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Cyclopenta-fused polyaromatic hydrocarbons: Synthesis and characterisation of a stable, carbon-centred helical radical

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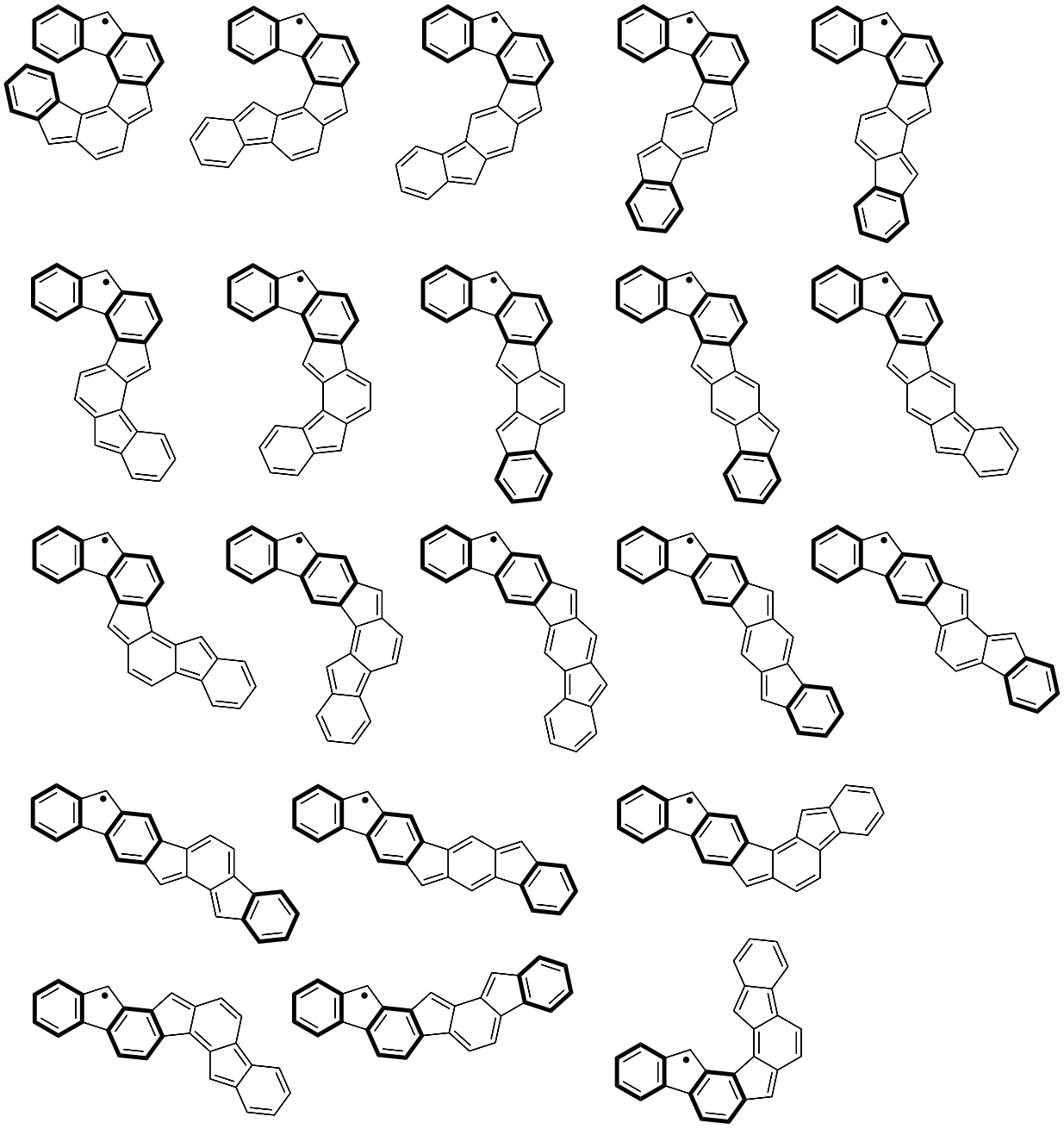
Electronic Supporting Information

Content:

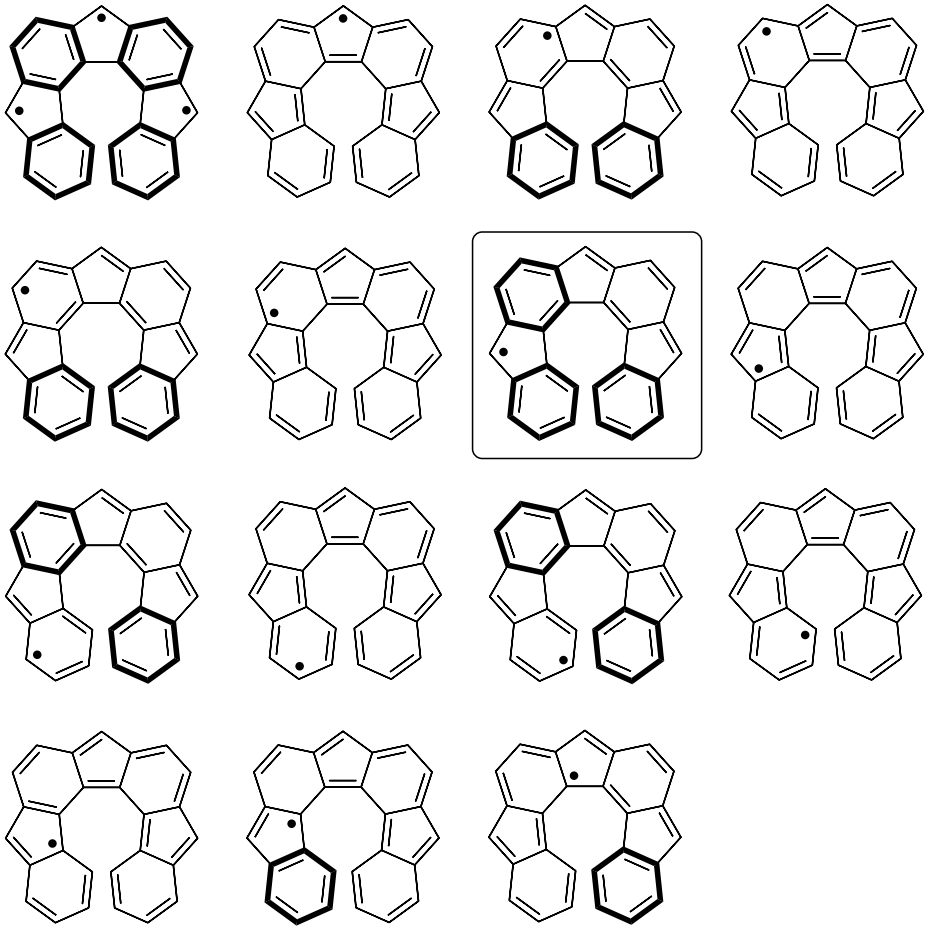
1. Possible Cyclopentadifluorene Radicals

The maximum number of full benzene rings for a monoradical is given; those are marked with bold bonds.



2. Resonance Formulas of 7

Fully intact benzene rings are given with bold bonds. Except for the first two formulas a second mirror image has to be considered for each resonance formula. The only monoradical resonance formula with three intact benzene rings is given in a box.

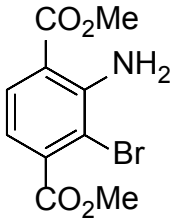


3. Experimental Procedures

General.

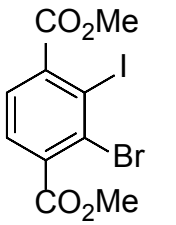
The pinacol boronates used for *Suzuki* couplings were synthesized according to published procedures.[1] Technical solvents (CH_2Cl_2, hexane, and n-pentane) were distilled prior to use. $CHCl_3$, MeOH, and MeCN were purchased as HPLC-grade solvents and used without further purification. THF was dried over sodium, CH_2Cl_2 was dried over CaH_2, and both were distilled prior to use. Anhydrous toluene (99.8%) was used as purchased without further purification. Flash column chromatography[2] was carried out using Merck SiO_2 60 (230–400 mesh) and thin layer chromatography (TLC) was carried out using commercially available Merck F254 pre-coated sheets. ^1H and ^{13}C NMR spectra were recorded with *Bruker* Avance 400 or Avance Neo instruments. NMR spectra at elevated temperatures were measured with a Bruker Avance DRX 500 spectrometer. Chemical shifts are given in ppm and are referenced by using the residual signals of the solvent as internal standard.[3] IR spectra were recorded with a *Bruker* Alpha FT-IR-spectrometer using the ATR technique and mass spectra were recorded with a *Finnigan* MAT-95 mass spectrometer. Melting points were determined with a *Laboratory Devices* Mel-Temp II melting point apparatus with a heating rate of 2 K/min. UV/Vis data were recorded with *Mettler Toledo* UV7 and *Perkin Elmer* Lambda 750 spectrophotometers; an UV/Vis/NIR spectrum was recorded on an Agilent Cary 5000 spectrophotometer. Cyclic voltammetry measurements were performed with a suitable potentiostat and an electrochemical cell within a glovebox. A freshly polished Pt disk as working electrode, a Pt wire as a counter electrode and an Ag wire as a (pseudo)reference electrode were used in 0.05mM $[NBu_4][Al\{OC(CF_3)_3\}_4]$ as electrolyte). Potentials were calibrated against the Fc/Fc^+ couple (internal standard). EPR spectra were recorded on a *Bruker* EMXplus X-band spectrometer (microwave frequency: 9.43 GHz). The spectra were simulated using the MATLAB/easyspin package.[4] Single crystals were mounted in perfluoropolyalkyl ether oil on a cryo loop and then brought into the cold nitrogen stream of a low-temperature device (*Oxford Cryosystems* Cryostream unit) so that the oil solidified. Diffraction data were collected using a *Stoe* IPDS II diffractometer and graphite-monochromated Mo-Kα (0.71073 Å) radiation. The structures were solved by direct methods with SHELXS[5] or by intrinsic phasing with SHELXT[6] followed by full-matrix least-squares refinement using SHELXL-2014/7[7] and the ShelXle GUI.[8] All non-hydrogen atoms were refined anisotropically. The contribution of the hydrogen atoms, in their calculated positions, was included in the refinement using a riding model.

Dimethyl 2-Amino-3-bromoterephthalate (9)



Following a published protocol[9] AcOH (1.45 mL, 1.50 g, 25.0 mmol) and then NBS (4.26 g, 23.9 mmol) were added to a solution of dimethyl-2-aminoterephthalate (**8**, 5.00 g, 23.9 mmol) in toluene (500 mL) and the mixture was stirred for 4 d at rt and washed with a solution of $NaHCO_3$ (5.00 g) in H_2O (500 mL). The organic layer was separated and the aqueous layer was extracted with EtOAc (3×150 mL). The combined organic layers were washed with brine (200 mL), dried (Na_2SO_4), concentrated at reduced pressure and purified by column chromatography (silica gel, hexane, EtOAc, 10:1) to yield **9** as a yellow solid (2.06 g, 7.15 mmol, 30%). R_f = 0.38 (hexane/EtOAc 4:1). ^1H NMR (400 MHz, $CDCl_3$): δ = 7.89 (d, ^3J = 8.3 Hz, 1 H, ArH), 6.87 (d, ^3J = 8.3 Hz, 1 H, ArH), 6.58 (br s, 2 H, NH_2), 3.93 (s, 3 H, OCH_3), 3.90 ppm (s, 3 H, OCH_3). The ^1H NMR data are in full agreement with published data.[10]

Dimethyl 2-Bromo-3-iodoterephthalate (10)



Following a published protocol[11] a solution of $NaNO_2$ (1.20 g, 17.4 mmol) in H_2O (12 mL) was added dropwise within 25 min to a cooled (0 °C) suspension of terephthalate **9** (2.00 g, 6.94 mmol) in a mixture of concd. HCl and H_2O (1:1, 45 mL) and stirring was continued for 30 min. The mixture was added slowly to a cooled (0 °C) solution of KI (6.91 g, 41.6 mmol) in H_2O (65 mL) and stirred vigorously for 18 h. Solid $Na_2S_2O_3$ was added to the stirred solution until the colour vanished and EtOAc (100 mL) was added. (If the organic layer turned dark, either more $Na_2S_2O_3$ was added or it was washed with saturated aqueous $NaHSO_3$ solution.) The organic layer was separated and the aqueous layer was extracted with EtOAc (2×100 mL). The combined organic layers were washed with saturated aqueous $NaHCO_3$ solution (150 mL), brine (100 mL), dried (Na_2SO_4), concentrated at reduced pressure, and purified by columns chromatography (silica gel, hexane/EtOAc, 6:1→5:1) to yield **10** as a slightly yellow solid (1.88 g, 4.71 mmol, 68%). R_f = 0.30 (hexane/EtOAc 4:1); ^1H NMR (400 MHz, $CDCl_3$): δ = 7.57 (d, ^3J = 7.9 Hz, 1 H, ArH), 7.46 (d, ^3J = 7.9 Hz, 1 H, ArH), 3.95 (s, 3 H, OCH_3), 3.95 ppm (s, 3 H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.6 (C), 166.7 (C), 143.1 (C), 137.2 (C), 130.09 (C), 129.2 (CH), 127.5 (CH), 103.9 (C), 53.3 (OCH_3), 53.2 ppm (OCH_3); IR (ATR): $\tilde{\nu}$ = 2953 (w), 1714 (m), 1579

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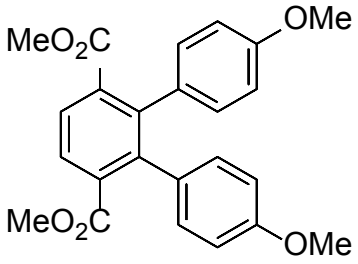
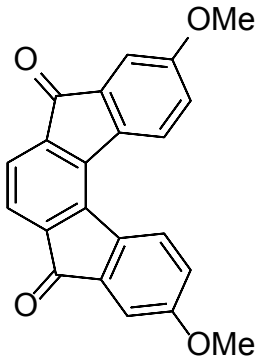
(w), 1448 (w), 1425 (w), 1343 (w), 1278 (m), 1243 (m), 1189 (m), 1152 (m), 1119 (m), 1057 (m), 949 (m), 863 (w), 842 (m), 821 (w), 791 (w), 752 (m), 726 (m), 698 (w), 529 (w), 475 (w) cm^{-1}; MS (FAB): *m/z* (%): 401.0 (35) $[M+1]^+$, 399.9 (14) $[M]^+$, 398.9 (35) $[M+1]^+$, 397.9 (11) $[M]^+$, 368.9 (15) $[M–OCH_3]^+$, 366.9 (15) $[M–OCH_3]^+$; HRMS (FAB): *m/z* calcd for $C_{10}H_9O_4{}^{79}BrI$: 398.8723 $[M+1]^+$; found: 398.8725.

Dimethyl 4,4''-Dimethoxy-[1,1':2',1''-terphenyl]-3',6'-dicarboxylate (12)



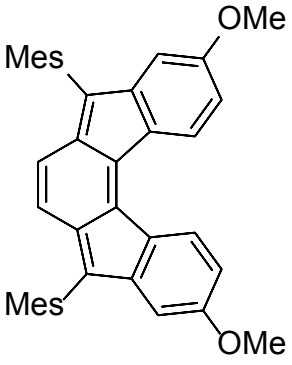
THF (2 mL) and H_2O (2 mL) were added to a mixture of terephthalate **10** (200 mL, 500 µmol), 2-(4-methoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolan[1a] (**11**, 260 mg, 1.11 mmol), and Na_2CO_3 (132 mg, 1.25 mmol). The solution was degassed by ultrasonication (15 min) and $PdCl_2(PPh_3)_2$ (8 mg, 11 µmol) was added. The mixture was heated for 15 h to 80 °C and cooled to rt. Half saturated aqueous NaCl solution (5 mL) and EtOAc (5 mL) were added and the aqueous layer was extracted with EtOAc (2×10 mL). The combined organic layers were dried (Na_2SO_4), concentrated at reduced pressure, and purified by columns chromatography (silica gel, hexane/EtOAc, 5:1) to yield **12** as a colourless, microcrystalline solid (124 mg, 305 µmol, 61%). R_f = 0.18 (hexane/EtOAc 4:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.72 (s, 2 H, ArH), 6.86–6.83 (m, 4 H, ArH), 6.70–6.66 (m, 4 H, ArH), 3.74 (s, 6 H, $ArOCH_3$), 3.57 ppm (s, 6 H, CO_2CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 169.0 (C), 158.4 (C), 141.6 (C), 135.5 (C), 131.0 (C), 130.9 (CH), 127.5 (CH), 113.0 (CH), 55.2 ($ArOCH_3$), 52.3 ppm (CO_2CH_3); IR (ATR): $\tilde{\nu}$ = 2953 (w), 1725 (m), 1609 (w), 1576 (w), 1511 (m), 1458 (w), 1429 (m), 1288 (m), 1240 (s), 1176 (m), 1142 (s), 1106 (m), 1077 (m), 1053 (m), 1029 (m), 958 (w), 872 (w), 836 (m), 758 (m), 641 (w), 608 (w), 564 (w), 542 (w), 497 (w) cm^{-1}; MS (FAB): *m/z* (%): 407.2 (47) $[M+1]^+$, 406.2 (100) $[M]^+$, 375.1 (27) $[M–OCH_3]^+$, 344.1 (16) $[M–2\ OCH_3]^+$, 343.1 (60); HRMS (FAB): *m/z* calcd for $C_{24}H_{22}O_6$: 406.1411 $[M^+]$; found: 406.1410.

3,10-Dimethoxyindeno[2,1-*c*]fluorene-5,8-dione (13)



Following a published protocol[12] terphenyl **12** (170 mg, 418 µmol) was dissolved under an argon atmosphere in Eaton's reagent (7.7% w/w P_2O_5 in $MeSO_3H$; 8 mL) and the solution was heated with vigorous stirring for 18 h to 80 °C, cooled to rt, poured on ice water (100 mL), and the precipitate was collected by filtration. It was washed successively with H_2O, saturated aqueous $NaHCO_3$ solution, H_2O, and acetone, and dried in high vacuum to yield **13** as a brown-red solid (75 mg, 220 µmol, 52%). ^{1}H NMR (400 MHz, $CDCl_3$ + 10% TFA): δ = 7.89 (d, ^3J = 8.4 Hz, 2 H, ArH), 7.53 (s, 2 H, ArH), 7.38 (d, ^4J = 2.6 Hz, 2 H, ArH), 7.21 (dd, ^3J = 8.4 Hz, ^4J = 2.6 Hz, 2 H, ArH), 3.94 ppm (s, 6 H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$ + 10% TFA): δ = 195.7 (C), 161.1 (C), 141.6 (C), 138.0 (C), 137.0 (C), 136.5 (C), 125.8 (CH), 125.5 (CH), 122.7 (CH), 110.9 (CH), 56.2 ppm (OCH_3); IR (ATR): $\tilde{\nu}$ = 3078 (w), 2847 (w), 1702 (s), 1601 (m), 1479 (s), 1442 (m), 1402 (m), 1340 (w), 1312 (m), 1289 (s), 1253 (m), 1229 (s), 1211 (m), 1112 (w), 1060 (m), 1024 (m), 959 (m), 899 (m), 814 (m), 796 (m), 759 (m), 725 (m), 607 (w), 571 (m), 484 (w), 435 (vw), 407 (vw) cm^{-1}; MS (EI): *m/z* (%): 343.3 (25) $[M+1]^+$, 342.3 (100) $[M]^+$, 327.2 (35) $[M–CH_3]^+$; HRMS (FAB): *m/z* calcd for $C_{22}H_{14}O_4$: 342.0887 $[M^+]$; found: 342.0886.

3,10-Dimethoxy-5,8-bis(2,4,6-trimethylphenyl)indeno[2,1-*c*]fluorene (15)



Following a published protocol[13] BuLi (2.5M in hexane; 0.57 mL, 1.43 mmol) was added dropwise within 5 min under an argon atmosphere to a cooled (–78 °C) solution of mesityl bromide (0.24 mL, 312 mg, 1.57 mmol) in anhydrous THF (4 mL) and the mixture was stirred for 20 min. It was transferred via a cannula to a cooled (–78 °C) suspension of diketone **13** (100 mg, 292 µmol) in anhydrous THF (12 mL) and stirred for 15 h at rt. Saturated aqueous NH_4Cl solution (20 mL) was added and stirring was continued for 10 min. The mixture was extracted with Et_2O (3×25 mL) and the combined organic layers were dried ($MgSO_4$) and concentrated at reduced pressure. High vacuum was applied to the residue (**14**) for 1 h, the vessel was backfilled with argon and anhydrous toluene (20 ml) was added as solvent. $SnCl_2$ (209 mg, 1.10 mmol) and trifluoroacetic acid (0.05 ml) were added at positive argon pressure and the mixture was heated for 18 h to 50 °C. The mixture was allowed to cool to rt, filtered, concentrated at reduced pressure and purified by column chromatography (silica gel, hexane/CH_2Cl_2, 4:1→1:1) to furnish an oily product, which was digested with CH_2Cl_2 (2 mL) and precipitated with MeOH to yield **15** as a black powder (79 mg, 144 µmol, 49%). R_f = 0.38 (hexane/CH_2Cl_2 1:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.92 (d, ^3J = 8.3 Hz, 2 H, ArH), 6.95 (s, 4 H, $Ar_{Mes}H$), 6.61 (dd, ^3J = 8.3 Hz, ^4J = 2.5 Hz, 2 H, ArH), 6.24 (d, ^4J = 2.5 Hz, 2 H, ArH), 6.02 (s, 2 H, ArH), 3.76 (s, 6 H, OCH_3), 2.34 (s, 6 H, Ar-CH_3), 2.14 ppm (s, 12 H, Ar-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.0 (C), 148.3 (C), 142.7 (C), 137.8 (C), 137.5 (C), 137.3 (C), 137.0 (C), 130.0 (C), 129.3 (C), 128.3 (CH), 126.1 (CH), 121.2 (CH), 110.5 (CH), 108.5 (CH), 55.6 (OCH_3), 21.3 (Ar-CH_3), 20.5 ppm (Ar-CH_3) ; IR (ATR): $\tilde{\nu}$ = 2912 (w), 1595 (m), 1460 (m), 1428 (m), 1340 (w), 1287 (w), 1213 (m), 1125 (m), 1030 (m), 849 (m), 808 (m), 692 (w), 654 (w), 623 (w), 546 (w), 421 (vw) cm^{-1}; MS (FAB): *m/z* (%): 550.3 (20) $[M+2]^+$, 549.3 (61) $[M+1]^+$, 548.3 (100) $[M]^+$; HRMS (FAB): *m/z* calcd for $C_{40}H_{36}O_2$: 548.2710 $[M^+]$; found: 548.2712.

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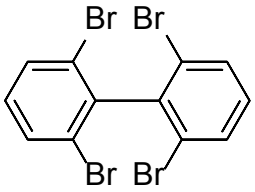
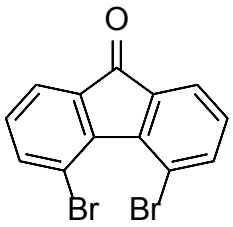
2,2',6,6'-Tetrabromo-1,1'-biphenyl (17)



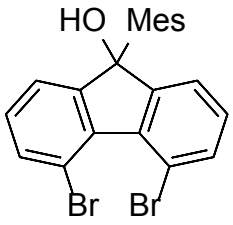
According to a published procedure[14] BuLi (2.5M in hexane; 16.6 mL, 41.4 mmol) was added dropwise within 20 min under an argon atmosphere to a cooled (–78 °C) solution of iPr_2NH (5.80 mL, 4.19 g, 41.4 mmol) in anhydrous THF (80 mL) and the mixture was stirred for 40 min. 1,3-Dibromobenzene (**16**, 5.00 mL, 9.76 g, 41.4 mmol) was added dropwise within 20 min at –78 °C and stirring was continued for 2 h. A solution of CuCN (1.85 g, 20.7 mmol) and LiCl (877 mg, 20.7 mmol) in anhydrous THF (45 mL), prepared under an argon atmosphere, was slowly added via a cannula and the mixture was stirred for 2 h at –78 °C. 1,4-Benzoquinone (6.71 g, 62.1 mmol) was added portionwise at positive argon pressure and the mixture was let come to rt over night. H_2O (30 mL) was added, the mixture was stirred for 10 min and extracted with Et_2O (3×200 mL). The combined organic layers were washed with H_2O (2×150 mL), dried ($MgSO_4$), concentrated at reduced pressure, and purified by column chromatography (silica gel, pentane) and recrystallization from MeCN (75 mL) to yield **17** as colourless, crystalline needles (4.10 g, 8.73 mmol, 42%). R_f = 0.34 (pentane); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67 (d, ^3J = 8.1 Hz, 4 H, ArH), 7.17 ppm (t, ^3J = 8.1 Hz, 2 H, ArH). The ^{1}H NMR data are in full agreement with published data.[15]

4,5-Dibromo-9*H*-fluoren-9-one (18)



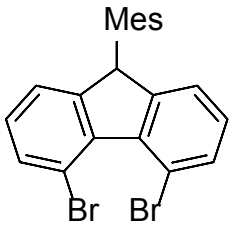
In slight variation of a published procedure[16] BuLi (2.5M in hexane; 5.60 mL, 14.0 mmol) was added dropwise within 30 min under an argon atmosphere to a cooled (–78 °C) solution of biphenyl **17** (3.00 g, 6.39 mmol) in anhydrous THF (75 mL) and the mixture was stirred for 40 min. $ClCO_2Et$ (1.50 mL, 1.83 g, 19.4 mmol) was added in one portion at –78 °C and stirring was continued for 2 h. The mixture was let come to rt, H_2O (50 mL) was added, and stirring was continued for 10 min. The mixture was extracted with CH_2Cl_2 (3×50 mL), dried ($MgSO_4$), concentrated at reduced pressure, and purified by column chromatography (silica gel, hexane/CH_2Cl_2, 2:1) to yield **18** as a yellow solid (1.67 g, 4.94 mmol, 77%). R_f = 0.27 (hexane/CH_2Cl 2:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.75 (dd, ^3J = 8.0 Hz, ^4J = 1.2 Hz, 2 H, ArH), 7.72 (dd, ^3J = 7.2, ^4J = 1.2 Hz, 2 H), 7.23 ppm (dd, ^3J = 8.0, ^3J = 7.2 Hz, 2 H). The ^{1}H NMR data are in full agreement with published data.[16]

4,5-Dibromo-9-(2,4,6-trimethylphenyl)-9*H*-fluoren-9-ol (19)



Following a published protocol[17] MesMgBr (1M in THF; 3.60 mL, 3.60 mmol) was added under an argon atmosphere within 5 min to a cooled (0 °C) solution of fluorenone **18** (800 mg, 2.37 mmol) in anhydrous THF (20 mL). The cooling bath was removed and stirring was continued for 15 h at rt. Saturated aqueous NH_4Cl solution (30 mL) was added and the mixture was stirred for 10 min and extracted with Et_2O (3×30 mL). The combined organic layers were dried ($MgSO_4$), concentrated at reduced pressure, and purified by column chromatography (silica gel, hexane/CH_2Cl_2, 2:1) and recrystallization from hexane (22 mL) to yield **19** as colourless crystalline needles (940 mg, 2.05 mmol, 86%). R_f = 0.15 (hexane/CH_2Cl 2:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.62 (dd, ^3J = 7.9 Hz, ^4J = 1.2 Hz, 2 H, ArH), 7.23 (dd, ^3J = 7.4 Hz, ^4J = 1.2 Hz, 2 H, ArH), 7.13 (t, ^3J = 7.6 Hz, 2 H, ArH), 6.97 (s, 1 H, ArH), 6.62 (s, 1 H, ArH), 2.90 (s, 3 H, CH_3), 2.24 (s, 3 H, CH_3), 2.08 (s, 1 H, OH), 1.25 ppm (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 154.7 (C), 139.0 (C), 138.7 (C), 136.8 (C), 136.2 (C), 136.1 (CH), 134.4 (C), 132.7 (CH), 131.1 (CH), 130.5 (CH), 123.0 (CH), 116.7 (C), 85.9 (C), 25.8 (CH_3), 21.6 (CH_3), 20.7 ppm (CH_3); IR (ATR): $\tilde{\nu}$ = 3555 (w), 2966 (w), 1718 (vw), 1609 (w), 1556 (w), 1479 (w), 1454 (w), 1417 (w), 1400 (m), 1379 (w), 1237 (w), 1210 (w), 1191 (w), 1168 (w), 1103 (m), 1049 (w), 1007 (m), 937 (w), 901 (w), 852 (m), 793 (m), 770 (m), 739 (m), 705 (w), 693 (m), 542 (vw), 440 (vw) cm^{-1}; MS (FAB): *m/z* (%): 458.0 (15) [*M*]$^+$, 457.0 (18), 443.0 (52) [*M*–OH]$^+$, 441.0 (100) [*M*–OH]$^+$, 439.0 (52) [*M*–OH]$^+$, 379.1 (15) [*M*–Br]$^+$, 377.1 (15) [*M*–Br]$^+$, 361.1 (27), 340.9 (14) [*M*–Mes]$^+$, 338.9 (30) [*M*–Mes]$^+$, 336.9 (15) [*M*–Mes]$^+$, 280.1 (21), 266.1 (16); HRMS (FAB): *m/z* calcd for $C_{22}H_{18}O^{79}Br^{81}Br$: 457.9698 [*M*]$^+$; found: 457.9701.

