H	0.596373	3.047445	-4.052262
H	-2.490889	-1.733096	-3.041882
H	-2.040134	-1.842942	-1.323278
H	0.413638	-2.308581	-2.315299
H	-0.525644	-2.991077	-3.677515
H	-1.997425	8.118624	-3.234800
H	2.243170	7.679529	-3.817156
H	0.189107	9.072236	-3.933233
H	3.334522	5.779506	-3.341485
H	2.491344	4.354656	-3.901090
H	3.166233	2.473983	-2.834498
H	3.824641	2.360984	1.419236
H	3.505993	4.187708	2.742631
H	4.110627	5.667594	2.032839
C	3.764315	7.241680	-0.612462
H	-3.997801	-7.661392	-0.091829
H	-3.823607	-7.612319	1.675935
C	-2.480782	-9.007882	0.686487
C	-2.103874	9.092500	0.272075
H	-3.318764	7.600538	1.287578
H	-3.557536	7.660240	-0.470727
H	3.402954	-7.356508	0.370829
H	3.108950	-7.343201	-1.382787
C	1.817745	-8.696237	-0.269977
C	3.239649	8.667487	-0.544468
H	4.285689	7.060977	-1.572298
H	4.505283	7.058157	0.189237
H	-1.751665	-9.007151	1.513907
H	-1.890054	-9.027286	-0.244938
C	-3.390587	-10.234200	0.770652
H	-1.553434	9.166806	-0.680615
H	-1.341786	9.131755	1.067803
C	-3.088418	10.254411	0.414944
H	1.027940	-8.697863	-1.039069
H	1.301814	-8.688501	0.704516
C	2.700128	-9.938366	-0.401183
H	2.689489	8.790788	0.402953
H	2.496102	8.802669	-1.346830
C	4.350142	9.712673	-0.661221
H	-4.107260	-10.267511	-0.067598
H	-3.975959	-10.245276	1.705742
H	-2.803705	-11.165405	0.739511
H	-3.631723	10.214244	1.374038
H	-3.841204	10.251978	-0.391437
H	-2.564814	11.222019	0.373843
H	3.476767	-9.971609	0.381852
H	3.213556	-9.975175	-1.377180
H	2.101998	-10.858472	-0.310313
H	4.893861	9.626616	-1.617160
H	5.091694	9.616240	0.149846
H	3.936920	10.731781	-0.608815
H	-4.397798	-1.816852	1.235470
H	1.843362	0.235965	1.966103
H	-3.708747	1.800789	0.086426
H	3.812988	-1.487442	-0.496224
H	-1.540423	0.405516	-4.355221
H	3.809663	1.212925	-0.791062
Ag	0.143907	2.887363	0.109323

Calculations were performed in ORCA 4.2.1 program package[S13] at the DFT level using B3LYP functional and def2-SVP basis set[S14] for all atoms except for Ag, for which SDD[S15] effective core potential was used.

References

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