4,5-Dibromo-9-(2,4,6-trimethylphenyl)-9*H*-fluorene (20)



Following a published protocol[17] $BF_3{\cdot}OEt_2$ (500 µL, 575 mg, 4.05 mmol) was added within 5 min under an argon atmosphere to a cooled (0 °C) solution of fluorenol **19** (930 mg, 2.03 mmol) and Et_3SiH (0.65 mL, 473 mg, 4.06 mmol) in anhydrous CH_2Cl_2 (13 mL) and stirring was continued for 1 h at 0 °C. Saturated aqueous Na_2CO_3 solution (10 mL) and brine (20 mL) were added, stirring was continued for 10 min and the aqueous layer was extracted with CH_2Cl_2 (2×20 mL). The combined organic layers were dried ($MgSO_4$), concentrated at reduced pressure, and purified by column chromatography (silica gel, hexane) and recrystallization from MeCN (10 mL) to yield **20** as pale pink crystalline needles (504 mg, 1.14 mmol, 56%). R_f = 0.18 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67–7.65 (m, 2 H, ArH), 7.15–7.10 (m, 4 H, ArH), 7.01 (s, 1 H, ArH), 6.67 (s, 1 H, ArH), 5.51 (s, 1 H, Ar_3CH), 2.62 (s, 3 H, CH_3), 2.28 (s, 3 H, CH_3), 1.09 ppm (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 151.1 (C), 139.7 (C), 137.8 (C), 137.0 (C), 134.2 (CH), 133.3 (C), 130.9 (CH), 129.1 (CH), 129.0 (CH), 122.6 (CH), 116.4 (C), 50.6 (CH), 21.8 (CH_3), 21.0 (CH_3), 18.9 ppm (CH_3), 1 signal is covered; IR (ATR): $\tilde{\nu}$ = 2961 (w), 2914 (w) 1707 (vw), 1553 (w), 1479 (w), 1454 (w), 1399 (w), 1279 (w), 1161 (w), 1121 (vw), 1102 (m), 1014 (w), 934 (vw), 905 (w), 854 (w), 815 (w), 773 (w), 754 (m), 705 (w), 680 (w), 666 (w), 618 (w), 560 (w), 544 (w), 507 (w), 472 (vw), 444 (w) cm^{-1}; MS (FAB):

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[14] Q. Perron, A. Alexakis, *Adv. Synth. Catal.* **2010**, *352*, 2611–2620.

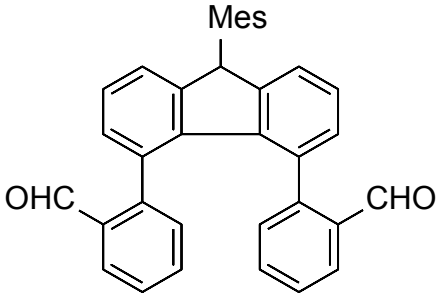
[15] J. Graff, E. Łastawiecka, L. Guénée, F. Leroux, A. Alexakis, *Adv.Synth. Catal*. **2015**, *357*, 2833–2839.

[16] H. Oyama, M. Akiyama, K. Nakano, M. Naito, K. Nobusawa, K. Nozaki, *Org. Lett.* **2016**, *18*, 3654–3657.

[17] G. C. Vougioukalakis, M. M. Roubelakis, M. Orfanopoulos, *J. Org. Chem.* **2010**, *75*, 4124–4130.

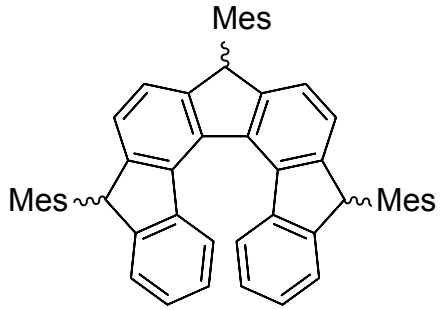
m/z (%): 444.0 (6) [*M*]$^+$, 442.0 (10) [*M*]$^+$, 440.1 (6) [*M*]$^+$, 363.1 (10) [*M*–Br]$^+$, 361.1 (10) [*M*–Br]$^+$, 324.9 (4) [*M*–Mes]$^+$, 322.9 (8) [*M*–Mes]$^+$, 320.9 (4) [*M*–Mes]$^+$; HRMS (FAB): *m/z* calcd for $C_{22}H_{18}{}^{79}Br^{81}Br$: 441.9749 [*M*]$^+$; found: 441.9749.

2,2'-[9-(2,4,6-trimethylphenyl)-9*H*-fluorene-4,5-diyl]dibenzaldehyde (22)



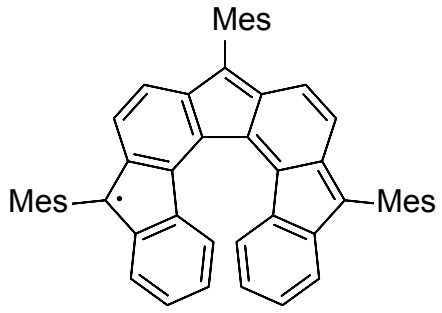
$PdCl_2(PPh_3)_2$ (18 mg, 26 µmol) was added with positive argon pressure to a degassed (ultrasonication) solution of fluorene **20** (200 mg, 452 µmol), 2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzaldehyde[1b] (**21**, 262 mg, 1.13 mmol), and Na_2CO_3 (220 mg, 2.06 mmol) in THF/H_2O (5:4, 9 mL), placed in a Schlenk tube. The flask was closed and the mixture was heated to 80 °C for 15 h. The mixture was cooled to rt, half-concentrated brine (5 mL) was added, and the mixture was extracted with EtOAc (3×15 mL). The combined organic layers were dried (Na_2SO_4), concentrated at reduced pressure, and purified by column chromatography (silica gel, hexane/EtOAc, 10:1) to yield **22** as a colourless solid (115 mg, 233 µmol, 52%). The product was obtained as a mixture of atropisomers. R_f = 0.38 (hexane/EtOAc 4:1); IR (ATR): $\tilde{\nu}$ = 2842 (vw), 2749 (vw), 1689 (m), 1594 (w), 1447 (w), 1392 (w), 1247 (w), 1194 (w), 1159 (vw), 854 (vw), 829 (w), 757 (m), 715 (w), 644 (w), 578 (vw), 449 (vw) cm^{-1}; MS (FAB): *m/z* (%): 493.3 (16) [*M*+1]$^+$, 492.3 (15) [*M*]$^+$, 475.3 (28), 474.3 (23); HRMS (FAB): *m/z* calcd for $C_{36}H_{28}O_2$: 492.2084 [*M*$^+$]; found: 492.2085.

4,8,11-Tris(2,4,6-trimethylphenyl)-8,11-dihydro-4*H*-cyclopenta[1,2-*c*:4,3-*c*']difluorene (24)



Following a published protocol[18] MesMgBr (1M in THF; 1.15 mL, 1.15 mmol) was added dropwise within 5 min under argon atmosphere to a cooled (0 °C) solution of fluorene **22** (115 mg, 233 µmol) in anhydrous THF (6 mL). The cooling bath was removed and the mixture was stirred for 15 at rt. Saturated aqueous NH_4Cl solution (20 mL) was added, stirring was continued for 10 min, and the mixture was extracted with CH_2Cl_2 (3×25 mL). The combined organic layers were dried ($MgSO_4$) and concentrated at reduced pressure. The residue (**23**) was dissolved in anhydrous CH_2Cl_2 (25 mL), cooled to 0 °C, and $BF_3{\cdot}OEt_2$ (0.15 mL, 173 mg, 1.22 mmol) was added within 5 min. Stirring was continued for 1 h at rt and saturated aqueous NH_4Cl solution (25 mL) was added. The mixture was stirred for 10 min and extracted with CH_2Cl_2 (2×20 mL). The organic layers were dried ($MgSO_4$), concentrated at reduced pressure, and purified by column chromatography (silica gel, hexane/CH_2Cl_2, 4:1) furnishing an oil, which was digested in CH_2Cl_2 (2 mL) and precipitated with MeOH to yield **24** as a white powder (117 mg, 167 µmol, 63%). The product was obtained as a mixture of isomers; reasonable NMR spectra could thus not be measured. R_f = 0.17 (hexane/CH_2Cl_2 4:1); IR (ATR): $\tilde{\nu}$ = 2914 (vw), 1611 (vw), 1447 (w), 1401 (vw), 1377 (vw), 1342 (vw), 1016 (vw), 849 (w), 814 (vw), 774 (w), 732 (m), 709 (w), 661 (vw), 632 (vw), 551 (vw), 439 (vw) cm^{-1}; MS (FAB): *m/z* (%): 698.4 (32) [*M*+2]$^+$, 697.4 (85) [*M*+1]$^+$, 696.4 (100) [*M*]$^+$, 695.4 (34) [*M*–1]$^+$, 578.3 (34), 577.3 (75) [*M*–Mes]$^+$, 576.3 (30), 458.2 (15) [*M*–2 Mes]$^+$; HRMS (FAB): *m/z* calcd for $C_{54}H_{48}$: 696.3751 [*M*]$^+$; found: 696.3752.

5,8,11-Tris(2,4,6-trimethylphenyl)cyclopenta[1,2-*c*:4,3-*c*']difluoren-5-yl (7)



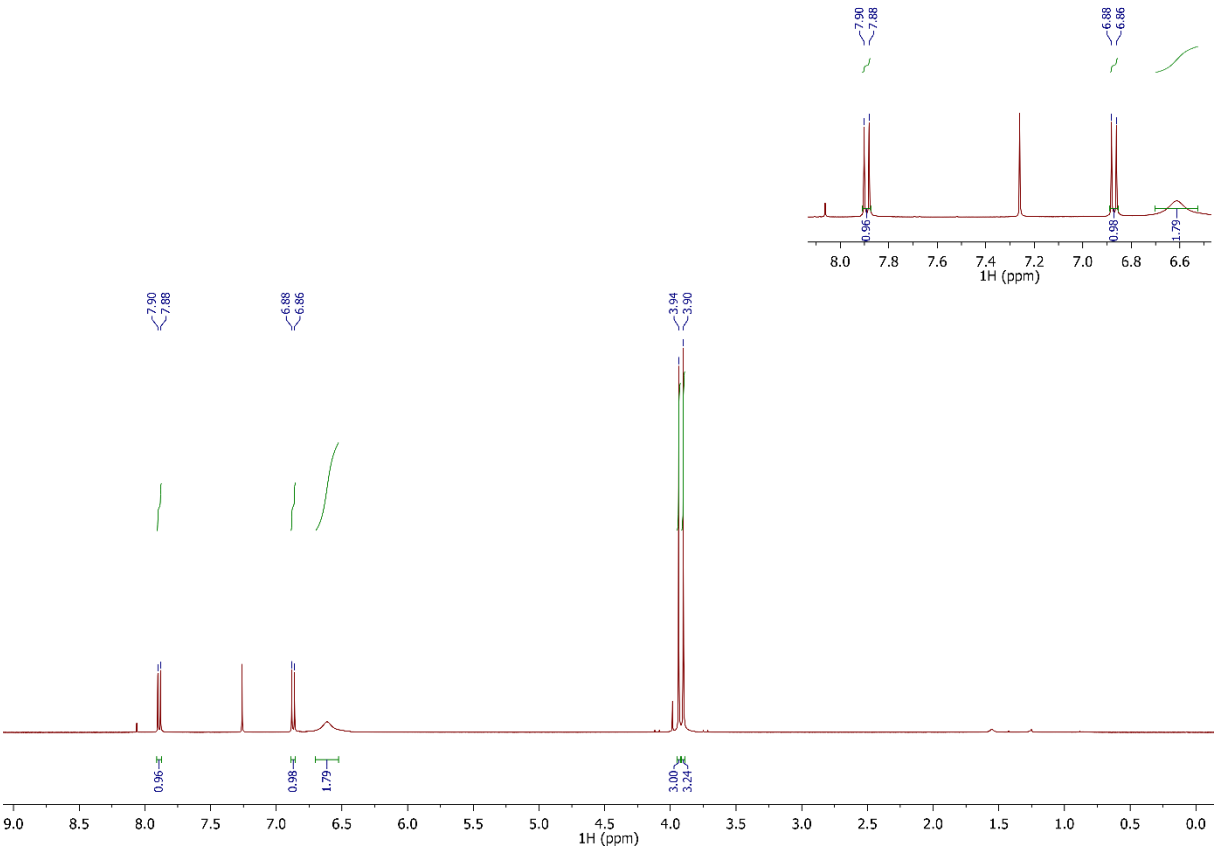
Following a published protocol[19] heptacycle **24** (100 mg, 144 µmol) and *t*BuOK (229 mg, 2.04 mmol), placed in a Schlenk tube, were dissolved under an argon atmosphere in anhydrous THF (7 mL) and the mixture was heated to 60 °C for 16 h. The mixture was cooled to rt, chloranil (160 mg, 649 µg) was added, and after a short stirring (4 min) the mixture was concentrated at reduced pressure. The residue was purified by column chromatography (silica gel, hexane/CH_2Cl_2, 4:1) to furnish **7** as a black solid (84 mg, 121 µmol, 84%). It was digested in degassed $CHCl_3$ (2 mL) and covered with degassed MeOH (3 mL). Slow, undisturbed diffusion yielded black, rod-shaped crystals, suitable for X-ray crystallography. R_f = 0.35 (hexane/CH_2Cl_2 4:1); m.p. 241 °C ($CHCl_3$/EtOH); IR (ATR): $\tilde{\nu}$ = 2962 (w), 2914 (w), 1737 (vw), 1610 (w), 1561 (vw), 1459 (w), 1442 (w), 1376 (w), 1347 (w), 1260 (w), 1189 (w), 1140 (w), 1090 (w), 1014 (w), 941 (w), 911 (vw), 847 (w), 807 (m), 793 (m), 745 (m), 692 (m), 576 (vw), 549 (w), 438 (vw) cm^{-1}; UV/Vis (CH_2Cl_2): λ_{max} (ε) = 262 (54,000), 315 (33,000), 348 (22,000), 449 (27,000), 769 (6,000), 855 nm (12,000 mol$^{-1}{\cdot}$dm$^3{\cdot}$cm^{-1}); MS (FAB): *m/z* (%): 694.4 (20) [*M*+1]$^+$, 693.4 (19) [*M*]$^+$; HRMS (FAB): *m/z* calcd for $C_{54}H_{45}$: 693.3516 [*M*]$^+$; found: 693.3518.

[18] H. Sharma, P. K. Sharma, S. Das, *Chem. Commun.*, **2020**, *56*, 11319–11322.

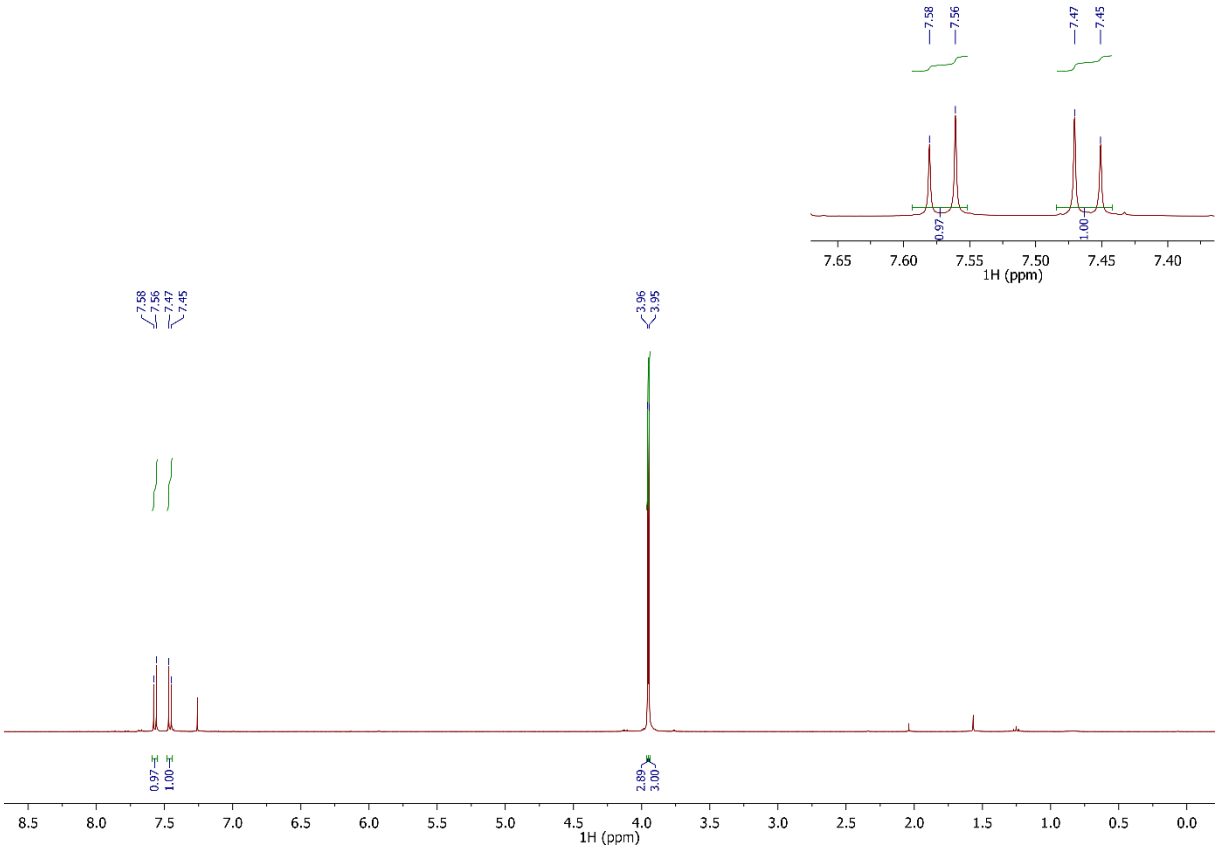
[19] X. Yang, D. Zhang, Y. Liao, D. Zhao, *J. Org. Chem.* **2020**, *85*, 5761–5770.

4. NMR Spectra of New Compounds, Mass and IR Spectra of 7

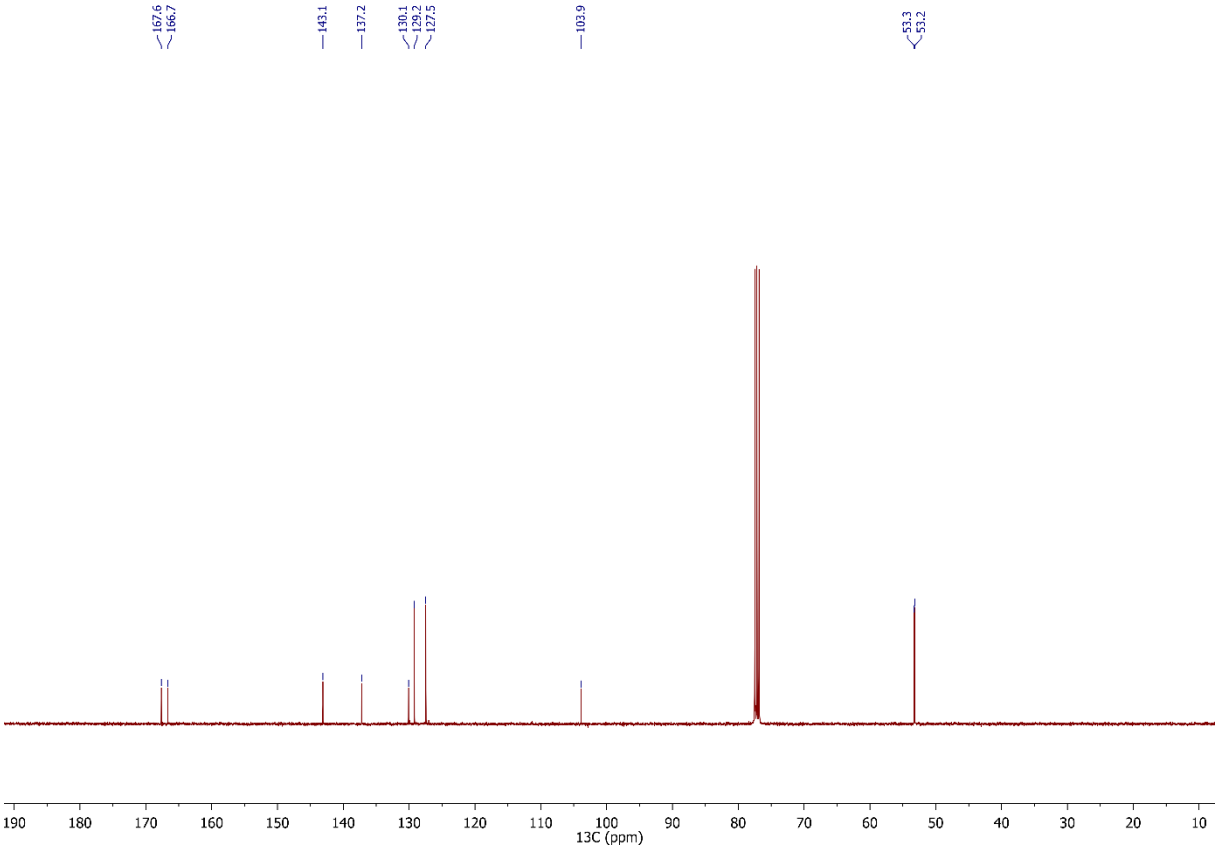
^{1}H NMR Spectrum of Dimethyl 2-Amino-3-bromoterephthalate (400 MHz, $CDCl_3$) (9)



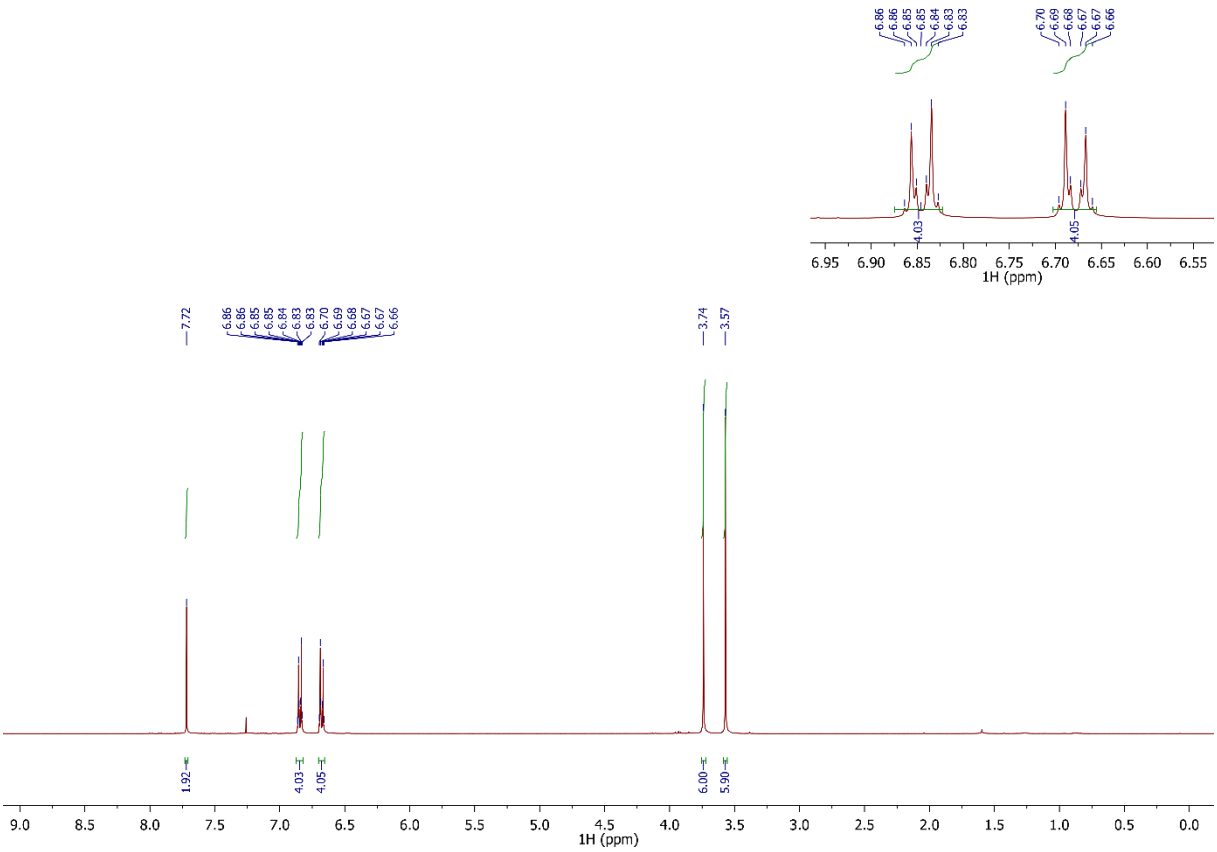
^{1}H NMR Spectrum of Dimethyl 2-Bromo-3-iodoterephthalate (400 MHz, $CDCl_3$) (10)



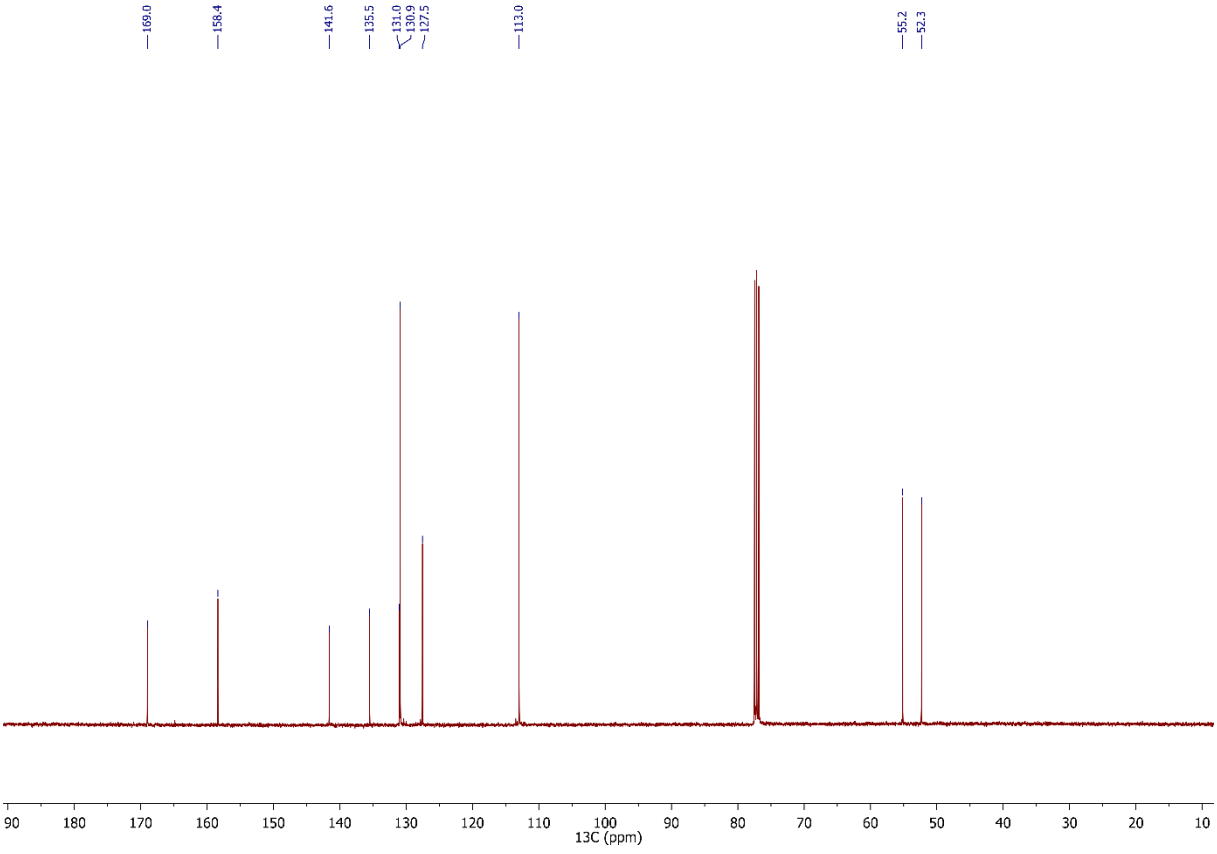
^{13}C NMR Spectrum of Dimethyl 2-Bromo-3-iodoterephthalate (100 MHz, $CDCl_3$) (10)



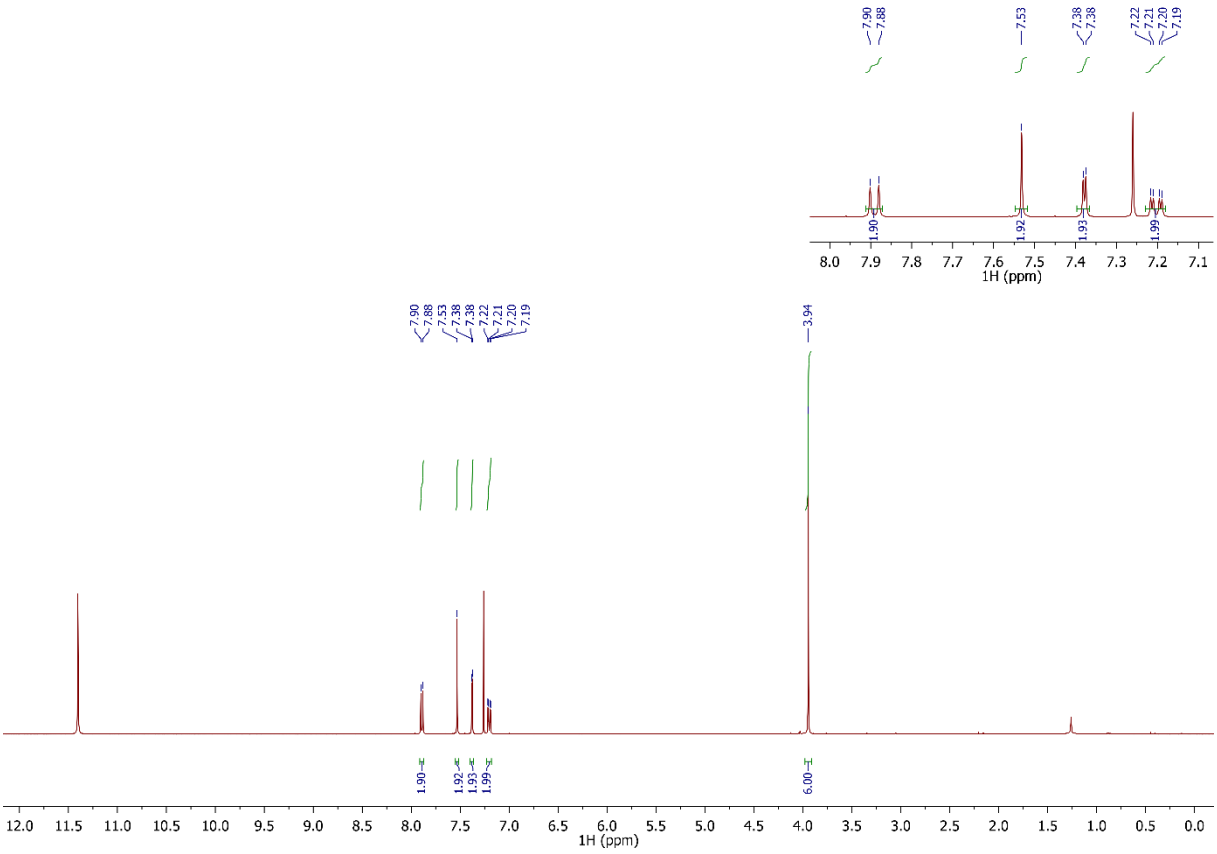
^{1}H NMR Spectrum of Dimethyl 4,4''-Dimethoxy-[1,1':2',1''-terphenyl]-3',6'-dicarboxylate (400 MHz, $CDCl_3$) (12)



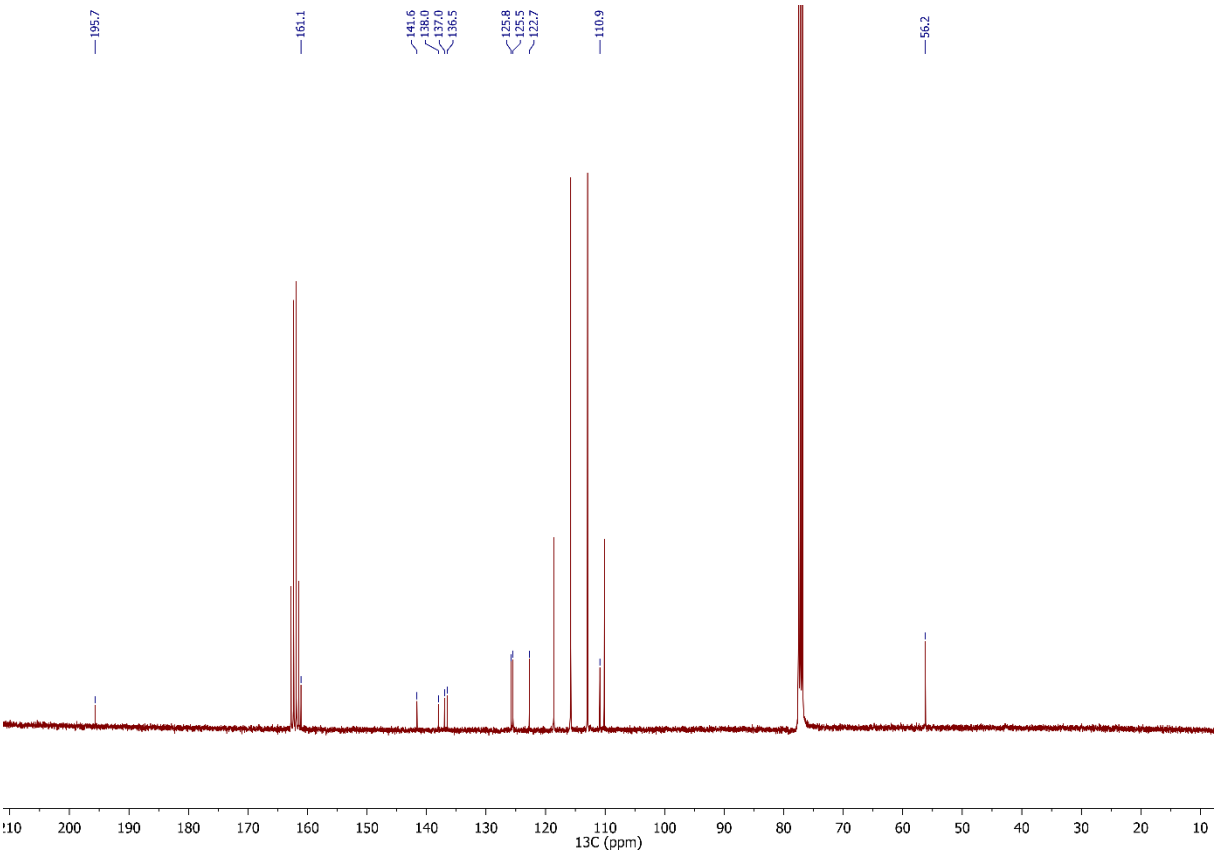
^{13}C NMR Spectrum of Dimethyl 4,4''-Dimethoxy-[1,1':2',1''-terphenyl]-3',6'-dicarboxylate (100 MHz, $CDCl_3$) (12)



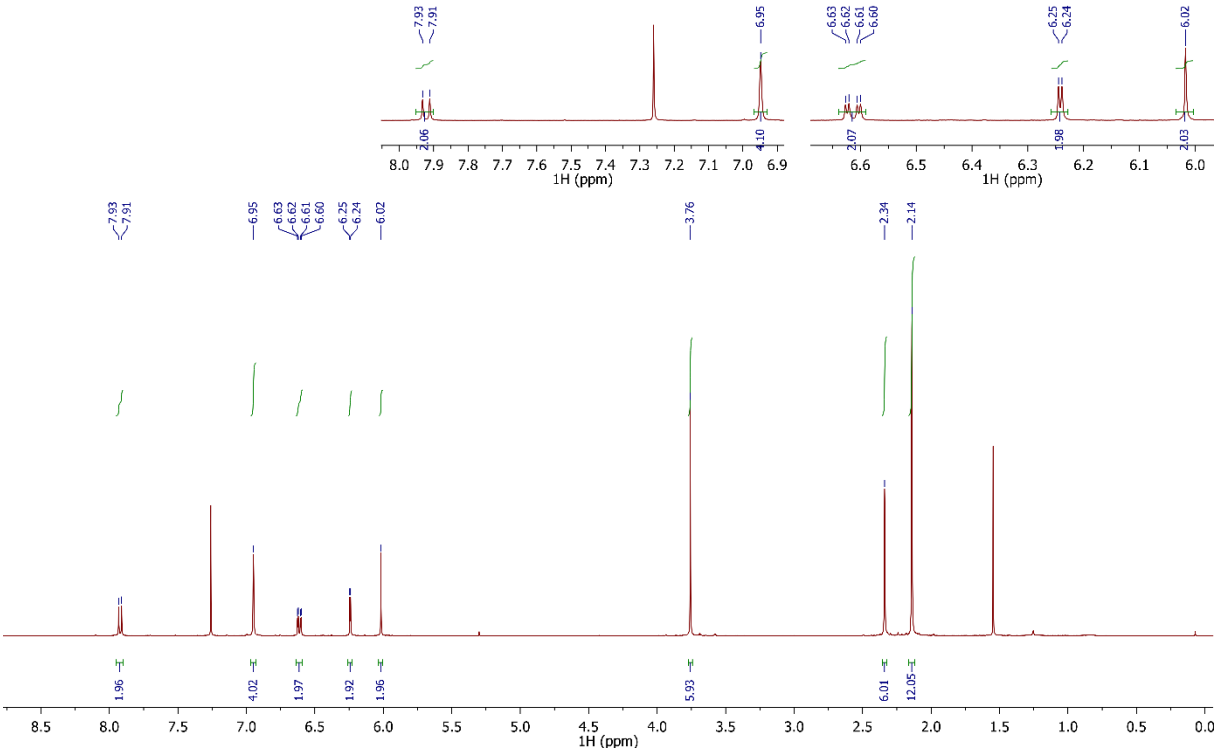
^{1}H NMR Spectrum of 3,10-Dimethoxyindeno[2,1-*c*]fluorene-5,8-dione (400 MHz, $CDCl_3$ + 10% TFA) (13)



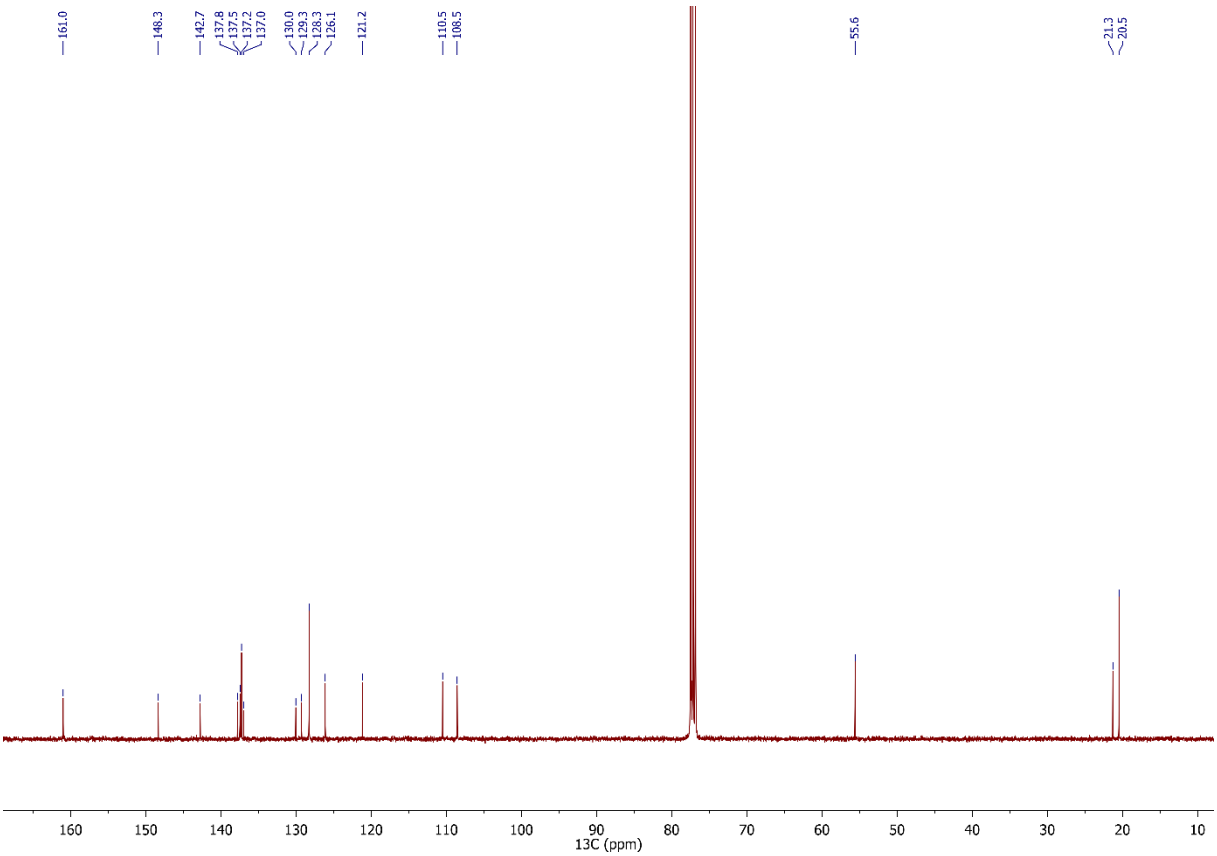
^{13}C NMR Spectrum of 3,10-Dimethoxyindeno[2,1-*c*]fluorene-5,8-dione (100 MHz, $CDCl_3$ + 10% TFA) (13)



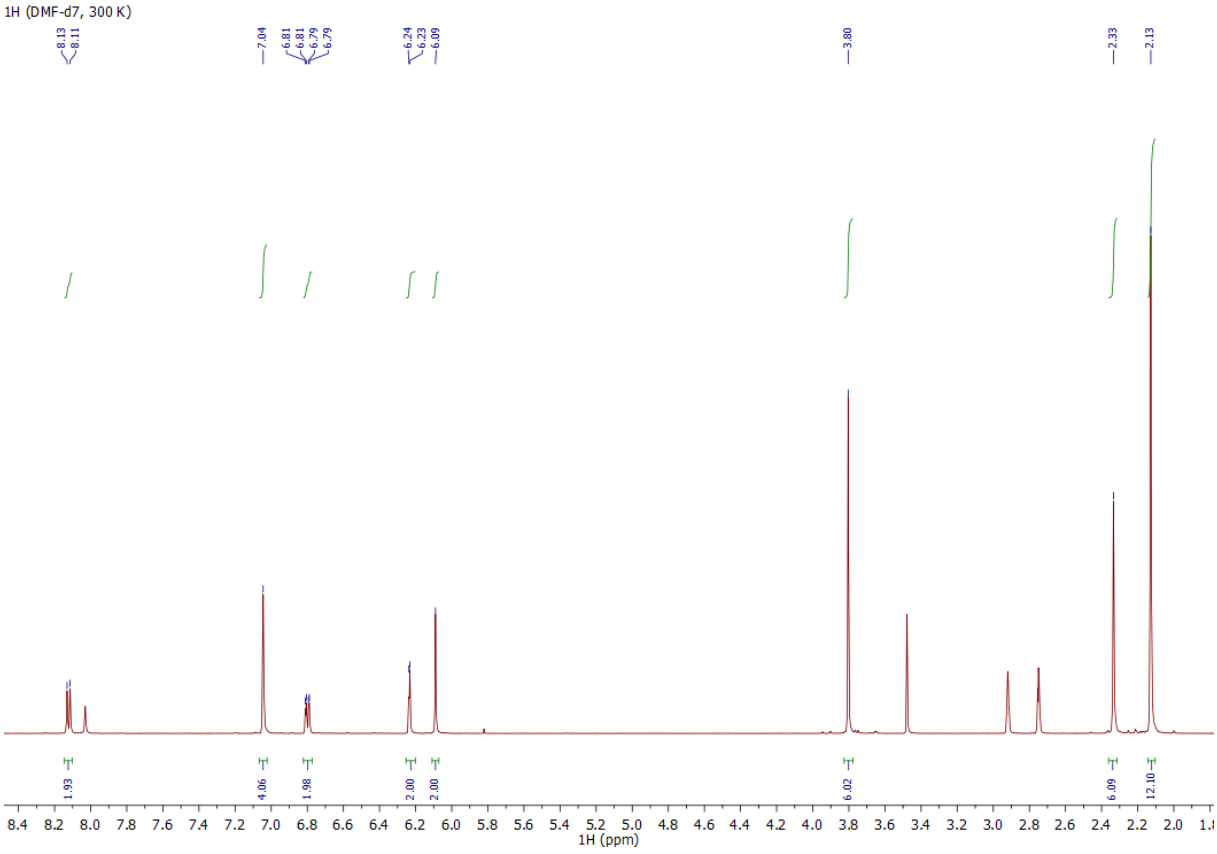
^{1}H NMR Spectrum of 3,10-Dimethoxy-5,8-bis(2,4,6-trimethylphenyl)indeno[2,1-*c*]fluorene (400 MHz, $CDCl_3$) (15)

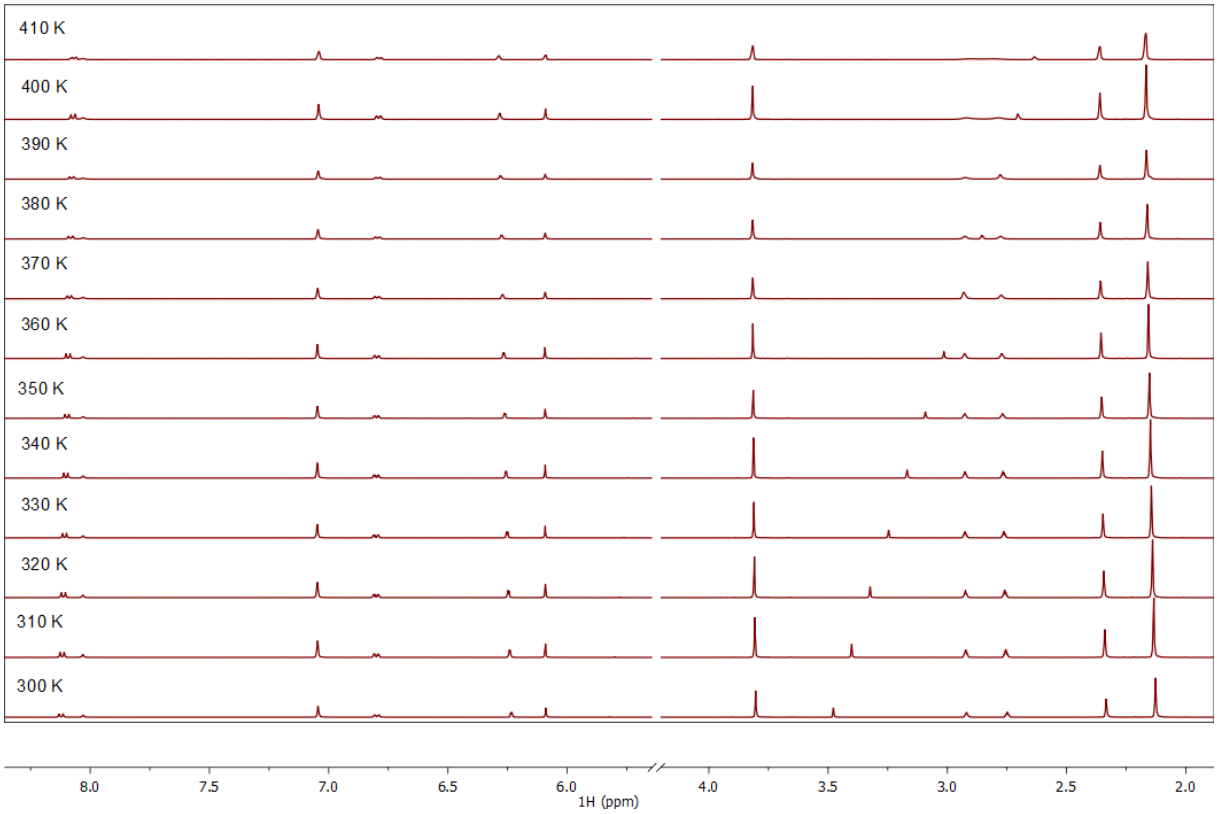


^{13}C NMR Spectrum of 3,10-Dimethoxy-5,8-bis(2,4,6-trimethylphenyl)indeno[2,1-*c*]fluorene (100 MHz, $CDCl_3$) (15)

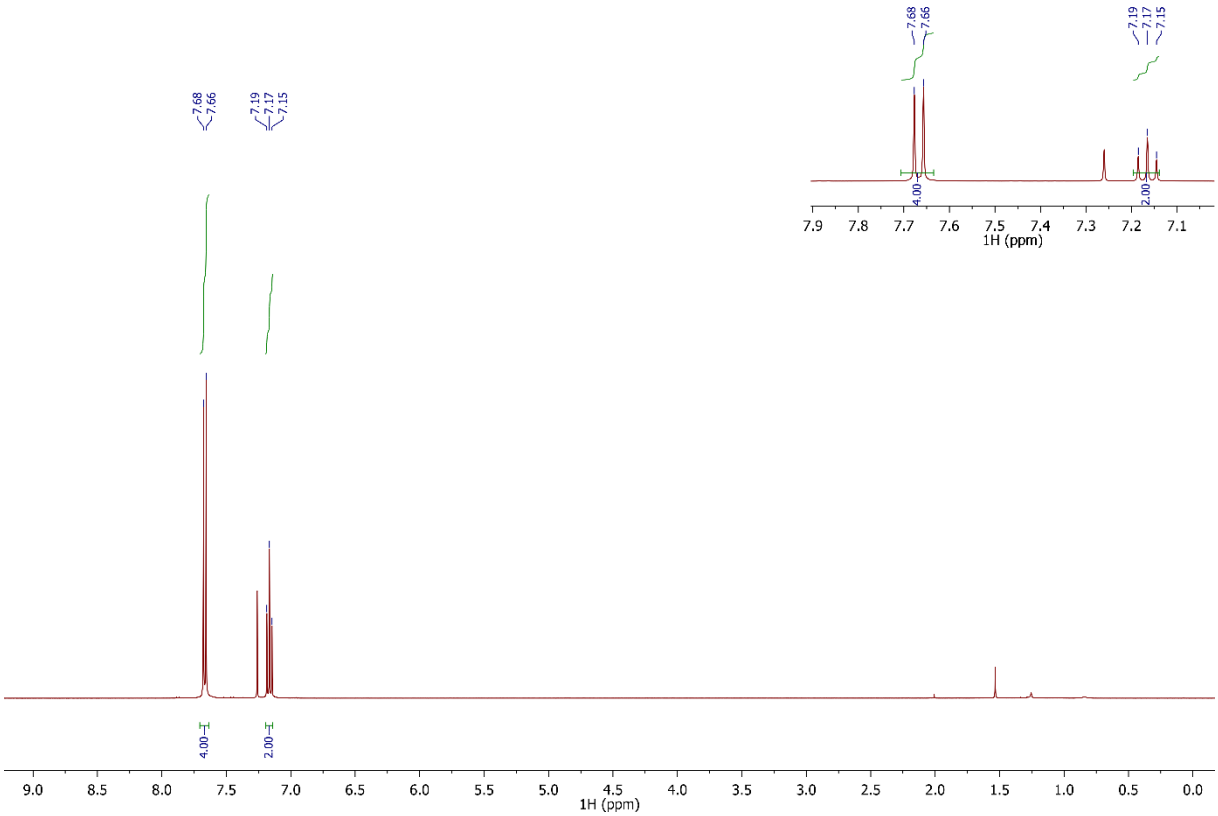


^{1}H NMR Spectra of 3,10-Dimethoxy-5,8-bis(2,4,6-trimethylphenyl)indeno[2,1-*c*]fluorene (500 MHz, DMF-d_7) (15) at Elevated Temperatures

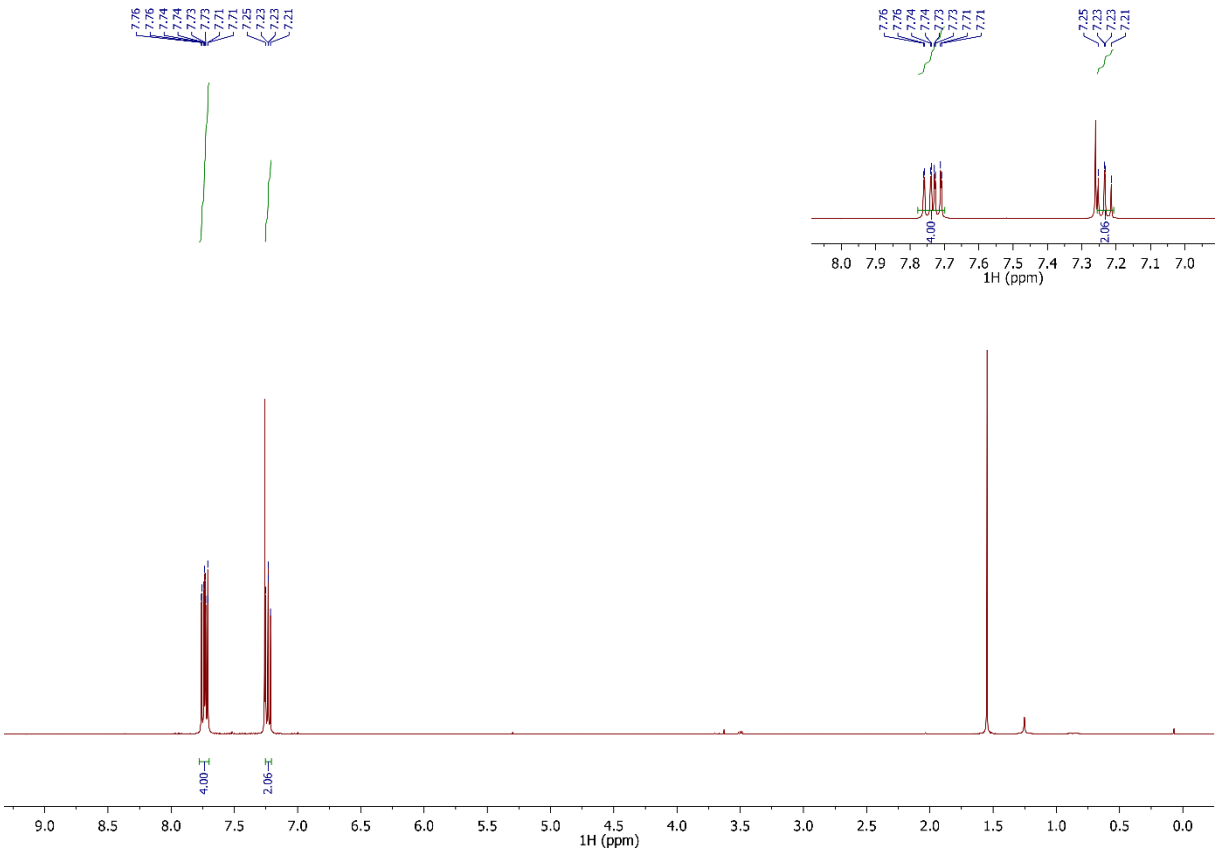



410 K
400 K
390 K
380 K
370 K
360 K
350 K
340 K
330 K
320 K
310 K
300 K
8.0
7.5
7.0
6.5
6.0
4.0
3.5
3.0
2.5
2.0
1H (ppm)

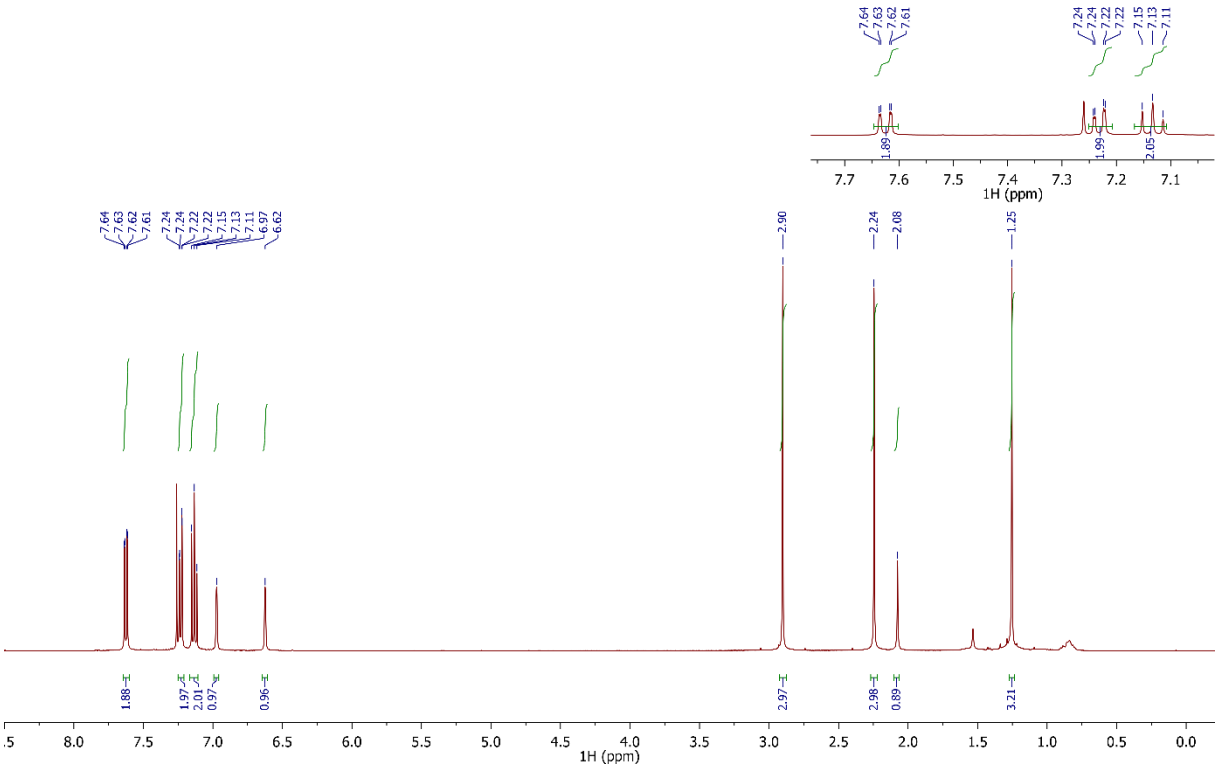
^{1}H NMR Spectrum of 2,2',6,6'-Tetrabromo-1,1'-biphenyl (400 MHz, $CDCl_3$) (17)



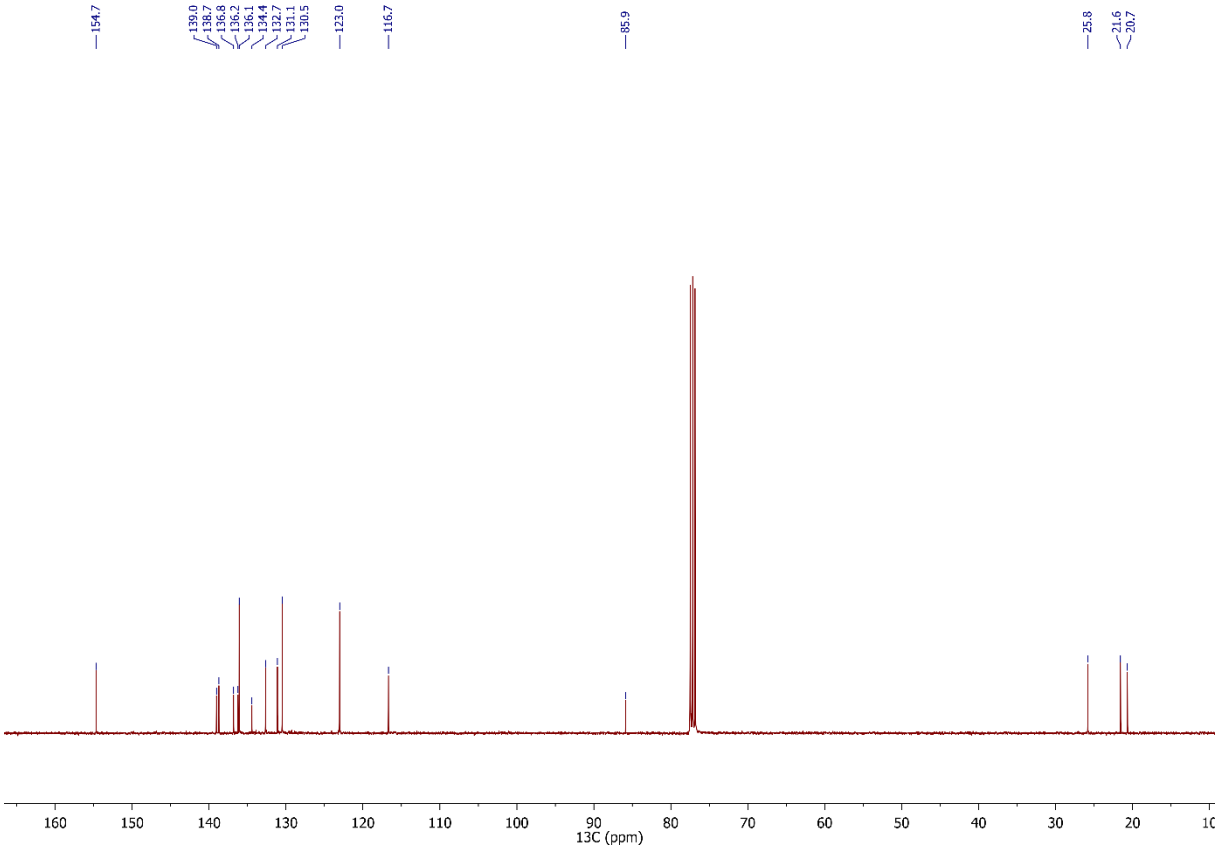
^{1}H NMR Spectrum of 4,5-Dibromo-9*H*-fluoren-9-one (400 MHz, $CDCl_3$) (18)



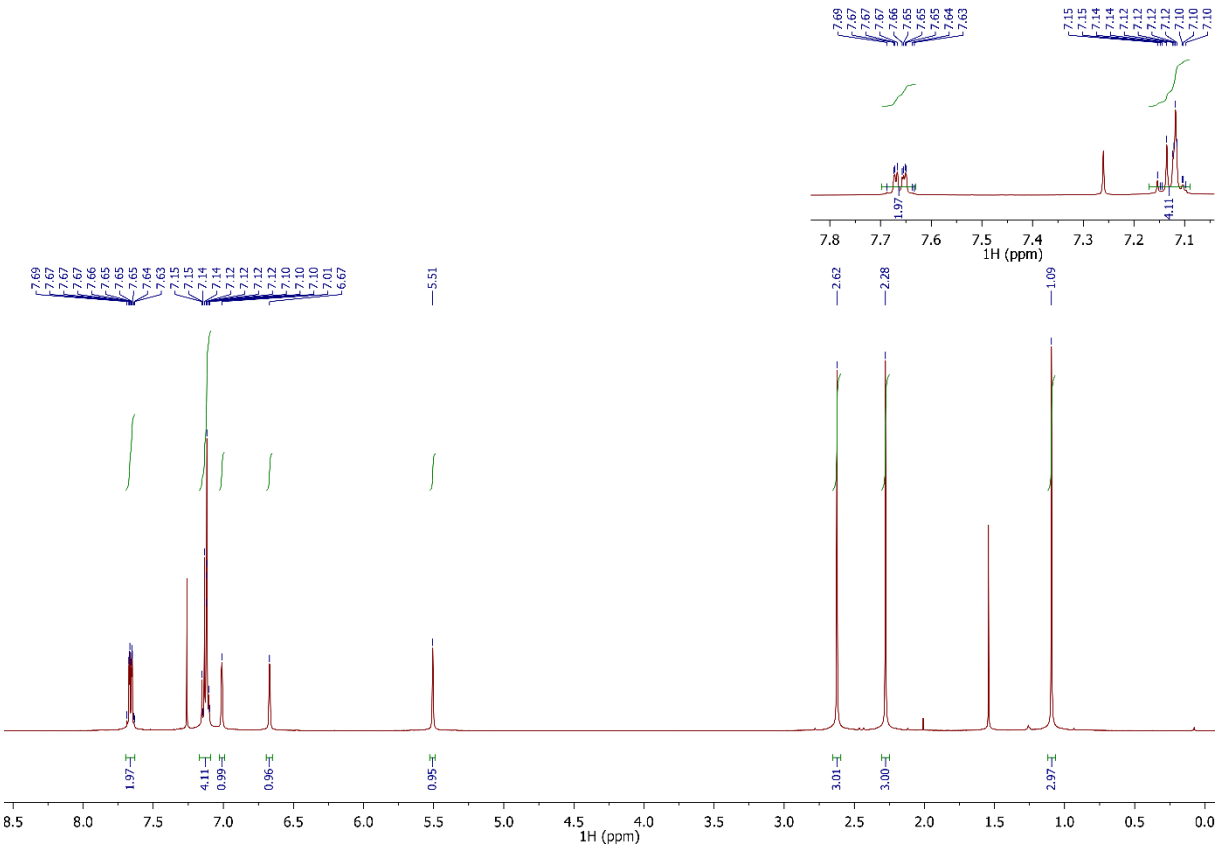
^{1}H NMR Spectrum of 4,5-Dibromo-9-(2,4,6-trimethylphenyl)-9*H*-fluoren-9-ol (400 MHz, $CDCl_3$) (19)



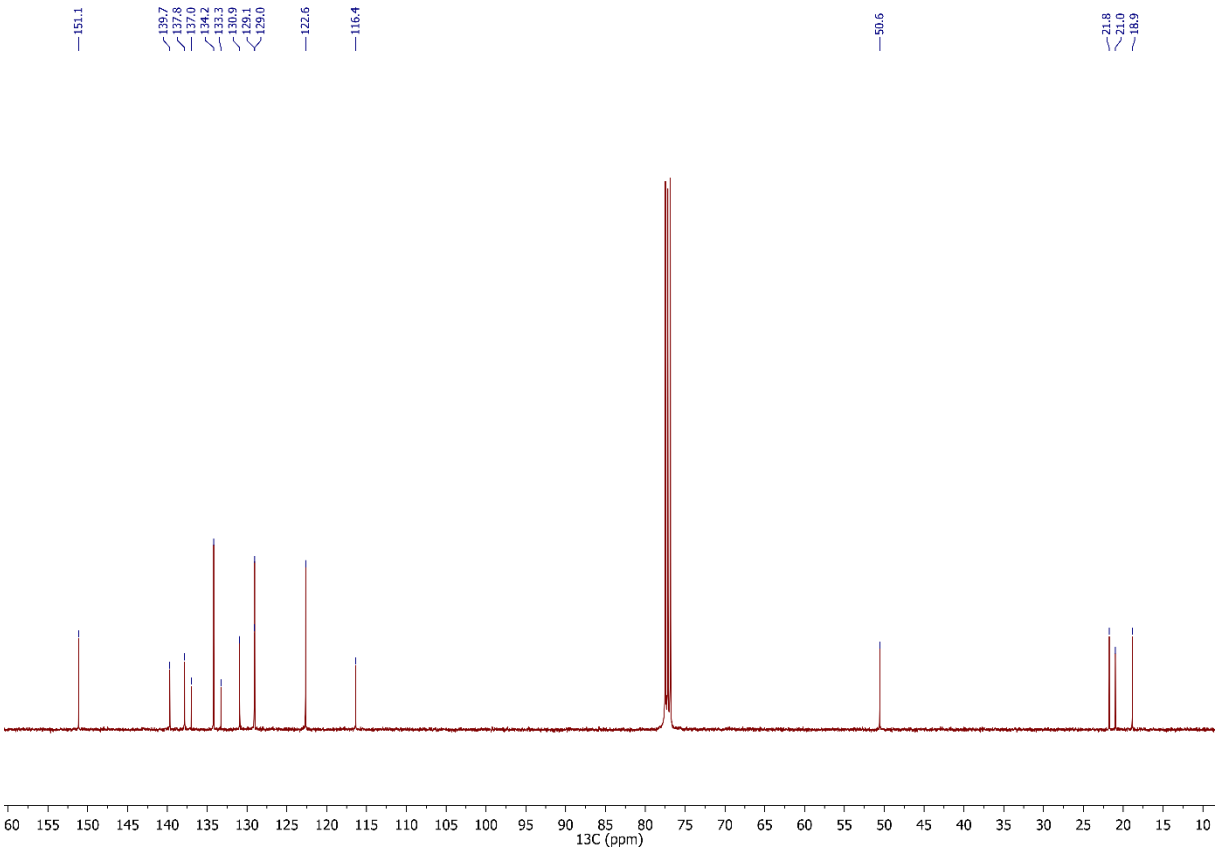
^{13}C NMR Spectrum of 4,5-Dibromo-9-(2,4,6-trimethylphenyl)-9*H*-fluoren-9-ol (100 MHz, $CDCl_3$) (19)



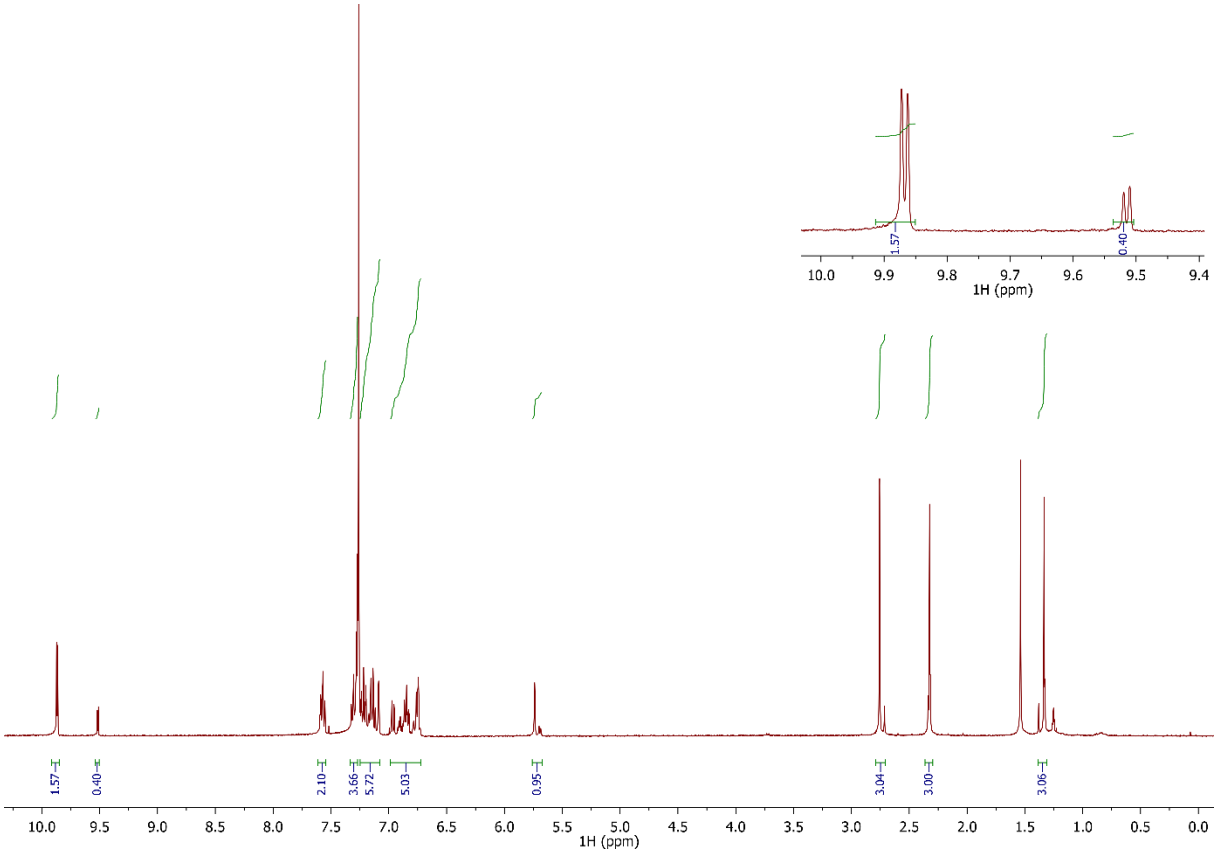
^{1}H NMR Spectrum of 4,5-Dibromo-9-(2,4,6-trimethylphenyl)-9*H*-fluorene (400 MHz, $CDCl_3$) (20)



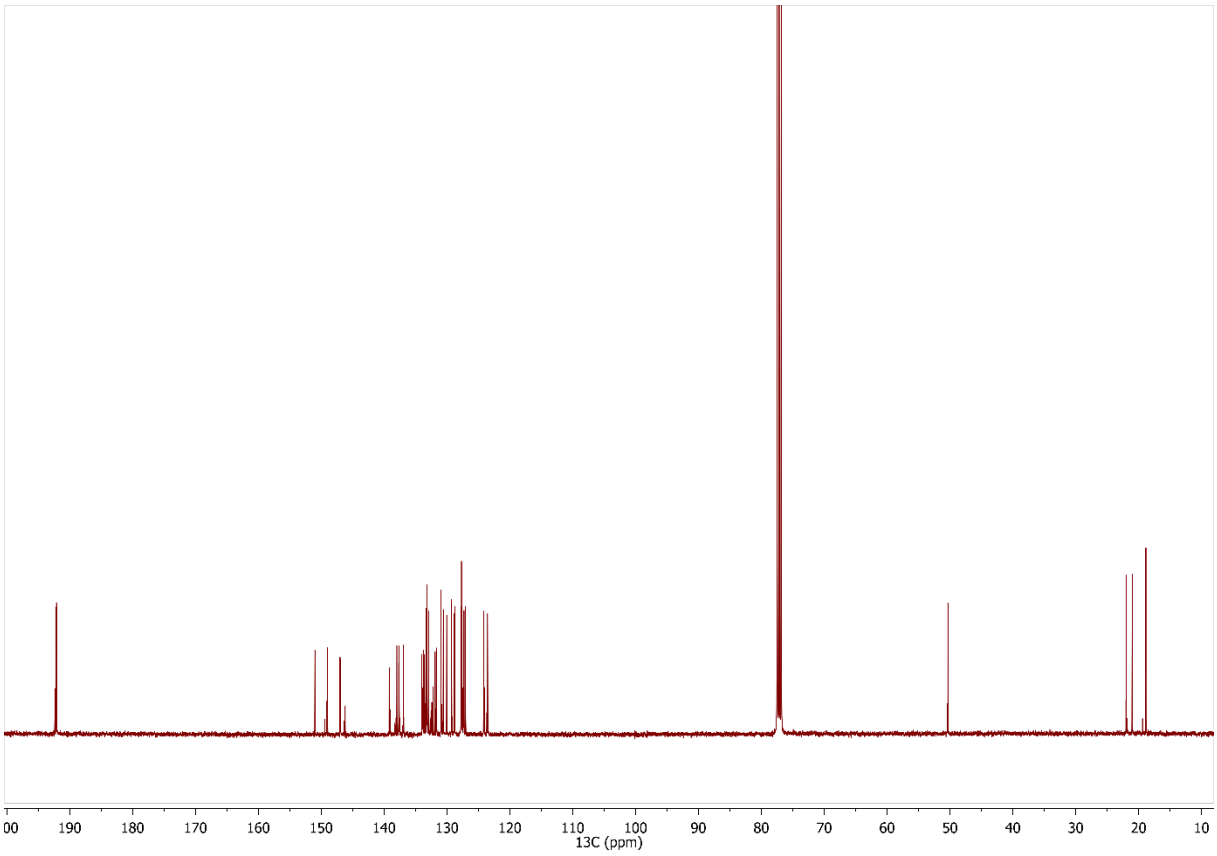
^{13}C NMR Spectrum of 4,5-Dibromo-9-(2,4,6-trimethylphenyl)-9*H*-fluorene (100 MHz, $CDCl_3$) (20)



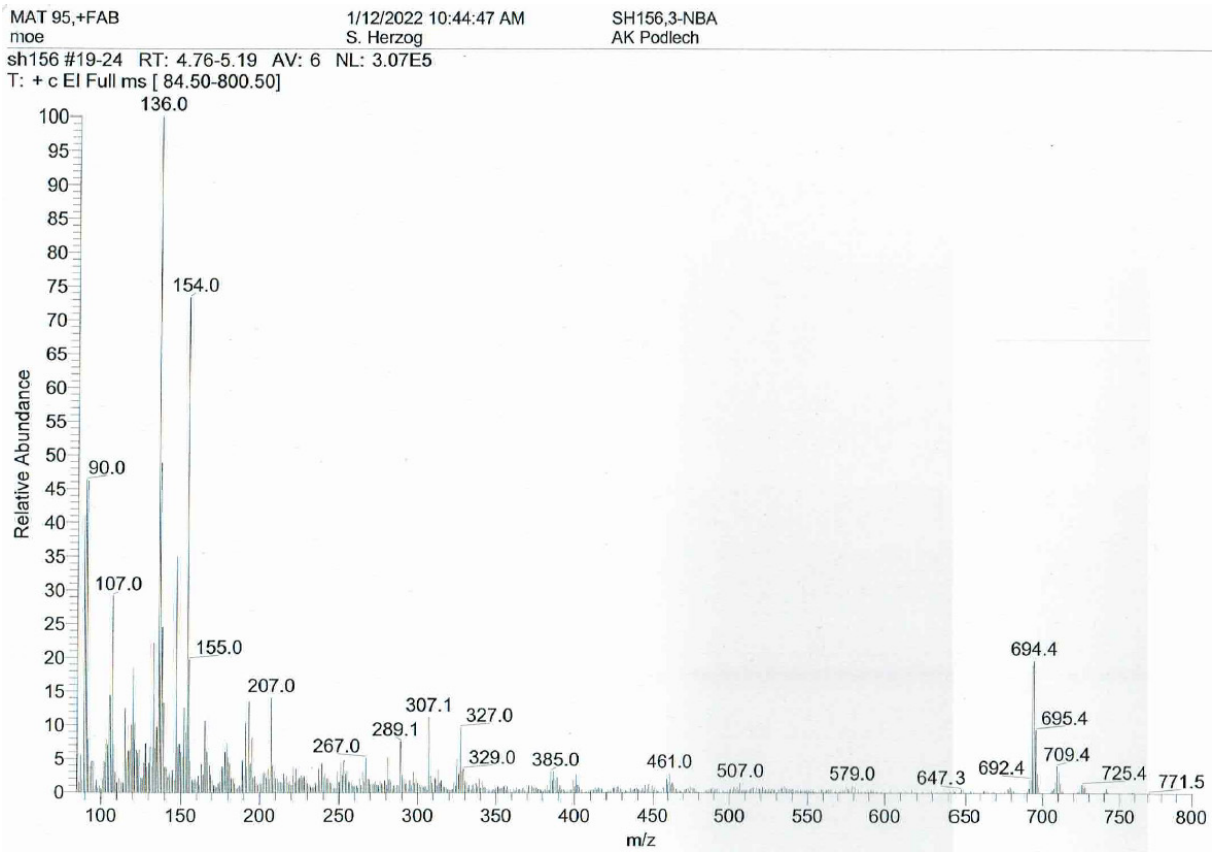
^{1}H NMR Spectrum of 2,2'-[9-(2,4,6-trimethylphenyl)-9*H*-fluorene-4,5-diyl]dibenzaldehyde (22)

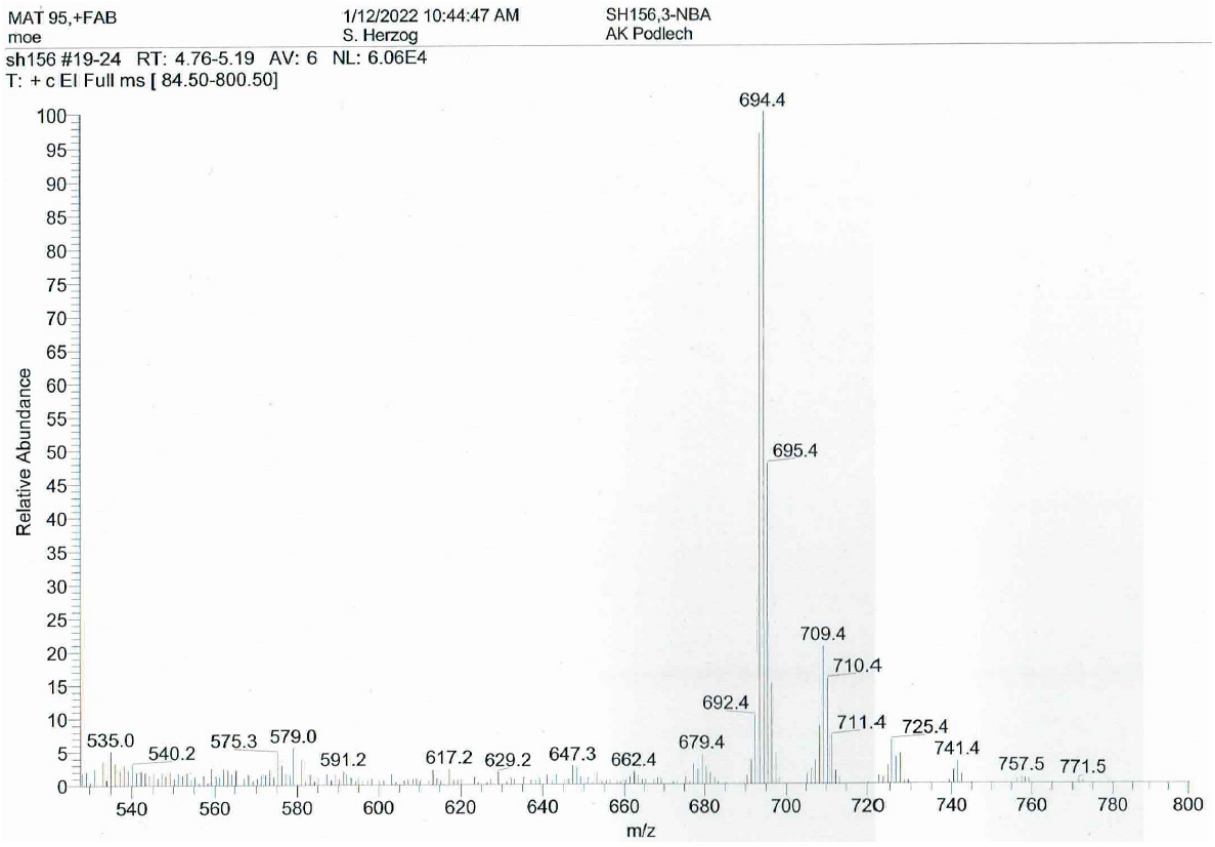


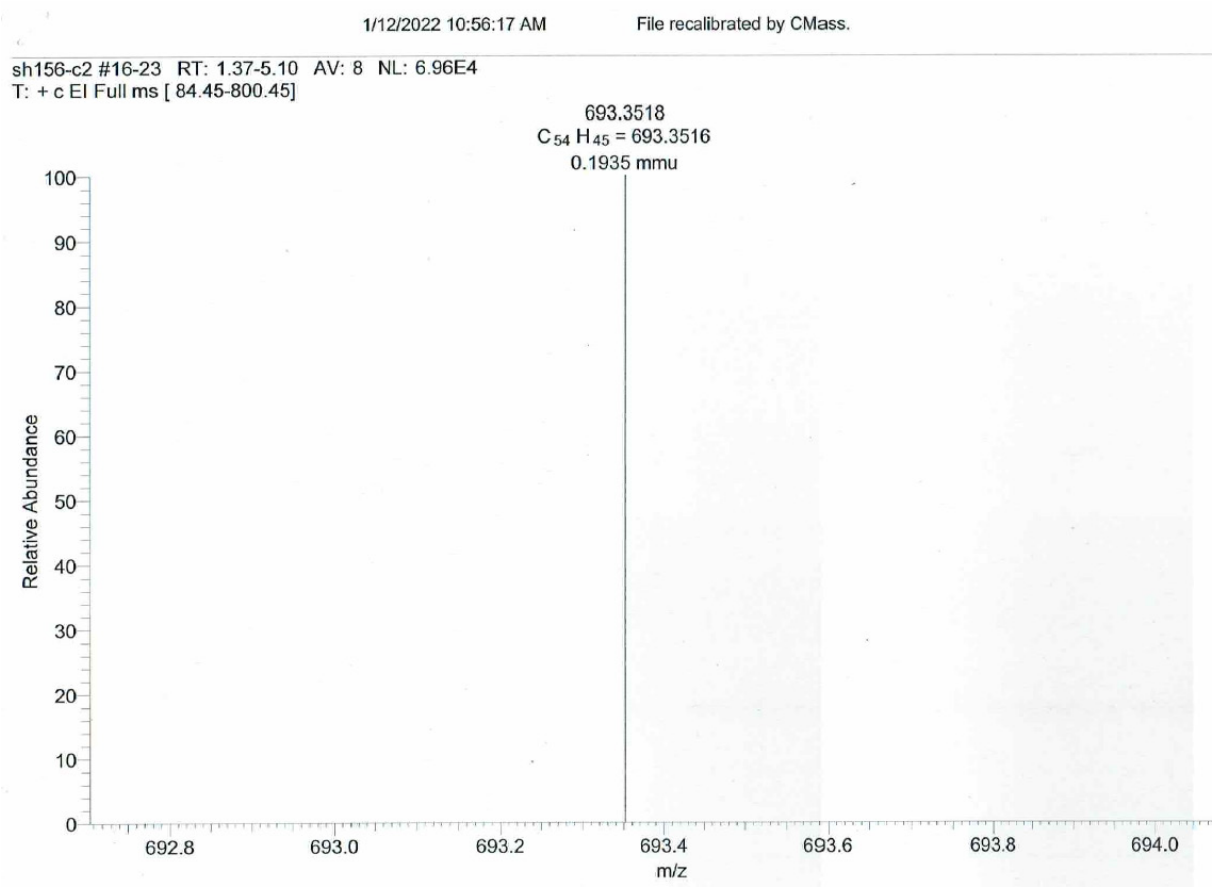
^{13}C NMR Spectrum of 2,2'-[9-(2,4,6-trimethylphenyl)-9*H*-fluorene-4,5-diyl]dibenzaldehyde (22)



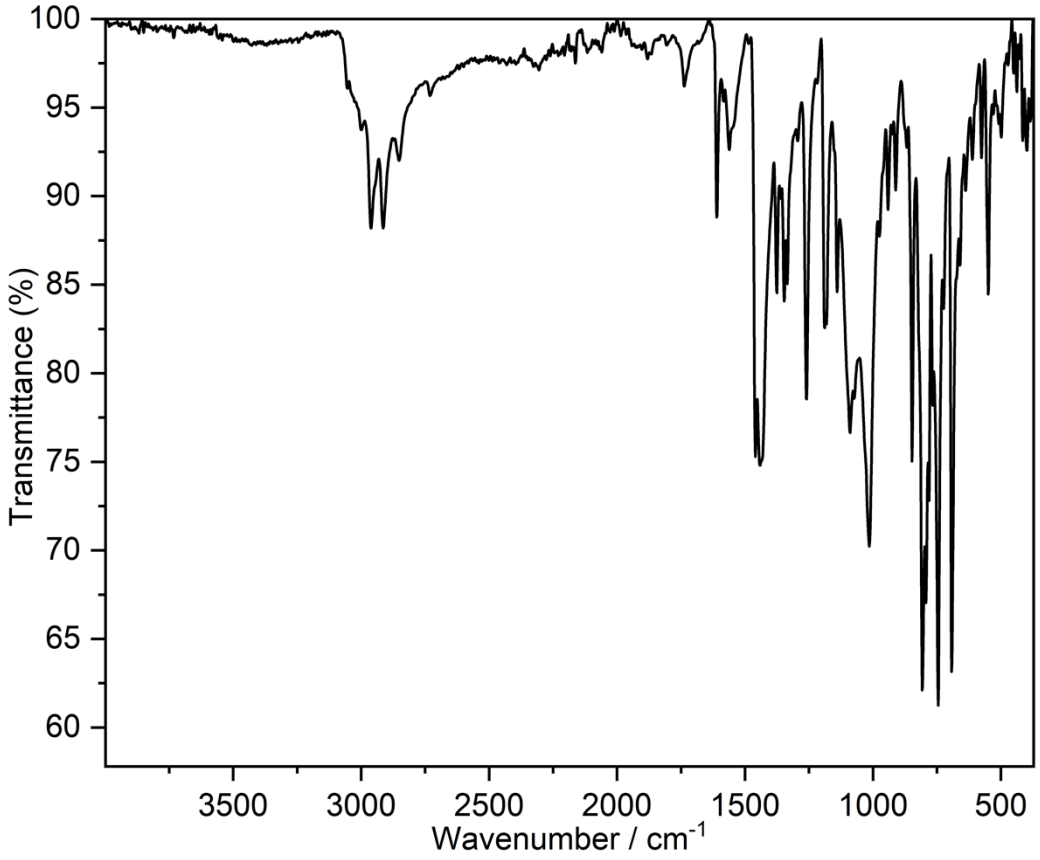
Mass Spectrum of 5,8,11-Tris(2,4,6-trimethylphenyl)cyclopenta[1,2-*c*:4,3-*c*']difluoren-5-yl (7)





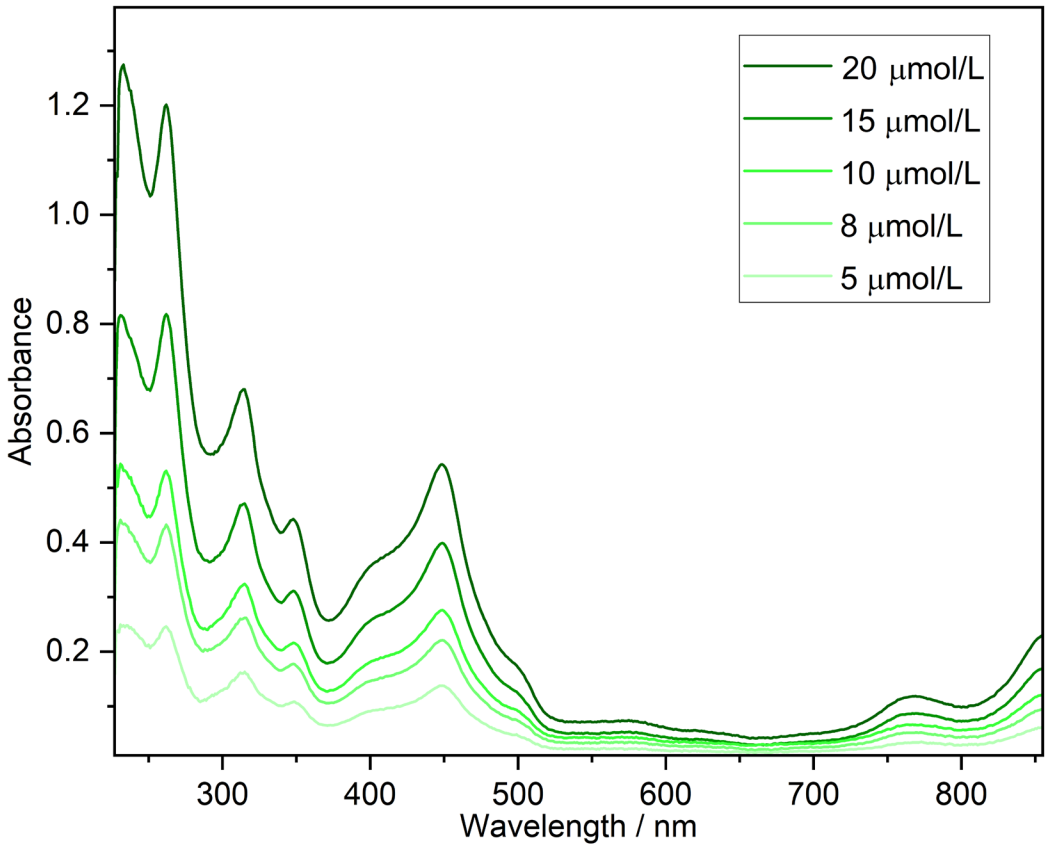


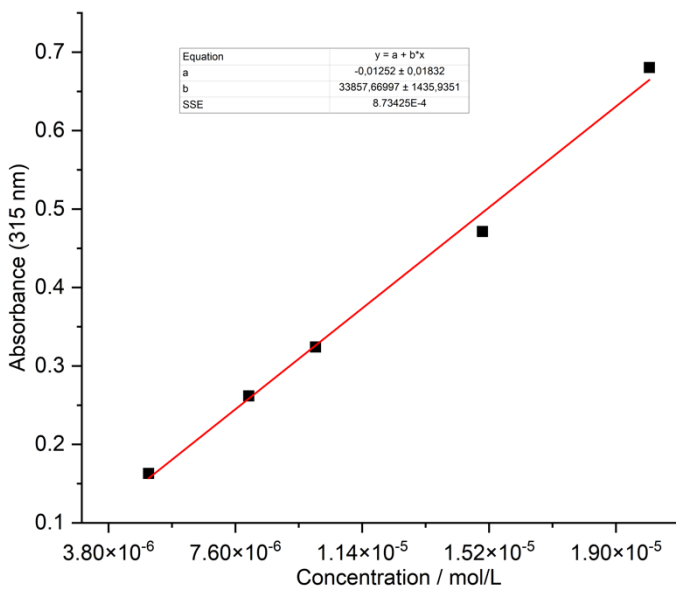
IR Spectrum of 5,8,11-Tris(2,4,6-trimethylphenyl)cyclopenta[1,2-*c*:4,3-*c*']difluoren-5-yl (7)

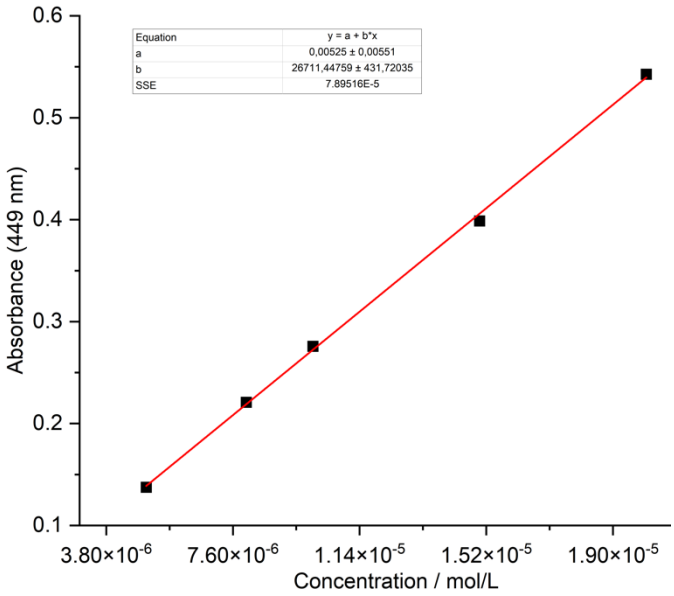


5. Measured UV/Vis Spectra of 7 and 15 in CH_2Cl_2

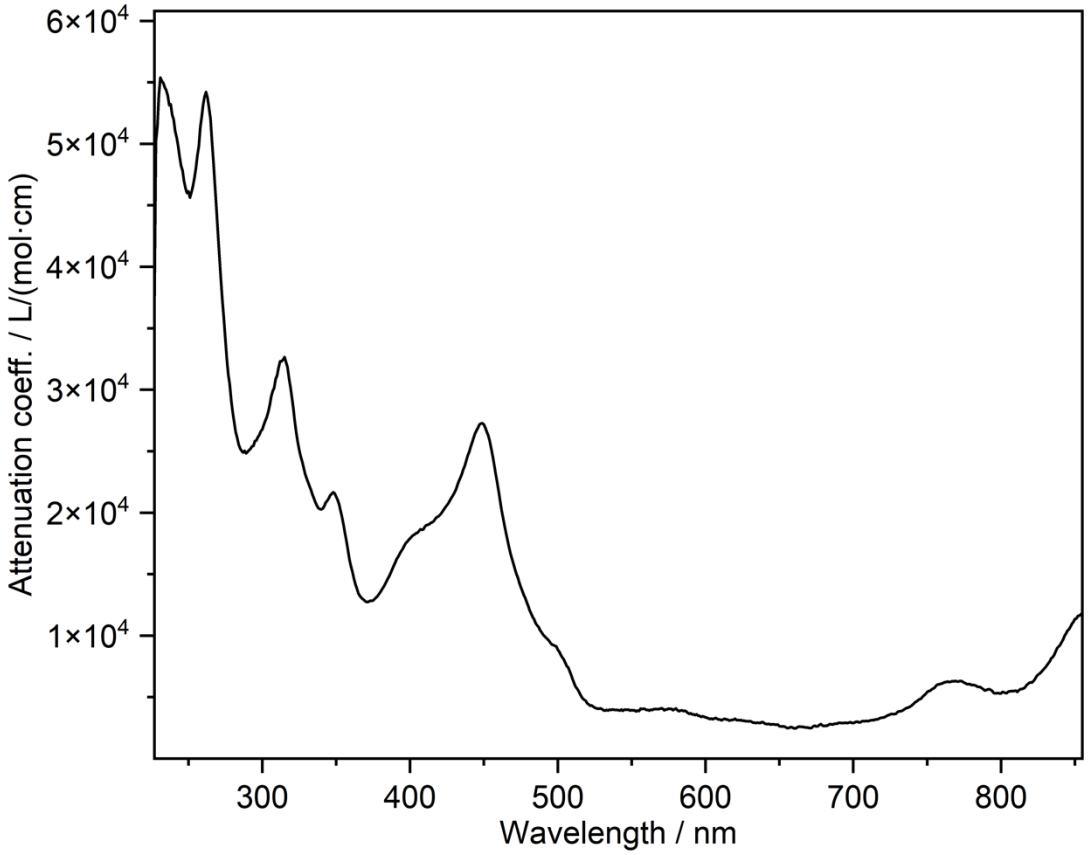
Compound 7:



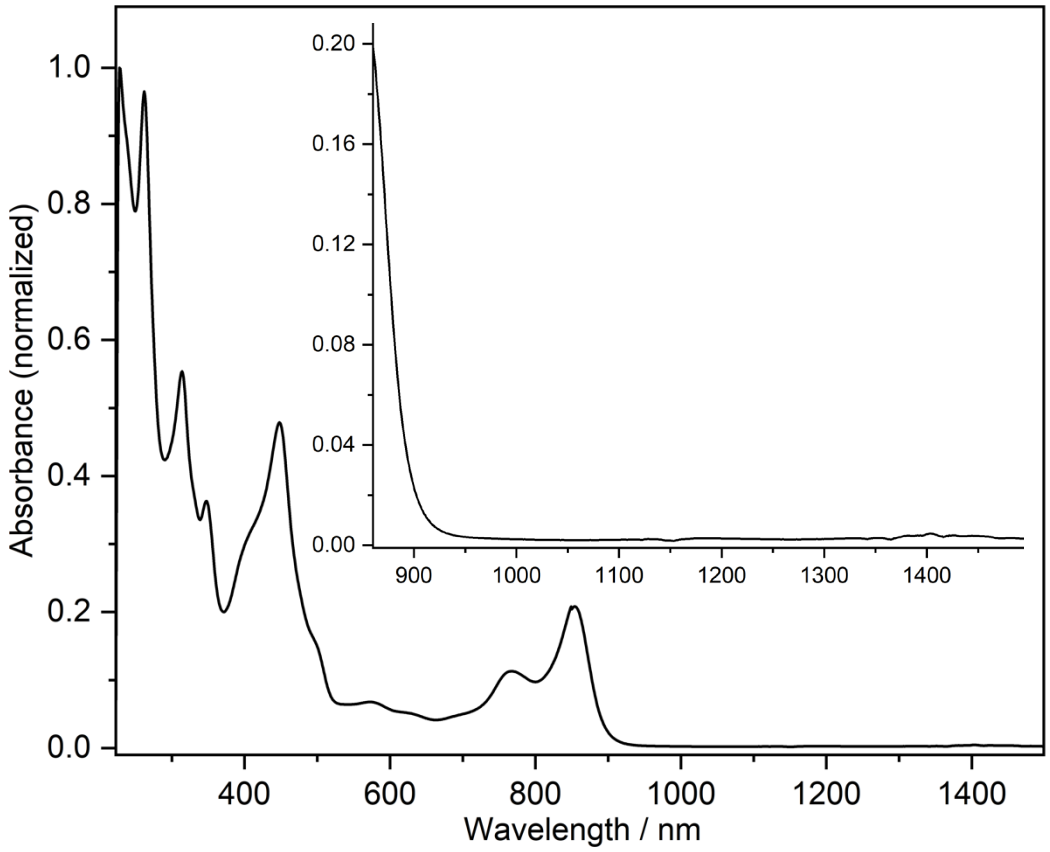




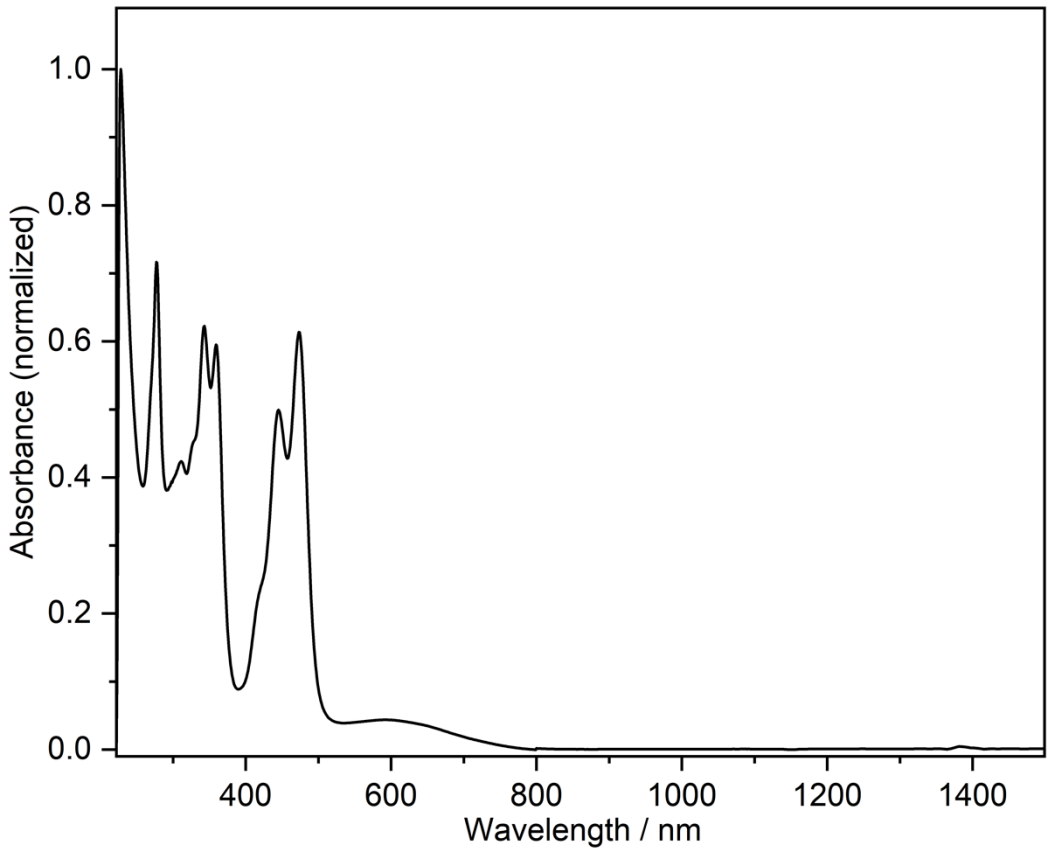
Quantitative UV/Vis spectrum of **7**:



UV/Vis/NIR Spectrum of **7** with magnified section:



UV/Vis/NIR Spectrum of **15**:



6. Cyclic Voltammograms of 7

Half-wave potentials, peak potential differences and corresponding i_{pc}/i_{pa} values of **7** in CH_2Cl_2 and THF vs. Fc/Fc^+(internal standard); conditions: Pt/$[NBu_4][Al\{OC(CF_3)_3\}_4]$/Ag; v(THF) = 200 mV s^{-1}, $v(CH_2Cl_2)$ = 500 mV s^{-1}. Corresponding redox processes in both solvents are highlighted with identical colours.

Redox wave	Solvent	$E^0_{½}$ [V]	ΔE_p [mV]	i_{pc}/i_{pa}
$E^0_{½}(1)$	THF	–2.73	180	~0.5
$E^0_{½}(2)$		–2.15	160	~1
$E^0_{½}(3)$		–1.36	140	~1
$E^0_{½}(4)$		–0.05	130	~1
$E^0_{½}(1)$	CH_2Cl_2	–2.14	220	~0.9
$E^0_{½}(2)$		–1.37	190	~1
$E^0_{½}(3)$		–0.16	190	~1
$E^0_{½}(4)$		+1.11	200	~1
$E^0_{½}(5)$		+1.55	200	~1

7. Computational Details

Compound **7** (in its doublet and in its quartet state, respectively) and **25** were optimized at the uM06[20]/6-311++g(d,p)[21] level by using the Gaussian 09 software package.[22] Except for the frequency analyses all calculations were performed using the thus obtained geometries. Frequency analyses[23] at the B3LYP[24]/6-311g(d,p)//B3LYP/6-311g(d,p) level confirmed the structures to be minima (no imaginary frequencies). An IR spectrum of **7** was visualized with GaussSum[25] [full width at half maximum (FWHM) of 10 cm^{-1}] using a scaling factor of 0.9619.[26] UV/Vis/NIR and ECD spectra were calculated with a time-dependent DFT calculation (td=nstates=50)[27] at the uM06/6-311g(d,p) level using a modelled solvent field of methylene chloride with the cpcm-scrf method.[28] These spectra were again visualized with GaussSum. An FWHM of 1500 cm^{-1} was chosen for the UV/Vis/NIR spectrum and a σ of 0.2 eV was used for the ECD spectrum. $NICS_{zz}$ values[29] were determined at the B3LYP/6-311g(d,p) level, *g* values, hyperfine coupling constants (EPR), and NMR shifts were calculated at the uM06/6-311g(d,p) level with the keywords nmr=giao[30] and prop=epr.[31] Frontier orbitals and spin densities were visualized with GaussView.[32] The triradical character of **7** was determined at the uhf[33]/6-311g(d,p), at the B3LYP/6-311g(d,p), and at the CAM-B3LYP[34]/6-311g(d,p) level using the pop=no keyword.[35]

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8. Archive Entry for a Single Point Calculation on a Minimum Structure of 7 (Doublet)

uM06/6-311++g(d,p)//uM06/6-311++g(d,p)

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9. Archive Entry for a Single Point Calculation on a Minimum Structure of 7 (Quartet)

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45287997,13,106.86257325,12,174.47107661,0\C,18,1.42972881,13,107.0380
9737,12,-179.79103505,0\C,20,1.39432523,18,128.37394585,13,-179.772302
78,0\C,19,1.39471496,14,135.65298924,13,-162.24361462,0\H,21,1.0876537
3,20,119.64877004,18,5.04795598,0\C,22,1.42703034,19,118.46020252,14,-
175.14764971,0\C,21,1.39024043,20,119.2542757,18,-174.32144389,0\H,25,
1.08754573,21,121.15986675,20,-178.92870801,0\C,22,1.45530986,19,134.8
7825684,14,10.88668269,0\C,24,1.44849704,22,109.13407224,19,178.512681
01,0\C,28,1.41454193,24,107.01621074,22,4.21882558,0\C,27,1.38682709,2
2,132.56594465,19,6.58254182,0\C,29,1.40171881,28,129.95726013,24,175.
31626418,0\H,31,1.08778916,29,119.85026675,28,5.38554123,0\H,30,1.0851
9968,27,120.83769297,22,-3.22878609,0\C,31,1.38174632,29,118.75568171,
28,-173.25606837,0\C,30,1.39146939,27,119.21601809,22,176.79093004,0\H
,35,1.08601385,30,119.25913385,27,179.41801791,0\H,34,1.08577538,31,12
0.0585084,29,179.68273322,0\H,6,1.08519901,5,120.8368928,4,-175.938469
93,0\H,1,1.0860133,6,119.25891365,5,179.41749327,0\C,9,1.47116883,4,12
6.99786864,3,-2.51185856,0\C,18,1.47082339,13,126.46184096,12,0.203327
32,0\C,28,1.47116907,24,125.96016739,22,-177.92127561,0\C,40,1.4004467
8,9,120.07502113,4,86.13252333,0\C,40,1.40247327,9,119.65371173,4,-94.
31193743,0\C,41,1.40082694,18,119.90432476,13,93.70855413,0\C,41,1.402
63782,18,119.87690078,13,-86.00430779,0\C,42,1.40247623,28,119.6541172
9,24,88.26067589,0\C,42,1.40044484,28,120.07475523,24,-91.31890081,0\C
,43,1.39171766,40,118.95022997,9,179.59324923,0\C,44,1.38941462,40,119
.00666817,9,-179.62768734,0\C,45,1.39144402,41,119.00189929,18,-179.82
247629,0\C,46,1.38954796,41,118.99565619,18,179.66607421,0\C,47,1.3894
1264,42,119.00648499,28,-179.65354264,0\C,48,1.39172217,42,118.950381,
28,179.62004992,0\H,50,1.08948558,44,119.0461498,40,179.88628644,0\H,4
9,1.08908785,43,118.96121506,40,-179.72346134,0\H,52,1.08950039,46,118
.98962403,41,-179.94062327,0\H,51,1.08917217,45,118.97080516,41,179.59
927194,0\H,54,1.08908851,48,118.96166822,42,-179.72749594,0\H,53,1.089
48803,47,119.04599762,42,179.88966648,0\C,54,1.38953443,48,121.7519126
5,42,0.11456832,0\C,51,1.38958778,45,121.74903433,41,0.04963951,0\C,49
,1.38953645,43,121.7521691,40,0.11390468,0\C,45,1.49861249,41,120.3206
6159,18,-0.54809594,0\H,64,1.09635555,45,111.23261851,41,-57.64282062,
0\H,64,1.09616152,45,111.51660316,41,61.10751319,0\H,64,1.0931664,45,1
11.16624691,41,-178.2267637,0\C,46,1.49856279,41,120.26921605,18,-0.69
369168,0\H,68,1.09634798,46,111.20851716,41,-57.45830312,0\H,68,1.0961
5475,46,111.53601864,41,61.28757279,0\H,68,1.0931644,46,111.16170302,4
1,-178.0259887,0\C,62,1.49771958,51,121.11846637,45,-178.84809875,0\H,
72,1.09365572,62,111.51548265,51,-19.29404617,0\H,72,1.09644211,62,111
.06671004,51,100.49868326,0\H,72,1.09457246,62,111.43256653,51,-140.22
930106,0\C,47,1.49852947,42,120.17385986,28,0.52289704,0\H,76,1.096472
53,47,111.42534306,42,-59.26294771,0\H,76,1.09650675,47,111.20650526,4
2,59.49472748,0\H,76,1.09319711,47,111.22208836,42,-179.95405833,0\C,4
8,1.49857981,42,120.32003139,28,-0.20698827,0\H,80,1.09620623,48,111.3
4059354,42,-61.61062152,0\H,80,1.09628562,48,111.37515483,42,57.111320
48,0\H,80,1.09316683,48,111.20908588,42,177.78791648,0\C,61,1.49774518
,54,121.11951763,48,178.79665985,0\H,84,1.09466581,61,111.42582354,54,

138.69067659,0\H,84,1.09635409,61,111.05865046,54,-102.05779742,0\H,84
,1.09356709,61,111.51183875,54,17.7727265,0\C,44,1.49853178,40,120.174
06624,9,0.54394429,0\H,88,1.09647503,44,111.42564488,40,-59.26828143,0
\H,88,1.09650476,44,111.20704225,40,59.49014621,0\H,88,1.0931972,44,11
1.22181118,40,-179.95847467,0\C,63,1.49774541,49,121.11807737,43,178.8
0203473,0\H,92,1.09466373,63,111.42587536,49,138.73375174,0\H,92,1.096
355,63,111.05954341,49,-102.01316829,0\H,92,1.09356875,63,111.51119641
,49,17.81637031,0\C,43,1.4985785,40,120.31930425,9,-0.23037242,0\H,96,
1.0962059,43,111.33994667,40,-61.58365314,0\H,96,1.09628706,43,111.375
10292,40,57.13860996,0\H,96,1.09316644,43,111.20931227,40,177.81399596
,0\\Version=EM64L-G09RevA.02\State=4-A\HF=-2083.7182071\S2=3.804742\S2
-1=0.\S2A=3.751494\RMSD=4.997e-09\Dipole=0.1946488,-0.0683618,-0.08601
63\Quadrupole=-0.3902727,-7.4637544,7.8540271,-3.0547761,2.525842,-0.7
744928\PG=C01 [X(C54H45)]\\@

10. Archive Entry for a Single Point Calculation on a Minimum Structure of 25

uM06/6-311++g(d,p)//uM06/6-311++g(d,p)

1\1\GINC-SERVER-LAB406\SP\UM06\6-311++G(d,p)\C27H15(2)\PODLECH\08-Dec-
2021\0\\# uM06/6-311++g(d,p) geom=connectivity\\Title Card Required\\0
,2\C\C,1,1.38973797\C,2,1.39214531,1,120.73657436\C,3,1.38816616,2,118
.85144929,1,1.15810463,0\C,4,1.42068205,3,120.43238788,2,1.95620139,0\
C,5,1.382959,4,119.94013237,3,-4.46042613,0\H,2,1.08595007,1,119.57747
189,6,179.55606442,0\H,3,1.08660853,2,120.59928168,1,-177.4257485,0\C,
4,1.43951244,3,130.89461579,2,-173.23701488,0\C,9,1.38299489,4,108.839
34622,3,174.68810384,0\C,10,1.41548311,9,129.96179657,4,-172.72239399,
0\C,11,1.36985167,10,119.5009292,9,173.20775056,0\C,12,1.40979169,11,1
19.48331682,10,4.66159969,0\C,13,1.45197454,12,121.75865849,11,3.65697
414,0\C,14,1.36745774,13,117.88451782,12,-13.5568975,0\H,11,1.08640601
,10,119.3706746,9,-3.18418178,0\H,12,1.08625862,11,121.05712275,10,-17
4.89941849,0\C,13,1.40088588,12,129.77606657,11,-171.70431912,0\C,14,1
.46897441,13,106.13582194,12,174.433516,0\C,18,1.40084825,13,109.81518
826,12,179.49615857,0\C,20,1.40981451,18,129.77641881,13,179.49586869,
0\C,19,1.3674478,14,135.30397079,13,-158.6664439,0\H,21,1.08625895,20,
119.4572572,18,7.86645258,0\C,22,1.4602884,19,118.5173404,14,-176.5185
0925,0\C,21,1.36983188,20,119.4836724,18,-171.70201356,0\H,25,1.086405
83,21,121.02827125,20,-179.0082561,0\C,22,1.46139739,19,135.13377569,1
4,6.08341152,0\C,24,1.38296987,22,108.77831666,19,176.14124903,0\C,27,
1.4206784,22,107.21901997,19,-177.28673679,0\C,27,1.38295839,22,132.53
15742,19,9.31717755,0\C,29,1.38815923,27,120.43261984,22,-178.84795651
,0\H,31,1.08660921,29,120.53419569,27,-179.45911813,0\H,30,1.08473712,
27,121.0342917,22,-2.99669118,0\C,31,1.39215,29,118.85131363,27,1.9558
8327,0\C,34,1.38973476,31,120.7365696,29,1.15846052,0\H,35,1.08549212,
34,119.79138928,31,178.06208632,0\H,34,1.08595103,31,119.67114874,29,1
79.7575749,0\H,6,1.08473647,5,121.03416277,4,-175.71398995,0\H,1,1.085
49232,2,119.79134592,3,178.06208609,0\H,28,1.08433329,24,125.75797473,
22,-178.75254191,0\H,18,1.084871,13,125.09189565,12,-0.50397279,0\H,9,
1.08433371,4,125.33118779,3,-2.37065639,0\\Version=AM64L-G09RevA.02\St
ate=2-A\HF=-1037.2988147\S2=0.958824\S2-1=0.\S2A=0.771365\RMSD=7.082e-
09\Dipole=0.0669467,-0.0266319,-0.0247726\Quadrupole=3.5191433,-10.226
8782,6.7077349,-6.4212449,0.2959492,0.0519131\PG=C01 [X(C27H15)]\\@

11. Archive Entry for a Single Point Calculation on a Minimum Structure of 15 (Singlet)

uM06/6-311++g(d,p)//uM06/6-311++g(d,p)

1\1\GINC-SERVER-LAB406\SP\UM06\6-311++G(d,p)\C40H36O2\PODLECH\25-Feb-2
022\0\\# sp uM06/6-311++g(d,p) geom=connectivity\\Title Card Required\
\0,1\C\C,1,1.39131684\C,2,1.40044661,1,120.26972313\C,3,1.37711804,2,1
18.71323321,1,1.19170852,0\C,4,1.41935343,3,121.885765,2,1.08048938,0\
C,5,1.37951138,4,118.31547224,3,-3.0789806,0\H,3,1.08729466,2,119.3947
6507,1,-177.83202101,0\C,4,1.45495726,3,129.05457884,2,-176.16655574,0
\C,5,1.46555179,4,106.97240468,3,-179.49768531,0\C,8,1.36520415,4,108.
08840402,3,177.40105245,0\C,10,1.43338466,8,128.16967534,4,-178.085293
86,0\C,9,1.36028625,5,135.63915838,4,-175.60259845,0\H,11,1.0875058,10
,118.71738024,8,0.90650517,0\C,12,1.46888405,9,118.46844299,5,-175.698
07991,0\C,11,1.35062226,10,119.53036053,8,-179.92287646,0\H,15,1.08752
172,11,121.74892663,10,-178.86973309,0\C,12,1.46556349,9,135.63932236,
5,2.62809667,0\C,14,1.36520671,12,109.95790755,9,175.74978892,0\C,17,1
.41936672,12,106.97145257,9,-175.61978216,0\C,17,1.3795093,12,134.5814

7931,9,8.80454298,0\C,19,1.37711851,17,121.88616825,12,-179.49326287,0
\H,21,1.08727594,19,121.88120072,17,-179.92095896,0\H,20,1.08296317,17
,121.33236861,12,0.14131044,0\C,21,1.40044066,19,118.71315772,17,1.077
28387,0\C,24,1.39130954,21,120.26992607,19,1.19177828,0\H,25,1.0834470
5,24,120.89246668,21,178.0673753,0\C,8,1.47369433,4,124.68823587,3,-1.
88144006,0\C,18,1.47369449,14,127.21925836,12,-178.76834629,0\C,27,1.4
0058745,8,119.88833051,4,88.94812985,0\C,27,1.40164808,8,119.87959066,
4,-90.30933241,0\C,28,1.40037152,18,119.9030008,14,90.25041965,0\C,28,
1.40183963,18,119.86779197,14,-89.94999232,0\C,29,1.39156578,27,118.99
800695,8,-179.58128799,0\C,30,1.39044751,27,118.99845056,8,179.6010831
2,0\C,31,1.39176707,28,119.0002344,18,-179.97775643,0\C,32,1.39026925,
28,118.99511654,18,-179.99635677,0\H,34,1.08934631,30,118.97333353,27,
-179.88181283,0\H,33,1.08918551,29,118.94263619,27,179.86156695,0\H,36
,1.08942083,32,118.95803727,28,-179.67531335,0\H,35,1.08912936,31,118.
95675058,28,179.63504153,0\C,35,1.38943454,31,121.75947456,28,-0.23477
6,0\C,33,1.38975558,29,121.75748755,27,-0.03586756,0\C,29,1.49864379,2
7,120.43905107,8,0.5259518,0\H,43,1.09628917,29,111.44905683,27,-57.97
705157,0\H,43,1.09614914,29,111.32543017,27,60.87530536,0\H,43,1.09322
796,29,111.11644578,27,-178.57481992,0\C,30,1.4986039,27,120.44004961,
8,-0.47291302,0\H,47,1.09609781,30,111.34663571,27,-60.36958077,0\H,47
,1.09637345,30,111.44078499,27,58.51973105,0\H,47,1.09326448,30,111.09
28981,27,179.0542705,0\C,42,1.49788235,33,121.05615465,29,-178.6047911
5,0\H,51,1.0938556,42,111.50620509,33,-23.97059024,0\H,51,1.09658017,4
2,111.06708215,33,95.69616561,0\H,51,1.09430405,42,111.45562108,33,-14
4.91517599,0\C,31,1.4986379,28,120.48035413,18,-0.41452955,0\H,55,1.09
610362,31,111.37362695,28,-60.49891239,0\H,55,1.09636612,31,111.418413
61,28,58.39343451,0\H,55,1.09326978,31,111.0961209,28,178.90310637,0\C
,32,1.49862109,28,120.39747353,18,0.48829339,0\H,59,1.09627876,32,111.
42668138,28,-57.80523274,0\H,59,1.09617347,32,111.33925666,28,61.04058
193,0\H,59,1.09322708,32,111.11425877,28,-178.38801116,0\C,41,1.497803
51,35,121.02778059,31,-178.66797238,0\H,63,1.09374022,41,111.47758665,
35,-21.46363485,0\H,63,1.09652837,41,111.07707263,35,98.25233518,0\H,6
3,1.0945429,41,111.47051766,35,-142.40536482,0\H,6,1.08296135,5,121.33
153746,4,-175.0450481,0\H,1,1.08344817,2,120.89263382,3,178.0684636,0\
O,2,1.3533396,1,124.39217948,6,179.48941761,0\O,24,1.35337118,21,115.3
3309207,19,-179.65726114,0\C,69,1.40532827,2,118.4057123,1,0.14529977,
0\C,70,1.40533449,24,118.40294607,21,-178.95825892,0\H,72,1.09784227,7
0,111.59533278,24,-60.95690377,0\H,72,1.09016036,70,106.4761911,24,-17
9.82794861,0\H,72,1.09780428,70,111.59897473,24,61.32504776,0\H,71,1.0
9015986,69,106.47537673,2,-179.82589837,0\H,71,1.09784478,69,111.59569
92,2,-60.9535656,0\H,71,1.09780555,69,111.60018302,2,61.32895174,0\\Ve
rsion=AM64L-G09RevA.02\State=1-A\HF=-1695.529902\S2=0.\S2-1=0.\S2A=0.\
RMSD=3.245e-09\Dipole=-0.7878022,0.1055738,-0.4623549\Quadrupole=10.12
38648,-10.8353015,0.7114367,-1.3567312,7.5426085,-2.6532436\PG=C01 [X(
C40H36O2)]\\@

12. Archive Entry for a Single Point Calculation on a Minimum Structure of 15 (Triplet)

uM06/6-311++g(d,p)//uM06/6-311++g(d,p)

1\1\GINC-OCH-C3-131\SP\UM06\6-311++G(d,p)\C40H36O2(3)\PODLECH\23-Feb-2
022\0\\# sp uM06/6-311++g(d,p) geom=connectivity\\Title Card Required\
\0,3\C\C,1,1.39921298\C,2,1.38945124,1,120.07000165\C,3,1.39310969,2,1
18.94359516,1,1.07435249,0\C,4,1.43037941,3,121.60503069,2,1.3685383,0
\C,5,1.38270247,4,117.93527277,3,-3.34816757,0\H,3,1.087313,2,119.6110
0319,1,-177.91480317,0\C,4,1.41857724,3,129.02503597,2,-175.79613966,0
\C,5,1.46099687,4,107.81250191,3,-179.57925088,0\C,9,1.43260611,5,106.
29594139,4,2.96816986,0\C,10,1.38674458,9,122.87311489,5,176.3174216,0
\C,9,1.38961082,5,135.66391128,4,-177.15128934,0\H,11,1.08770246,10,11
9.84874651,9,-179.46664375,0\C,12,1.43260387,9,118.0400747,5,-174.6068
2359,0\C,14,1.38675346,12,122.87289086,9,-3.59676669,0\H,15,1.08771863
,14,119.84866542,12,-179.46131788,0\C,12,1.46100595,9,135.66385179,5,5
.53337852,0\C,14,1.44357494,12,109.42135154,9,177.14314552,0\C,18,1.41
855517,14,107.05822196,12,1.83276951,0\C,17,1.38270324,12,134.11062637
,9,7.46741781,0\C,19,1.39310607,18,129.02330883,14,177.52826821,0\H,21
,1.08729451,19,121.43441223,18,3.16146168,0\H,20,1.08309456,17,121.220
31571,12,0.10909885,0\C,21,1.38943605,19,118.94376099,18,-175.80779583
,0\C,20,1.39585239,17,120.60495418,12,177.89258929,0\H,25,1.08381695,2
0,118.69957724,17,-179.99667158,0\C,8,1.47059381,4,126.7347224,3,-1.59
841897,0\C,18,1.47060127,14,126.20987381,12,-179.03109038,0\C,27,1.401
07408,8,119.86839576,4,88.62451652,0\C,27,1.4011511,8,119.86646156,4,-

91.05112084,0\C,28,1.40124085,18,119.86683447,14,89.60834997,0\C,28,1.
40098831,18,119.86762731,14,-90.14396465,0\C,29,1.39083902,27,118.9932
9751,8,-179.8379819,0\C,30,1.39075511,27,118.9945904,8,179.83126439,0\
C,31,1.39065826,28,118.99314941,18,-179.71929342,0\C,32,1.39093235,28,
118.99392246,18,179.73303695,0\H,34,1.08926166,30,118.98610962,27,-179
.71822301,0\H,33,1.08927315,29,118.96513187,27,179.74625778,0\H,36,1.0
8925984,32,118.96545047,28,-179.76685764,0\H,35,1.08928554,31,118.9890
0067,28,179.76720339,0\C,36,1.3904545,32,121.7193744,28,0.131926,0\C,3
4,1.39049905,30,121.72287354,27,0.10014766,0\C,29,1.49846381,27,120.17
644053,8,-0.17731927,0\H,43,1.09634049,29,111.27336467,27,-60.09032439
,0\H,43,1.09640525,29,111.35151337,27,58.59587671,0\H,43,1.09321199,29
,111.22886129,27,179.2875241,0\C,30,1.49845703,27,120.22011572,8,0.184
2374,0\H,47,1.09637657,30,111.35375922,27,-59.06997284,0\H,47,1.096373
42,30,111.28200571,27,59.67142717,0\H,47,1.09326611,30,111.20578844,27
,-179.72502385,0\C,42,1.49784088,34,120.78822167,30,178.53738016,0\H,5
1,1.09407574,42,111.51216454,34,151.49192796,0\H,51,1.09659321,42,111.
05575221,34,-88.98541312,0\H,51,1.09401534,42,111.47598138,34,30.51165
338,0\C,31,1.49845094,28,120.22132271,18,0.24961838,0\H,55,1.09637052,
31,111.38543032,28,-59.20598352,0\H,55,1.09637537,31,111.25332369,28,5
9.53631295,0\H,55,1.09326721,31,111.20470677,28,-179.88852378,0\C,32,1
.49846885,28,120.17849927,18,-0.19899467,0\H,59,1.09632721,32,111.2560
4891,28,-59.92653148,0\H,59,1.09642147,32,111.36906684,28,58.75932504,
0\H,59,1.09320967,32,111.22911113,28,179.46972168,0\C,41,1.49784002,36
,120.92527635,32,178.53528151,0\H,63,1.0940663,41,111.47704624,36,149.
6197499,0\H,63,1.09658059,41,111.03883132,36,-90.91488868,0\H,63,1.094
03536,41,111.52063804,36,28.62365227,0\H,6,1.08309063,5,121.21607059,4
,-174.89876623,0\H,1,1.08381822,6,118.69964792,5,180.,0\O,2,1.3564429,
1,124.00611199,6,179.46111318,0\O,24,1.35646476,21,115.91641404,19,-17
9.8299992,0\C,69,1.40441516,2,118.46845235,1,0.40325471,0\C,70,1.40443
251,24,118.46725541,21,-178.68363336,0\H,72,1.09812278,70,111.71974113
,24,-61.34955389,0\H,72,1.0902668,70,106.46287468,24,179.84709562,0\H,
72,1.09807036,70,111.70145666,24,61.06066117,0\H,71,1.09026962,69,106.
4659595,2,179.81745239,0\H,71,1.09812892,69,111.71734265,2,-61.3771673
,0\H,71,1.09807282,69,111.70165275,2,61.03118743,0\\Version=EM64L-G09R
evA.02\State=3-A\HF=-1695.5053871\S2=2.040541\S2-1=0.\S2A=2.001051\RMS
D=3.792e-09\Dipole=-0.6618069,0.084141,-0.3793441\Quadrupole=10.662543
3,-10.2802448,-0.3822985,-1.7127127,8.1481981,-2.7921637\PG=C01 [X(C40
H36O2)]\\@

13. Doublet and Quartet Energies of 7; Singlet and Triplet Energies of 15

7, doublet: HF = –2083.7500138 Hartree

7, quartet: HF = –2083.7182071 Hartree

Doublet-quartet gap: 0.0318 Hartree = 83.5 kJ/mol = 0.866 eV

15, singlet: HF = –1695.529902 Hartree

15, triplet: HF = –1695.5053871 Hartree

Singlet-triplet gap: 0.0245 Hartree = 64.4 kJ/mol = 0.668 eV

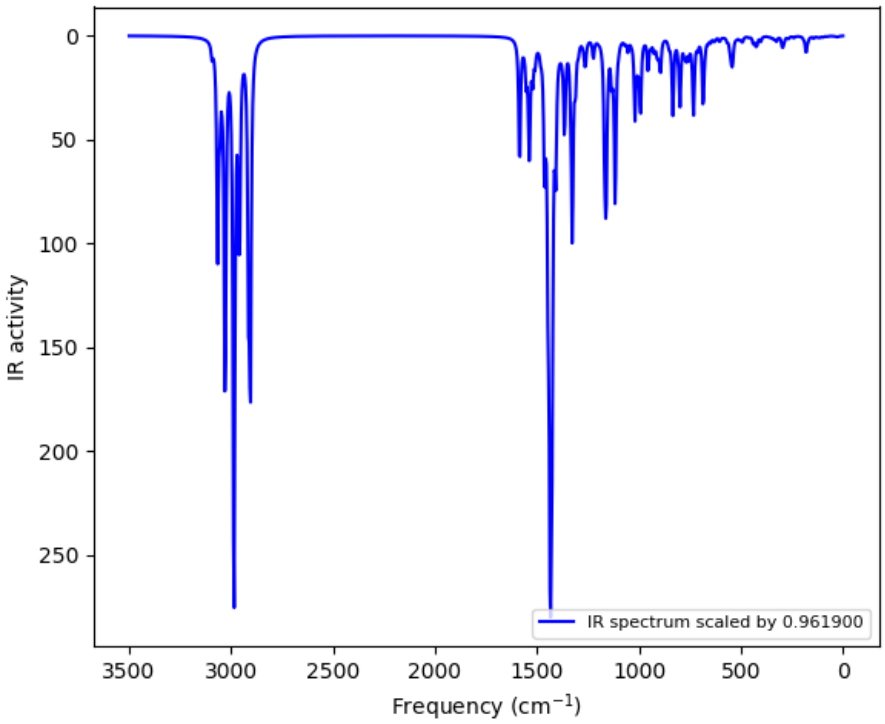
14. Frequency Analyses and Measured IR Spectrum of 7

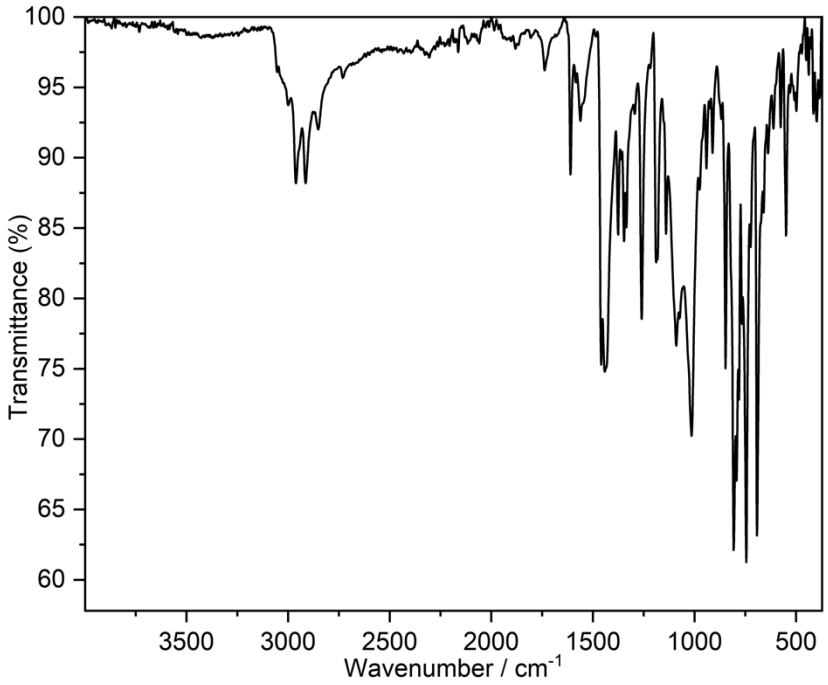
Frequency analyses of the doublet and of the quartet state, respectively, of **7** were performed at the B3LYP/6-311g(d,p) level; they show no imaginary frequencies. A frequency analysis for the doublet state showed lowest frequencies at $\tilde{\nu}$ = 10.0, 11.2, 15.3, 18.9, 21.7 cm^{-1}, etc. They are due to different twisting and bending modes of the mesityl groups and rotations of the methyl group. The lowest frequency for a twisting of the helicene core is 46.4 cm^{-1}.

Output of the frequency calculation for the doublet state of **7** (excerpt):

```
 Low frequencies ---   -4.1123   -2.5059   -0.4739   -0.0013   -0.0006    0.0017
 Low frequencies ---   10.0683   11.3989   15.3103
[...]
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole), reduced masses (AMU),
 force constants (mDyne/A):
                      1                      2                      3
                      A                      A                      A
 Frequencies --    10.0248               11.1685               15.2691
 Red. masses --     3.6212                3.4344                4.5037
 Frc consts  --     0.0002                0.0003                0.0006
 IR Inten    --     0.0277                0.0016                0.0389
[...]
                      4                      5                      6
                      A                      A                      A
 Frequencies --    18.9078               21.6899               22.9467
 Red. masses --     3.6569                4.2693                2.5536
 Frc consts  --     0.0008                0.0012                0.0008
 IR Inten    --     0.0015                0.0960                0.0652
[...]
                      7                      8                      9
                      A                      A                      A
 Frequencies --    27.7152               29.3041               31.5454
 Red. masses --     1.9956                1.9586                1.1051
 Frc consts  --     0.0009                0.0010                0.0006
 IR Inten    --     0.2941                0.0051                0.1199
[...]
                     10                     11                     12
                      A                      A                      A
 Frequencies --    34.7528               37.1066               43.0083
 Red. masses --     1.2784                2.3376                3.8520
 Frc consts  --     0.0009                0.0019                0.0042
 IR Inten    --     0.1471                0.0427                0.0333
[...]
                     13                     14                     15
                      A                      A                      A
 Frequencies --    46.4400               61.6480               67.0717
 Red. masses --     5.3494                5.0338                4.4757
 Frc consts  --     0.0068                0.0113                0.0119
 IR Inten    --     0.0943                0.0004                0.0735
```

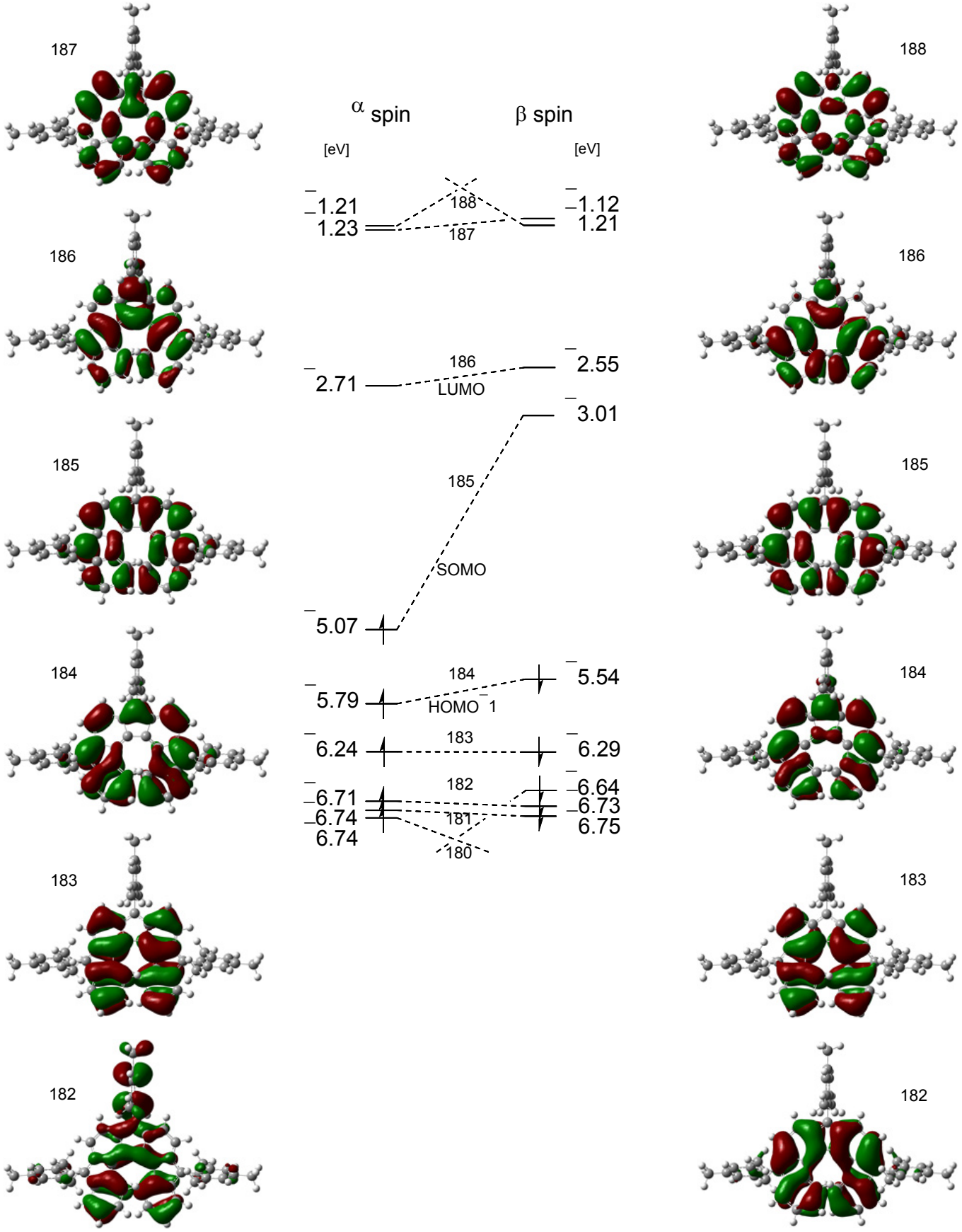
A calculated IR spectrum of **7** (doublet state, top) was obtained using a published scaling factor of 0.9619.[26] The spectrum was visualized with GaussSum: FWHM 10 cm^{-1}.The measured IR spectrum of **7** (bottom) is additionally given with an aligned frequency scale.





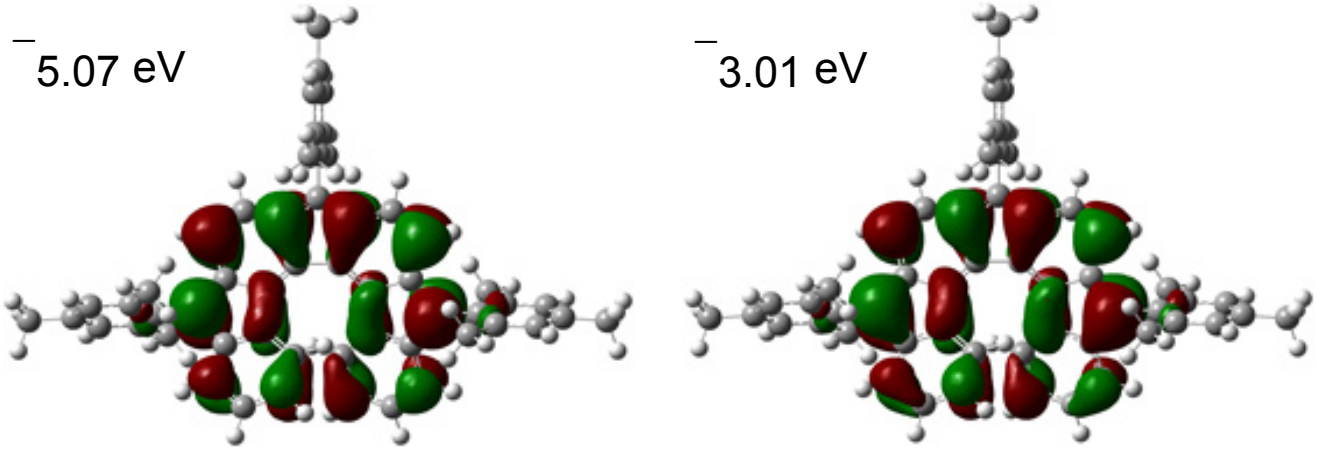
15. Frontier Orbitals of 7

M06/6-311++g(d,p)//M06/6-311++g(d,p) (isovalue: 0.02 electrons$^{1/2}$·bohr$^{-3/2}$)



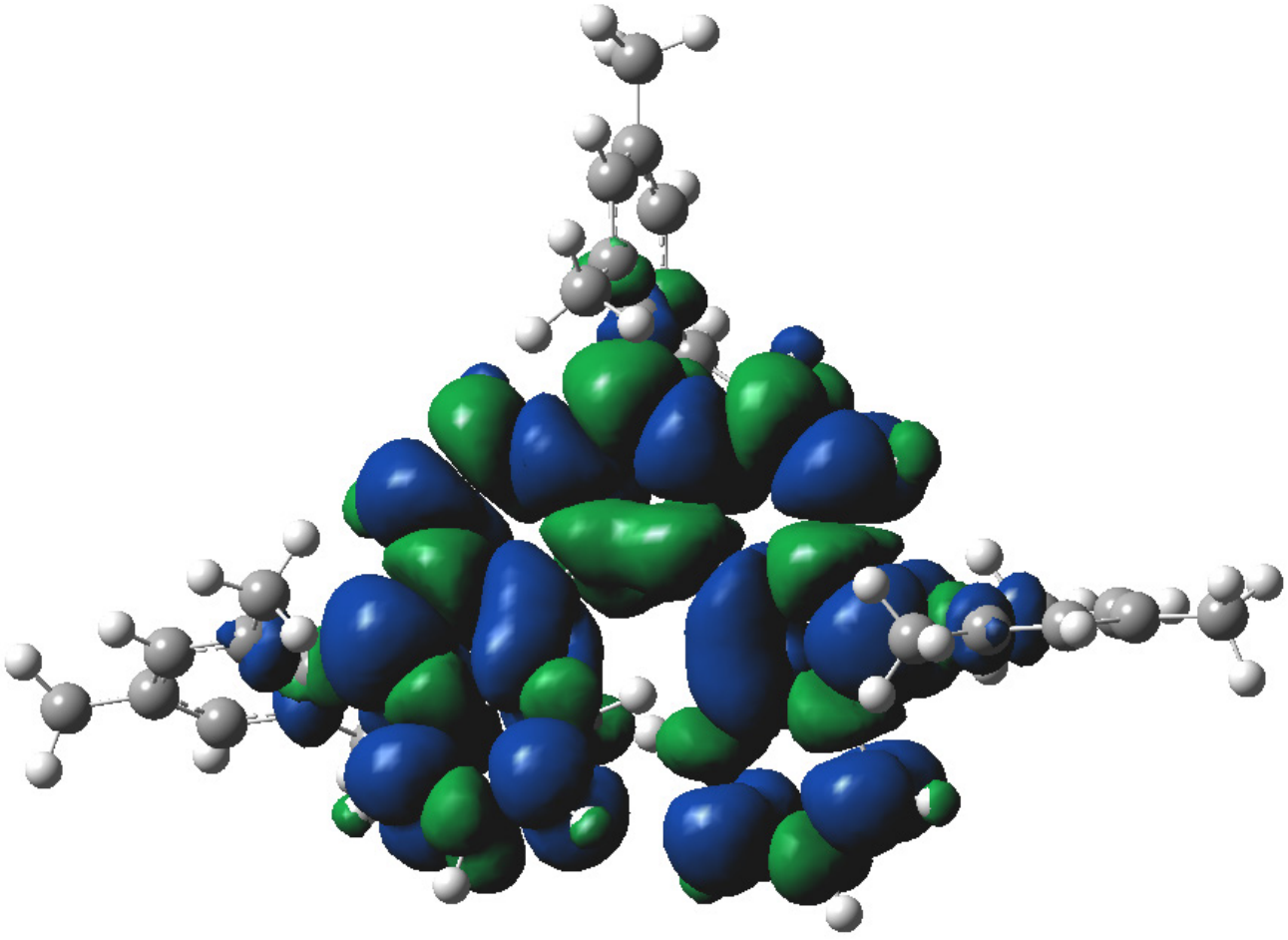
16. Enlarged Figure 6. Calculated SOMOs of α and β Electrons, respectively

M06/6-311++g(d,p)//M06/6-311++g(d,p) (isovalue: 0.02 electrons$^{1/2}$·bohr$^{-3/2}$)



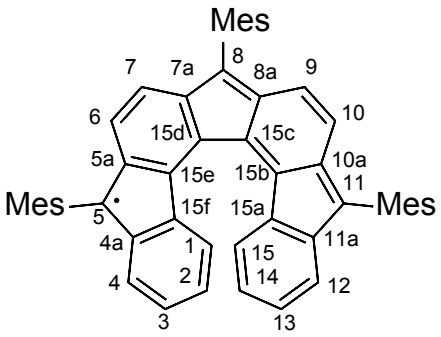
17. Enlarged Figure 5. Calculated Spin Density of 7

M06/6-311++g(d,p)//M06/6-311++g(d,p); blue and green surfaces represent α and β spin densities, respectively (isovalue: 0.004 electrons·bohr^{-3}).



18. Mulliken Atomic Spin Densities of the Helicene Carbon Atoms in 7

Atom number	Internal numbering		Spin density
1	6	C	-0.033953
2	1	C	0.098519
3	2	C	-0.040923
4	3	C	0.098743
4a	4	C	-0.060766
5	9	C	**0.341252**
5a	10	C	-0.161717
6	11	C	0.216903
7	12	C	-0.137102
7a	13	C	0.195714
8	18	C	**-0.242001**
8a	20	C	0.195778
9	21	C	-0.137369
10	25	C	0.217011
10a	24	C	-0.161648
11	28	C	**0.340758**
11a	29	C	-0.060842
12	31	C	0.098652
13	34	C	-0.040951
14	35	C	0.098397
15	30	C	-0.034032
15a	27	C	0.072678
15b	22	C	0.107303
15c	19	C	-0.079740
15d	14	C	-0.079278
15e	15	C	0.107216
15f	5	C	0.072734



19. Triradical Character of 7

Calculation at the uB3LYP/6-31g(d,p)//uM06/6-311++g(d,p) level:

Input:

```
%chk=Mes_Trirad5.chk
%mem=600MW
%nprocs=16
#p sp uhf/sto-3g

Title Card Required

0 2
// Coordinates for the uM06/6-311++g(d,p)-optimized structure

--Link1--
%nprocs=16
%mem=600MW
%chk=Mes_Trirad5.chk
#p uhf/3-21g guess=(read,mix) geom=allcheck

--Link1--
%nprocs=16
%mem=600MW
%chk=Mes_Trirad5.chk
#p uhf/6-31g(d,p) guess=(read,mix) geom=allcheck

--Link1--
%nprocs=16
%mem=600MW
%chk=Mes_Trirad5.chk
#p uB3LYP/6-31g(d,p) guess=(read,permute) pop=no geom=allcheck
```

Output (excerpt):

```
     Natural Orbital Coefficients:

                      181       182       183       184       185
     Eigenvalues --   1.99826   1.99716   1.99512   1.92910   1.00000
[...]
                      186       187       188       189       190
     Eigenvalues --   0.07090   0.00488   0.00284   0.00174   0.00173
```

The triradical character *y* was calculated with n_{HONO} = 1.92910 and n_{LUNO} = 0.07090 using *Yamaguchi*'s scheme:[36]

$$T = \frac{n_{\mathrm{HONO}} - n_{\mathrm{LUNO}}}{2}$$

$$y = 1 - \frac{2T}{1 + T^2}$$

$$y = 0.0027$$

[36] K. Yamaguchi, *Chem. Phys. Lett.* **1975**, *33*, 330–335; K. Kamada, K. Ohta, A. Shimizu, T. Kubo, R. Kishi, H. Takahashi, E. Botek, B. Champagne, M. Nakano, *J. Phys. Chem. Lett.* **2010**, *1*, 937–940.

Calculation at the uCAM-B3LYP/6-31g(d,p)//uM06/6-311++g(d,p) level:

Input (excerpt):

```
...

--Link1--
%nprocs=16
%mem=600MW
%chk=Mes_Trirad.chk
#p uhf/3-21g guess=(read,mix) geom=allcheck

--Link1--
%nprocs=16
%mem=600MW
%chk=Mes_Trirad.chk
#p uhf/6-31g(d,p) guess=(read,mix) geom=allcheck

--Link1--
%nprocs=16
%mem=600MW
%chk=Mes_Trirad.chk
#p uCAM-B3LYP/6-31g(d,p) guess=(read,permute) pop=no geom=allcheck
```

Output (excerpt):

```
     Natural Orbital Coefficients:

                       181       182       183       184       185
     Eigenvalues --   1.99379   1.99008   1.98195   1.79275   1.00000
[...]
                       186       187       188       189       190
     Eigenvalues --   0.20725   0.01805   0.00992   0.00621   0.00607
```

y = 0.026

Calculation at the uhf/6-31g(d,p)//uM06/6-311++g(d,p) level:

Input (excerpt):

```
...

--Link1--
%chk=Mes_Trirad3.chk
%mem=600MW
%nprocs=16
#p sp uhf/6-31g(d,p) guess=(read,permute) pop=no geom=allcheck
```

Output (excerpt):

```
     Natural Orbital Coefficients:

                       181       182       183       184       185
     Eigenvalues --   1.89078   1.88057   1.84037   1.44988   1.00000
[...]
                       186       187       188       189       190
     Eigenvalues --   0.55012   0.15963   0.11943   0.10922   0.10044
```

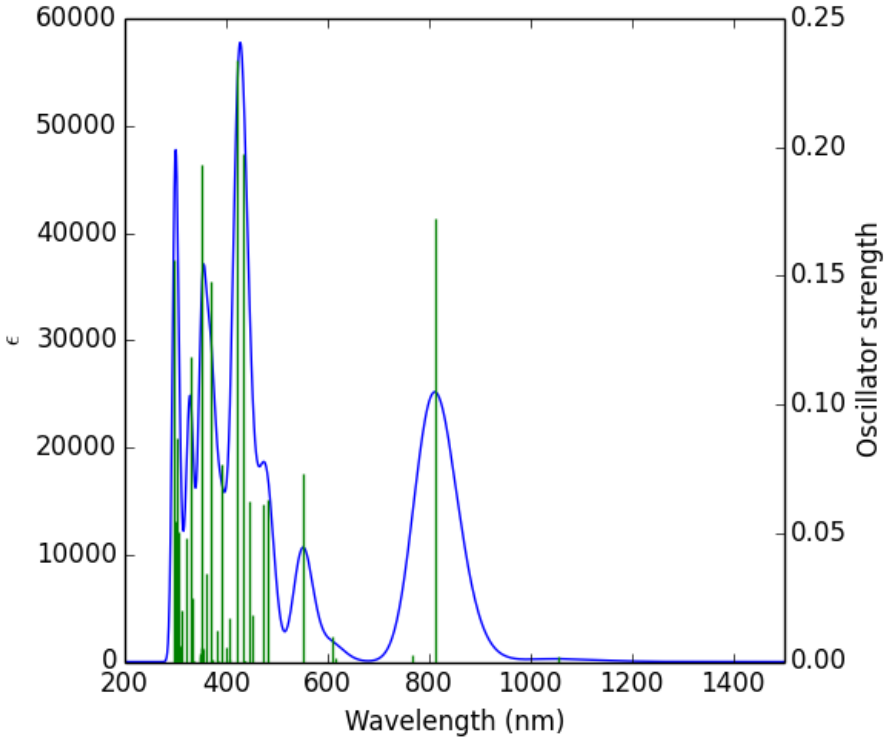
y = 0.252

The triradical character was also addressed by EPR spectroscopy. A solid sample of **7** (1% in KCl matrix) was irradiated with high microwave power for prolonged periods. The spectrum was checked for half-field resonances, but none could be detected.

Spin concentration was determined by NMR spectroscopy via the Evans method. The obtained values for sample magnetisation were considerably lower than expected (0.51 Bohr magnetons). Dilution of the sample lead to an increase of magnetic moment, hence, association in solution can be assumed. At higher dilution, spin concentration was determined by EPR spectroscopy by comparison with a TEMPO standard sample under the same measurement conditions. Integration of both signals yielded a normalised (intensity per molecule) difference of only 8% for the respective areas under the curve, giving a strong indication of the monoradical character of the helical species.

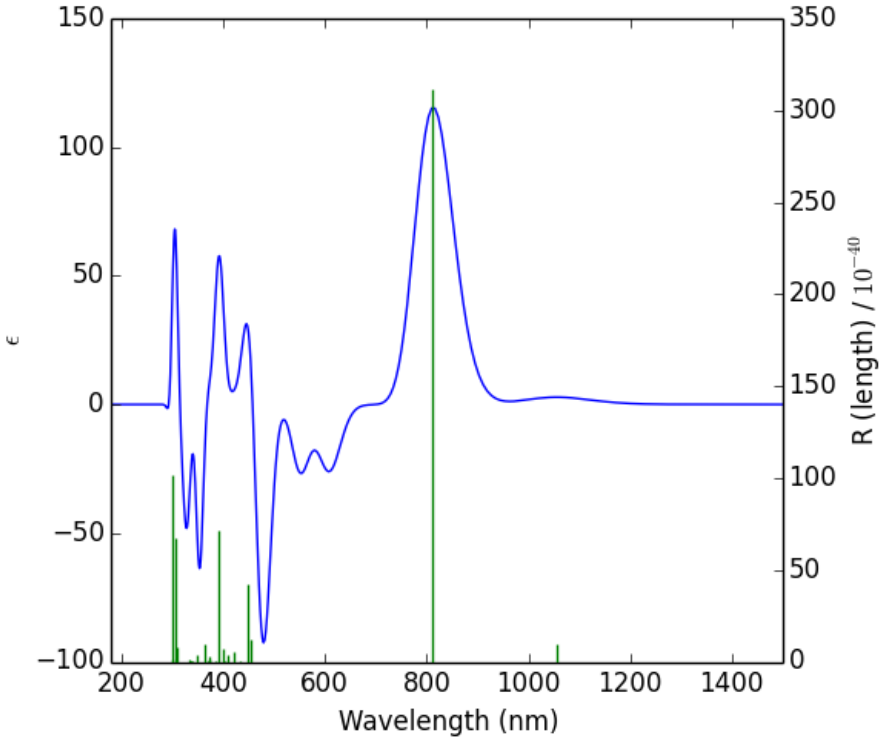
20. Calculated UV/Vis/NIR Spectra of 7

td(nstates=50)/M06/6-311g(d,p)/scrf(cpcm,CH_2Cl_2)//M06/6-311++g(d,p); Visualized with GaussSum: FWHM 1500 cm^{-1}

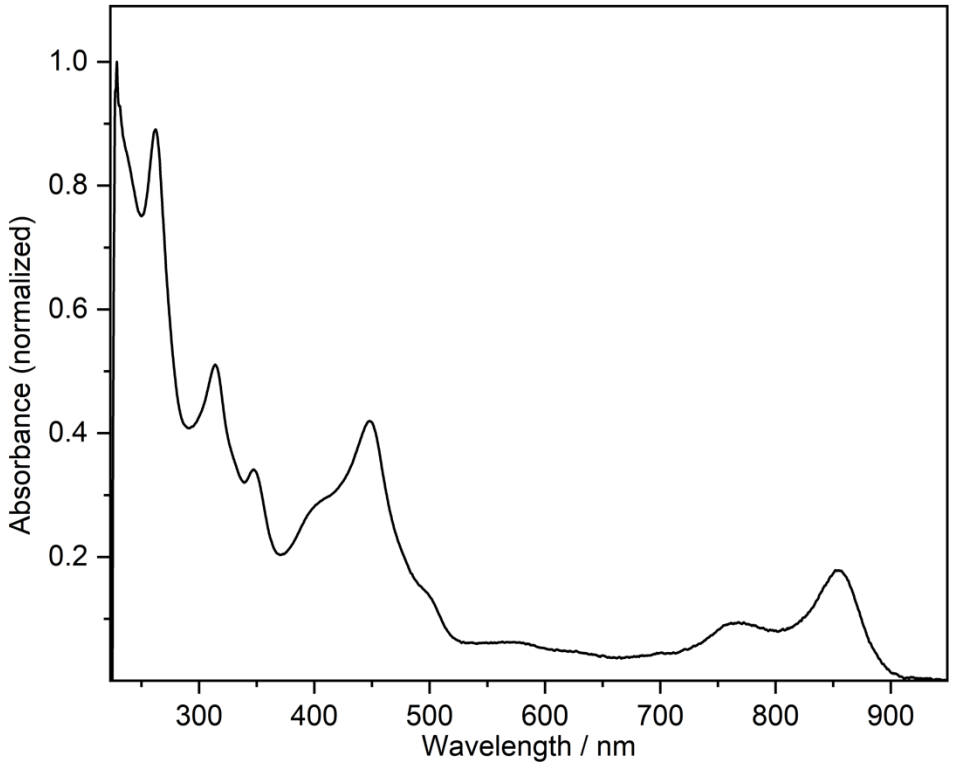


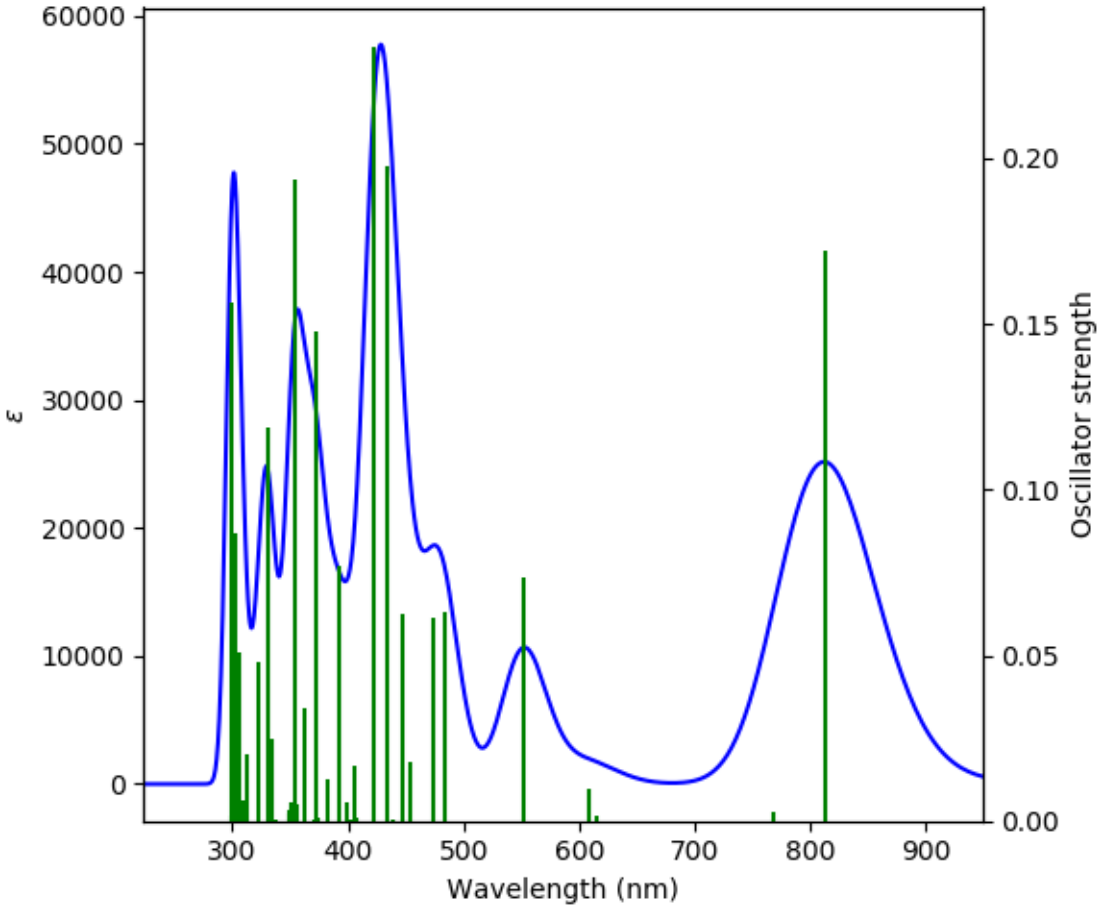
21. Calculated Electronic Circular Dichroism (ECD) Spectrum of 7

td(nstates=50)/M06/6-311g(d,p)/scrf(cpcm,CH_2Cl_2)//M06/6-311++g(d,p); Visualized with GaussSum: sigma 0.2 eV



UV/Vis spectra with identical section and scaling to allow for comparison: measured (top) and calculated (bottom) spectra:





22. TD Calculation of 7

TD(nstates=50)/M06/6-311g(d,p)/scrf(cpcm,CH_2Cl_2)//M06/6-311++g(d,p)

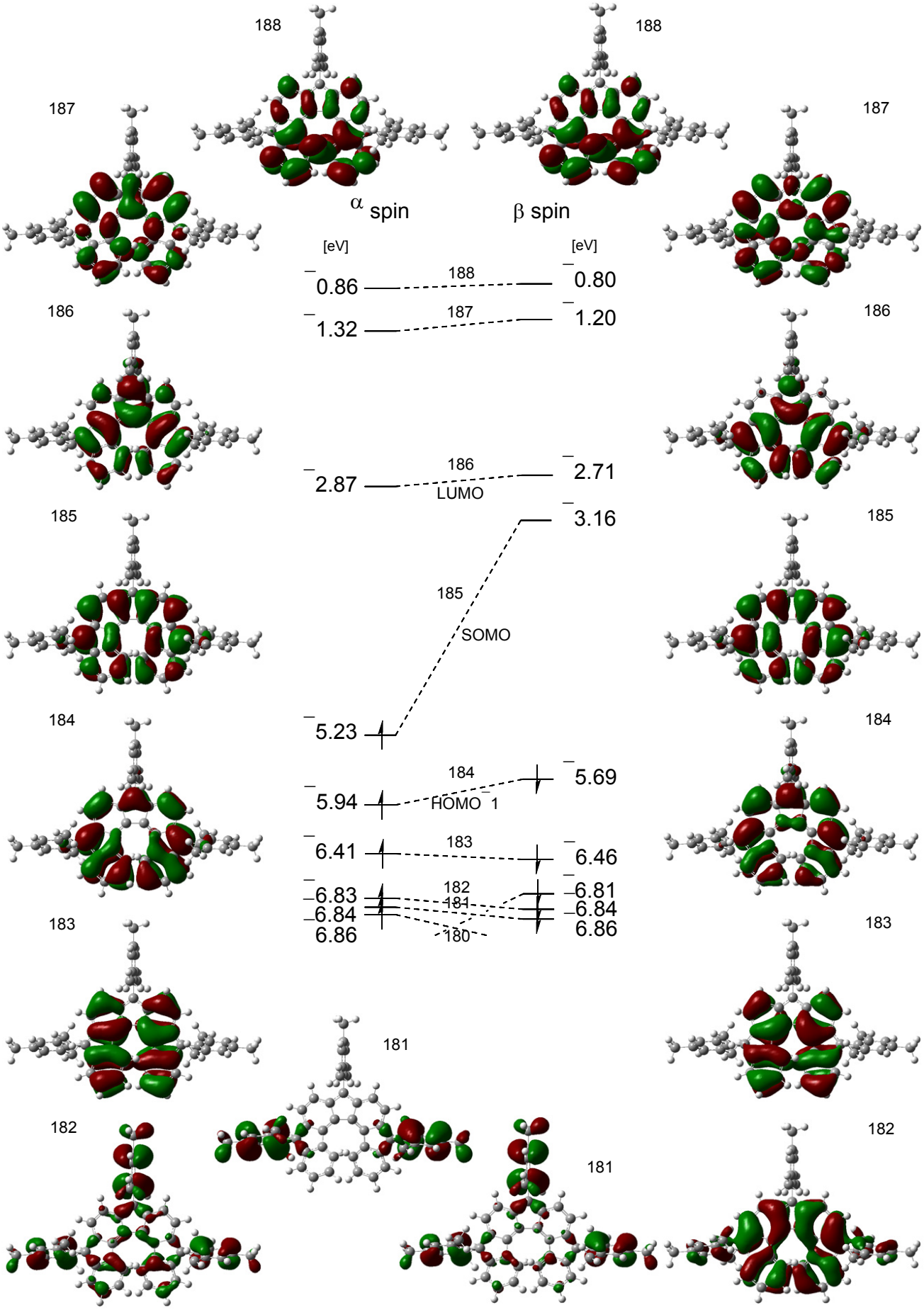
Output (excerpt; only a selection of transitions is given, Annotations after // were added by the authors):

```
 ********************************************************************
 Excited states from <AA,BB:AA,BB> singles matrix:
 ********************************************************************

Ground to excited state transition electric dipole moments (Au):
       state          X           Y           Z        Dip. S.      Osc.
         1        -0.2440     -0.0001      0.0898      0.0676      0.0019
         2         2.1201      0.0005     -0.3303      4.6040      0.1722
         3         0.0024      0.2647     -0.0001      0.0701      0.0028
         4        -0.1667     -0.0019      0.0060      0.0278      0.0014
         5         0.0020     -0.4458     -0.0005      0.1987      0.0099
         6         0.0003     -1.1541     -0.0006      1.3320      0.0733
         7         0.0023     -1.0011     -0.0011      1.0021      0.0629
         8        -0.9414     -0.0018      0.2681      0.9581      0.0613
         9         0.0025     -0.5177     -0.0008      0.2680      0.0180
        10        -0.9206     -0.0010      0.2622      0.9162      0.0622
[...]

Excitation energies and oscillator strengths:

 Excited State   1:  2.011-A      1.1746 eV 1055.53 nm  f=0.0019  <S**2>=0.761
    185A -> 186A       0.85152            // (SOMO   -> LUMO)
    184B -> 185B       0.51017            // (HOMO-1 -> SOMO)

 Excited State   2:  2.106-A      1.5262 eV  812.36 nm  f=0.1722  <S**2>=0.859
    185A -> 186A      -0.50330            // (SOMO   -> LUMO)
    185A -> 187A      -0.10539
    183B -> 186B      -0.19551            // (HOMO-2 -> LUMO)
    184B -> 185B       0.81917            // (HOMO-1 -> SOMO)

 Excited State   3:  3.158-A      1.6144 eV  767.97 nm  f=0.0028  <S**2>=2.243
    184A -> 186A       0.58905            // (HOMO-1 -> LUMO)
    182B -> 185B      -0.19119
    184B -> 186B       0.75353            // (HOMO-1 -> LUMO)

 Excited State   4:  3.390-A      2.0162 eV  614.93 nm  f=0.0014  <S**2>=2.624
    175A -> 186A       0.14614
    183A -> 186A       0.69797            // (HOMO-2 -> LUMO)
    183A -> 187A       0.12156
    174B -> 185B      -0.10406
    175B -> 185B      -0.19623
    183B -> 186B      -0.57864            // (HOMO-2 -> LUMO)

 Excited State   5:  2.395-A      2.0375 eV  608.50 nm  f=0.0099  <S**2>=1.184
    184A -> 186A       0.41733            // (HOMO-1 -> LUMO)
    175B -> 186B       0.20615
    183B -> 185B       0.80844            // (HOMO-2 -> SOMO)
    184B -> 186B      -0.24901            // (HOMO-1 -> LUMO)

 Excited State   6:  2.294-A      2.2446 eV  552.36 nm  f=0.0733  <S**2>=1.065
    176A -> 186A      -0.10803
    177A -> 186A      -0.12216
    179A -> 186A       0.13133
    180A -> 186A      -0.11428
    182A -> 186A      -0.12291
    184A -> 186A       0.63081            // (HOMO-1 -> LUMO)
    175B -> 186B      -0.10508
    182B -> 185B      -0.10996
    183B -> 185B      -0.39911            // (HOMO-2 -> SOMO)
    184B -> 186B      -0.54980            // (HOMO-1 -> LUMO)
    184B -> 187B      -0.12950

 Excited State   7:  2.356-A      2.5639 eV  483.59 nm  f=0.0629  <S**2>=1.137
    184A -> 186A       0.19610            // (HOMO-1 -> LUMO)
    174B -> 186B       0.13078
    175B -> 186B       0.13882
```

```
   180B -> 185B       0.24678
   182B -> 185B       0.87309
   184B -> 186B       0.10048            // (HOMO-1 -> LUMO)

Excited State   8:  2.284-A      2.6135 eV  474.40 nm  f=0.0613  <S**2>=1.055
   183A -> 186A      -0.49643            // (HOMO-2 -> LUMO)
   184A -> 188A      -0.11927
   185A -> 187A       0.52706
   175B -> 185B      -0.42079
   179B -> 185B      -0.19170
   181B -> 185B      -0.19763
   183B -> 186B      -0.39811            // (HOMO-2 -> LUMO)

Excited State   9:  3.237-A      2.7339 eV  453.51 nm  f=0.0180  <S**2>=2.369
   176A -> 186A       0.27013
   177A -> 186A       0.31064
   179A -> 186A      -0.33269
   180A -> 186A       0.34018
   182A -> 186A       0.37869
   175B -> 186B       0.36085
   179B -> 186B       0.14405
   181B -> 186B       0.13641
   183B -> 185B      -0.36104            // (HOMO-2 -> SOMO)
   184B -> 186B      -0.17508            // (HOMO-1 -> LUMO)
   184B -> 187B      -0.13669

Excited State  10:  3.192-A      2.7719 eV  447.28 nm  f=0.0622  <S**2>=2.296
   175A -> 186A       0.42798
   183A -> 186A      -0.30286            // (HOMO-2 -> LUMO)
   185A -> 187A      -0.14661
   174B -> 185B       0.19525
   175B -> 185B       0.14650
   179B -> 185B       0.16865
   180B -> 186B       0.17478
   183B -> 186B      -0.23955            // (HOMO-2 -> LUMO)
```

23. Frontier Orbitals of 7 as Obtained from the TD Calculation

TD(nstates=50)/M06/6-311g(d,p)/scrf(cpcm,CH_2Cl_2)//M06/6-311++g(d,p) (Isovalue: 0.02 electrons$^{1/2}$·bohr$^{-3/2}$).



24. HOMA Values of 7

HOMA values were calculated according to the following formula:[37]

$$\mathrm{HOMA} = 1 - \frac{\alpha}{n}\sum_{i=1}^{n}\left(d_{opt} - d_i\right)^2$$

α: 257.7 Å^{-2}; an empirical constant chosen to give HOMA = 0 for a hypothetical *Kekule* structure with alternating bonds and to result HOMA = 1 for the system with all bonds equal to the optimum value d_{opt}.
n: number of bonds considered
d_{opt}: 1.388 Å (for CC bonds)
d_i: the actually measured or calculated bond distance

Bond distances were either taken from the crystallographic data (here as the average from the two equivalent positions in the molecules, where two independent molecules in the unit cell were considered) or from the calculation [M06/6-311++g(d,p), gas phase; all the respective equivalent positions were identical within the relevant precision].

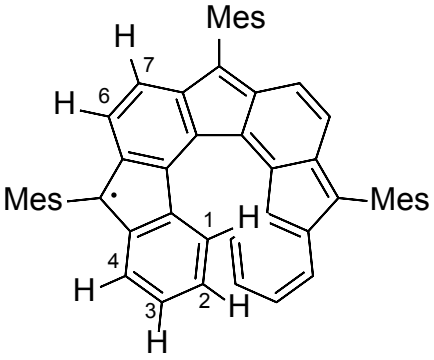
HOMA and $NICS_{zz}(1.0)$ values for comparison:

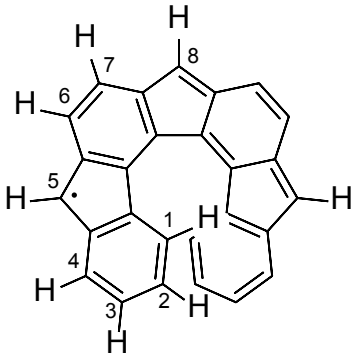
Compound	HOMA values[a]	$NICS_{zz}(1.0)$[b]
benzene	1.00	–29.4
cyclopentadienyl anion	0.89	–33.5
cyclopentadienyl radical	0.46	42.6
cyclopentadienyl cation	–1.03	216.7
cyclobutadiene	–3.44	58.6

[a] M06/6-311++g(d,p), gas phase;
[b] B3LYP/6-311g(d,p)//M06/6-311++g(d,p), gas phase

25. Calculated ^{1}H NMR Shifts of 7 and 25

nmr=gdiis/M06/6-311g(d,p)//M06/6-311++g(d,p)





Proton	Internal numbering	δ [ppm]
1-H	38	6.72
2-H	39	6.74
3-H	7	7.10
4-H	8	6.77
5-H	–	–
6-H	16	6.33
7-H	17	6.18
8-H	–	–

Proton	Internal numbering	δ [ppm]
1-H	38	6.55
2-H	39	6.60
3-H	7	7.04
4-H	8	7.16
5-H	42	6.66
6-H	16	6.77
7-H	17	6.62
8-H	41	6.43

[37] T. M. Krygowski, M. K. Cyrański, *Chem. Rev.* **2001**, *101*, 1385–1420.

26. Calculated EPR Data of 7

nmr=gdiis,prop=epr/M06/6-311g(d,p)//M06/6-311++g(d,p)

g value: $g_{xx} = 2.0023195 + 89.1 \cdot 10^{-6}$; $g_{yy} = 2.0023195 + 237.8 \cdot 10^{-6}$; $g_{zz} = 2.0023195 + 661.6 \cdot 10^{-6}$

$g_{iso} = (g_{xx} + g_{yy} + g_{zz}) / 3 = 2.0026$

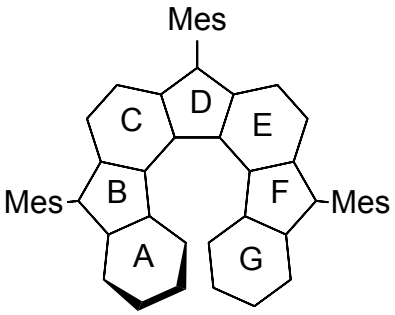
Output (excerpt):

		Isotropic Fermi Contact Couplings				
	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1	IUPAC numbering (selection)
1	C(13)	0.01104	12.41449	4.42980	4.14103	C-2
2	C(13)	-0.00783	-8.80699	-3.14255	-2.93770	C-3
3	C(13)	0.01120	12.59519	4.49428	4.20130	C-4
4	C(13)	-0.01902	-21.38436	-7.63047	-7.13306	C-4a
5	C(13)	0.00681	7.66070	2.73353	2.55533	C-15f
6	C(13)	-0.00626	-7.04076	-2.51232	-2.34855	C-1
7	H(1)	0.00058	2.57683	0.91948	0.85954	3-H
8	H(1)	-0.00207	-9.23908	-3.29673	-3.08183	4-H
9	C(13)	0.04122	46.33592	16.53381	15.45600	C-5
10	C(13)	-0.02951	-33.17879	-11.83902	-11.06725	C-5a
11	C(13)	0.02519	28.31714	10.10426	9.44558	C-6
12	C(13)	-0.02285	-25.68769	-9.16601	-8.56849	C-7
13	C(13)	0.03214	36.13480	12.89380	12.05327	C-7a
14	C(13)	-0.01209	-13.58683	-4.84812	-4.53208	C-15d
15	C(13)	0.01114	12.52365	4.46875	4.17744	C-15e
16	H(1)	-0.00398	-17.81112	-6.35545	-5.94115	6-H
17	H(1)	0.00273	12.21248	4.35772	4.07365	7-H
18	C(13)	-0.03505	-39.40466	-14.06056	-13.14398	C-8
19	C(13)	-0.01208	-13.57725	-4.84470	-4.52888	
20	C(13)	0.03215	36.14752	12.89834	12.05752	
21	C(13)	-0.02285	-25.69003	-9.16684	-8.56927	
22	C(13)	0.01113	12.51141	4.46438	4.17336	
23	H(1)	0.00273	12.21977	4.36032	4.07608	
24	C(13)	-0.02950	-33.16060	-11.83253	-11.06119	
25	C(13)	0.02519	28.31615	10.10391	9.44525	
26	H(1)	-0.00398	-17.81013	-6.35510	-5.94082	
27	C(13)	0.00681	7.65212	2.73047	2.55247	
28	C(13)	0.04117	46.28666	16.51623	15.43957	
29	C(13)	-0.01900	-21.36101	-7.62214	-7.12526	
30	C(13)	-0.00625	-7.03095	-2.50882	-2.34527	
31	C(13)	0.01119	12.57893	4.48848	4.19588	
32	H(1)	-0.00206	-9.22686	-3.29237	-3.07775	
33	H(1)	0.00036	1.62173	0.57867	0.54095	
34	C(13)	-0.00782	-8.79639	-3.13877	-2.93416	
35	C(13)	0.01103	12.39860	4.42413	4.13573	
36	H(1)	-0.00209	-9.34372	-3.33407	-3.11673	
37	H(1)	0.00058	2.57434	0.91859	0.85871	
38	H(1)	0.00036	1.62504	0.57986	0.54206	1-H
39	H(1)	-0.00209	-9.35610	-3.33849	-3.12086	2-H
40	C(13)	-0.01458	-16.38527	-5.84667	-5.46554	C_{Mes} at C-5
41	C(13)	0.00966	10.86226	3.87592	3.62326	C_{Mes} at C-8
42	C(13)	-0.01456	-16.36440	-5.83922	-5.45857	
43	C(13)	0.01388	15.60870	5.56957	5.20650	
44	C(13)	0.01387	15.59347	5.56414	5.20142	
45	C(13)	-0.00945	-10.62754	-3.79217	-3.54497	
46	C(13)	-0.00946	-10.62994	-3.79303	-3.54577	
47	C(13)	0.01385	15.57257	5.55668	5.19445	
48	C(13)	0.01387	15.59215	5.56367	5.20098	
49	C(13)	0.00109	1.22342	0.43655	0.40809	
50	C(13)	0.00094	1.06096	0.37858	0.35390	
51	C(13)	-0.00054	-0.60447	-0.21569	-0.20163	
52	C(13)	-0.00054	-0.60296	-0.21515	-0.20113	
53	C(13)	0.00094	1.05830	0.37763	0.35301	
54	C(13)	0.00109	1.22305	0.43641	0.40797	
55	H(1)	0.00035	1.56103	0.55701	0.52070	
56	H(1)	0.00035	1.58666	0.56616	0.52925	
57	H(1)	-0.00025	-1.09674	-0.39134	-0.36583	
58	H(1)	-0.00024	-1.08308	-0.38647	-0.36128	

59	H(1)	0.00035	1.58507	0.56559	0.52872
60	H(1)	0.00035	1.55854	0.55612	0.51987
61	C(13)	0.00008	0.09020	0.03219	0.03009
62	C(13)	-0.00022	-0.24350	-0.08689	-0.08122
63	C(13)	0.00008	0.09013	0.03216	0.03006
64	C(13)	-0.00054	-0.60915	-0.21736	-0.20319
65	H(1)	-0.00022	-0.96735	-0.34517	-0.32267
66	H(1)	-0.00023	-1.04692	-0.37357	-0.34922
67	H(1)	-0.00024	-1.05096	-0.37501	-0.35056
68	C(13)	-0.00054	-0.60333	-0.21528	-0.20125
69	H(1)	-0.00022	-0.98458	-0.35132	-0.32842
70	H(1)	-0.00023	-1.02072	-0.36422	-0.34048
71	H(1)	-0.00023	-1.05037	-0.37480	-0.35037
72	C(13)	0.00009	0.10229	0.03650	0.03412
73	H(1)	-0.00001	-0.02645	-0.00944	-0.00882
74	H(1)	-0.00006	-0.25012	-0.08925	-0.08343
75	H(1)	-0.00004	-0.18760	-0.06694	-0.06258
76	C(13)	0.00120	1.34619	0.48035	0.44904
77	H(1)	0.00028	1.25828	0.44899	0.41972
78	H(1)	0.00043	1.93463	0.69032	0.64532
79	H(1)	0.00035	1.54754	0.55220	0.51620
80	C(13)	0.00093	1.04634	0.37336	0.34902
81	H(1)	0.00040	1.76807	0.63089	0.58977
82	H(1)	0.00028	1.27030	0.45327	0.42373
83	H(1)	0.00030	1.35446	0.48330	0.45180
84	C(13)	-0.00007	-0.07581	-0.02705	-0.02529
85	H(1)	0.00001	0.06483	0.02313	0.02163
86	H(1)	0.00003	0.13728	0.04898	0.04579
87	H(1)	0.00001	0.06169	0.02201	0.02058
88	C(13)	0.00120	1.34678	0.48056	0.44924
89	H(1)	0.00028	1.26125	0.45005	0.42071
90	H(1)	0.00043	1.93499	0.69045	0.64544
91	H(1)	0.00035	1.55010	0.55311	0.51706
92	C(13)	-0.00007	-0.07583	-0.02706	-0.02529
93	H(1)	0.00001	0.06616	0.02361	0.02207
94	H(1)	0.00003	0.13712	0.04893	0.04574
95	H(1)	0.00001	0.06051	0.02159	0.02018
96	C(13)	0.00093	1.04842	0.37410	0.34971
97	H(1)	0.00040	1.76755	0.63071	0.58959
98	H(1)	0.00029	1.27479	0.45488	0.42522
99	H(1)	0.00030	1.35677	0.48413	0.45257

27. NICS Values of 7 and 25

B3LYP/6-311g(d,p)//M06/6-311++g(d,p)



Ring A

Top side

NICS@	isotropic	xx	yy	zz
0.0	-4.3368	-6.6258	-7.4871	1.1026
0.1	-4.3649	-6.6074	-7.2751	0.7878
0.2	-4.5698	-6.4364	-6.9132	-0.3599
0.3	-4.9107	-6.1202	-6.4250	-2.1870
0.4	-5.3288	-5.6750	-5.8419	-4.4694
0.5	-5.7592	-5.1241	-5.1994	-6.9541
0.6	-6.1430	-4.4965	-4.5325	-9.3999
0.7	-6.4349	-3.8230	-3.8721	-11.6095
0.8	-6.6070	-3.1332	-3.2420	-13.4459
0.9	-6.6491	-2.4528	-2.6588	-14.8356
1.0	-6.5652	-1.8024	-2.1319	**-15.7612**
1.1	-6.3701	-1.1969	-1.6659	-16.2475
1.2	-6.0847	-0.6459	-1.2618	-16.3464
1.3	-5.7324	-0.1548	-0.9186	-16.1239
1.4	-5.3362	0.2744	-0.6342	-15.6488
1.5	-4.9165	0.6424	-0.4056	-14.9864
1.6	-4.4905	0.9523	-0.2296	-14.1944
1.7	-4.0717	1.2082	-0.1021	-13.3212
1.8	-3.6696	1.4159	-0.0189	-12.4060
1.9	-3.2909	1.5816	0.0250	-11.4792
2.0	-2.9391	1.7120	0.0347	-10.5640
2.1	-2.6160	1.8139	0.0153	-9.6771
2.2	-2.3216	1.8935	-0.0280	-8.8303
2.3	-2.0549	1.9568	-0.0902	-8.0313
2.4	-1.8144	2.0086	-0.1672	-7.2847
2.5	-1.5981	2.0529	-0.2548	-6.5923
2.6	-1.4039	2.0928	-0.3499	-5.9545
2.7	-1.2298	2.1303	-0.4495	-5.3700
2.8	-1.0739	2.1665	-0.5514	-4.8366
2.9	-0.9344	2.2020	-0.6536	-4.3517
3.0	-0.8099	2.2368	-0.7543	-3.9121
3.1	-0.6988	2.2704	-0.8519	-3.5149
3.2	-0.6000	2.3021	-0.9446	-3.1573
3.3	-0.5122	2.3312	-1.0308	-2.8369
3.4	-0.4344	2.3569	-1.1085	-2.5518
3.5	-0.3658	2.3787	-1.1758	-2.3003
3.6	-0.3053	2.3960	-1.2307	-2.0812
3.7	-0.2523	2.4084	-1.2715	-1.8938
3.8	-0.2059	2.4157	-1.2965	-1.7370
3.9	-0.1656	2.4177	-1.3048	-1.6098
4.0	-0.1308	2.4145	-1.2960	-1.5108
4.1	-0.1009	2.4060	-1.2701	-1.4384
4.2	-0.0755	2.3922	-1.2284	-1.3903
4.3	-0.0542	2.3735	-1.1723	-1.3637
4.4	-0.0366	2.3498	-1.1041	-1.3556
4.5	-0.0225	2.3214	-1.0263	-1.3626
4.6	-0.0116	2.2885	-0.9418	-1.3814
4.7	-0.0034	2.2515	-0.8531	-1.4086
4.8	0.0023	2.2108	-0.7629	-1.4412
4.9	0.0057	2.1668	-0.6732	-1.4764
5.0	0.0073	2.1200	-0.5859	-1.5122

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	-4.3179	-7.0223	-7.0508	1.1195
0.1	-4.4783	-7.0938	-6.8948	0.5537
0.2	-4.8108	-7.0105	-6.5875	-0.8345
0.3	-5.2696	-6.7792	-6.1484	-2.8810
0.4	-5.7913	-6.4159	-5.6050	-5.3531
0.5	-6.3083	-5.9440	-4.9893	-7.9917
0.6	-6.7598	-5.3925	-4.3337	-10.5532
0.7	-7.1004	-4.7921	-3.6675	-12.8414
0.8	-7.3034	-4.1720	-3.0144	-14.7239
0.9	-7.3609	-3.5573	-2.3912	-16.1342
1.0	-7.2801	-2.9677	-1.8094	**-17.0631**
1.1	-7.0787	-2.4175	-1.2753	-17.5434
1.2	-6.7809	-1.9162	-0.7921	-17.6344
1.3	-6.4126	-1.4692	-0.3611	-17.4075
1.4	-5.9989	-1.0791	0.0180	-16.9356
1.5	-5.5618	-0.7458	0.3464	-16.2861
1.6	-5.1197	-0.4678	0.6260	-15.5174
1.7	-4.6868	-0.2421	0.8595	-14.6777
1.8	-4.2731	-0.0645	1.0499	-13.8048
1.9	-3.8855	0.0699	1.2011	-12.9273
2.0	-3.5277	0.1664	1.3171	-12.0665
2.1	-3.2013	0.2308	1.4021	-11.2368
2.2	-2.9063	0.2689	1.4605	-10.4482
2.3	-2.6414	0.2860	1.4964	-9.7067
2.4	-2.4047	0.2875	1.5137	-9.0154
2.5	-2.1938	0.2778	1.5160	-8.3753
2.6	-2.0063	0.2609	1.5064	-7.7861
2.7	-1.8396	0.2401	1.4876	-7.2463
2.8	-1.6913	0.2180	1.4618	-6.7537
2.9	-1.5594	0.1966	1.4308	-6.3055
3.0	-1.4418	0.1775	1.3961	-5.8990
3.1	-1.3367	0.1617	1.3590	-5.5309
3.2	-1.2428	0.1497	1.3203	-5.1982
3.3	-1.1584	0.1418	1.2806	-4.8977
3.4	-1.0826	0.1381	1.2407	-4.6265
3.5	-1.0141	0.1385	1.2008	-4.3816
3.6	-0.9522	0.1426	1.1612	-4.1605
3.7	-0.8960	0.1499	1.1223	-3.9604
3.8	-0.8449	0.1602	1.0842	-3.7791
3.9	-0.7982	0.1729	1.0469	-3.6144
4.0	-0.7554	0.1876	1.0107	-3.4644
4.1	-0.7161	0.2037	0.9755	-3.3274
4.2	-0.6798	0.2209	0.9414	-3.2017
4.3	-0.6462	0.2388	0.9084	-3.0859
4.4	-0.6151	0.2571	0.8766	-2.9789
4.5	-0.5861	0.2754	0.8460	-2.8796
4.6	-0.5590	0.2935	0.8165	-2.7870
4.7	-0.5337	0.3111	0.7882	-2.7003
4.8	-0.5099	0.3281	0.7610	-2.6189
4.9	-0.4876	0.3443	0.7350	-2.5421
5.0	-0.4665	0.3597	0.7101	-2.4693

Ring B

Top side

NICS@	isotropic	xx	yy	zz
0.0	7.2807	-10.4565	-9.4140	41.7127
0.1	7.2195	-10.5410	-9.0532	41.2526
0.2	7.0449	-10.3380	-8.6181	40.0910
0.3	6.7572	-9.8680	-8.0841	38.2238
0.4	6.3580	-9.1738	-7.4218	35.6697
0.5	5.8557	-8.3162	-6.6195	32.5028
0.6	5.2687	-7.3644	-5.6945	28.8652
0.7	4.6256	-6.3853	-4.6896	24.9516
0.8	3.9610	-5.4342	-3.6596	20.9769
0.9	3.3105	-4.5505	-2.6582	17.1402
1.0	2.7044	-3.7570	-1.7277	**13.5980**
1.1	2.1640	-3.0637	-0.8958	10.4515
1.2	1.7002	-2.4714	-0.1768	7.7489
1.3	1.3147	-1.9757	0.4257	5.4942
1.4	1.0022	-1.5698	0.9148	3.6615
1.5	0.7531	-1.2456	1.2978	2.2072
1.6	0.5565	-0.9947	1.5846	1.0798
1.7	0.4016	-0.8083	1.7859	0.2271
1.8	0.2786	-0.6774	1.9134	-0.4003
1.9	0.1799	-0.5925	1.9790	-0.8469
2.0	0.0995	-0.5441	1.9944	-1.1518
2.1	0.0331	-0.5227	1.9710	-1.3489
2.2	-0.0222	-0.5193	1.9194	-1.4668
2.3	-0.0687	-0.5255	1.8491	-1.5297
2.4	-0.1077	-0.5339	1.7683	-1.5574
2.5	-0.1404	-0.5386	1.6836	-1.5661
2.6	-0.1676	-0.5350	1.6002	-1.5679
2.7	-0.1902	-0.5201	1.5216	-1.5720
2.8	-0.2088	-0.4923	1.4503	-1.5843
2.9	-0.2240	-0.4511	1.3874	-1.6083
3.0	-0.2364	-0.3975	1.3333	-1.6452
3.1	-0.2466	-0.3328	1.2875	-1.6944
3.2	-0.2548	-0.2593	1.2493	-1.7543
3.3	-0.2614	-0.1792	1.2175	-1.8224
3.4	-0.2666	-0.0951	1.1911	-1.8959
3.5	-0.2707	-0.0093	1.1689	-1.9717
3.6	-0.2738	0.0761	1.1497	-2.0472
3.7	-0.2760	0.1592	1.1328	-2.1198
3.8	-0.2773	0.2386	1.1173	-2.1877
3.9	-0.2779	0.3131	1.1026	-2.2493
4.0	-0.2777	0.3820	1.0884	-2.3035
4.1	-0.2769	0.4449	1.0743	-2.3498
4.2	-0.2754	0.5015	1.0602	-2.3879
4.3	-0.2734	0.5517	1.0460	-2.4178
4.4	-0.2708	0.5957	1.0316	-2.4397
4.5	-0.2678	0.6338	1.0170	-2.4541
4.6	-0.2643	0.6662	1.0023	-2.4614
4.7	-0.2605	0.6934	0.9875	-2.4624
4.8	-0.2563	0.7157	0.9727	-2.4574
4.9	-0.2519	0.7337	0.9578	-2.4473
5.0	-0.2473	0.7476	0.9430	-2.4326

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	7.2944	-8.5446	-11.2592	41.6869
0.1	7.2380	-8.8533	-10.8724	41.4397
0.2	7.0589	-9.0383	-10.2375	40.4525
0.3	6.7510	-9.0422	-9.3982	38.6933
0.4	6.3135	-8.8126	-8.4141	36.1671
0.5	5.7560	-8.3269	-7.3553	32.9503
0.6	5.1013	-7.6025	-6.2924	29.1987
0.7	4.3833	-6.6911	-5.2861	25.1273
0.8	3.6430	-5.6629	-4.3800	20.9719
0.9	2.9205	-4.5895	-3.5981	16.9492
1.0	2.2500	-3.5314	-2.9468	**13.2281**
1.1	1.6545	-2.5325	-2.4210	9.9171
1.2	1.1460	-1.6206	-2.0084	7.0670
1.3	0.7257	-0.8097	-1.6951	4.6819
1.4	0.3877	-0.1043	-1.4670	2.7343
1.5	0.1214	0.4974	-1.3115	1.1783
1.6	-0.0853	1.0009	-1.2175	-0.0392
1.7	-0.2443	1.4141	-1.1747	-0.9723
1.8	-0.3663	1.7458	-1.1736	-1.6711
1.9	-0.4600	2.0055	-1.2049	-2.1807
2.0	-0.5323	2.2031	-1.2597	-2.5403
2.1	-0.5881	2.3482	-1.3291	-2.7834
2.2	-0.6311	2.4499	-1.4049	-2.9384
2.3	-0.6639	2.5167	-1.4794	-3.0291
2.4	-0.6884	2.5558	-1.5462	-3.0750
2.5	-0.7060	2.5737	-1.5998	-3.0919
2.6	-0.7177	2.5756	-1.6364	-3.0923
2.7	-0.7245	2.5655	-1.6535	-3.0855
2.8	-0.7271	2.5466	-1.6500	-3.0778
2.9	-0.7261	2.5212	-1.6261	-3.0735
3.0	-0.7222	2.4908	-1.5830	-3.0745
3.1	-0.7158	2.4567	-1.5227	-3.0813
3.2	-0.7073	2.4195	-1.4479	-3.0935
3.3	-0.6971	2.3796	-1.3615	-3.1094
3.4	-0.6855	2.3375	-1.2665	-3.1274
3.5	-0.6726	2.2934	-1.1658	-3.1455
3.6	-0.6588	2.2475	-1.0621	-3.1617
3.7	-0.6441	2.1999	-0.9577	-3.1746
3.8	-0.6288	2.1510	-0.8545	-3.1828
3.9	-0.6129	2.1010	-0.7542	-3.1854
4.0	-0.5965	2.0501	-0.6579	-3.1817
4.1	-0.5798	1.9985	-0.5665	-3.1715
4.2	-0.5629	1.9467	-0.4806	-3.1548
4.3	-0.5459	1.8947	-0.4005	-3.1318
4.4	-0.5288	1.8430	-0.3263	-3.1030
4.5	-0.5117	1.7916	-0.2580	-3.0687
4.6	-0.4947	1.7408	-0.1954	-3.0295
4.7	-0.4779	1.6907	-0.1383	-2.9862
4.8	-0.4614	1.6416	-0.0865	-2.9392
4.9	-0.4451	1.5934	-0.0395	-2.8893
5.0	-0.4292	1.5464	0.0029	-2.8368

Ring C

Top side

NICS@	isotropic	xx	yy	zz
0.0	1.9692	-7.7305	-8.9870	22.6252
0.1	1.9705	-7.9401	-8.4768	22.3285
0.2	1.8375	-8.0021	-7.8302	21.3447
0.3	1.5847	-7.9095	-7.0837	19.7472
0.4	1.2373	-7.6622	-6.2756	17.6497
0.5	0.8279	-7.2691	-5.4430	15.1957
0.6	0.3920	-6.7491	-4.6193	12.5444
0.7	-0.0359	-6.1296	-3.8313	9.8532
0.8	-0.4265	-5.4428	-3.0981	7.2615
0.9	-0.7583	-4.7214	-2.4314	4.8779
1.0	-1.0189	-3.9955	-1.8359	**2.7746**
1.1	-1.2049	-3.2903	-1.3122	0.9878
1.2	-1.3199	-2.6250	-0.8576	-0.4769
1.3	-1.3727	-2.0133	-0.4686	-1.6362
1.4	-1.3751	-1.4635	-0.1406	-2.5212
1.5	-1.3396	-0.9799	0.1307	-3.1697
1.6	-1.2781	-0.5633	0.3500	-3.6211
1.7	-1.2010	-0.2121	0.5223	-3.9131
1.8	-1.1163	0.0778	0.6525	-4.0792
1.9	-1.0303	0.3113	0.7462	-4.1485
2.0	-0.9472	0.4948	0.8088	-4.1451
2.1	-0.8694	0.6348	0.8458	-4.0889
2.2	-0.7984	0.7380	0.8626	-3.9958
2.3	-0.7346	0.8109	0.8640	-3.8786
2.4	-0.6778	0.8594	0.8543	-3.7472
2.5	-0.6277	0.8888	0.8372	-3.6092
2.6	-0.5836	0.9036	0.8159	-3.4703
2.7	-0.5449	0.9076	0.7926	-3.3347
2.8	-0.5109	0.9037	0.7691	-3.2055
2.9	-0.4811	0.8944	0.7469	-3.0844
3.0	-0.4549	0.8814	0.7267	-2.9728
3.1	-0.4320	0.8662	0.7091	-2.8711
3.2	-0.4118	0.8496	0.6943	-2.7793
3.3	-0.3941	0.8325	0.6823	-2.6972
3.4	-0.3785	0.8154	0.6732	-2.6241
3.5	-0.3648	0.7984	0.6666	-2.5594
3.6	-0.3527	0.7819	0.6623	-2.5023
3.7	-0.3420	0.7660	0.6600	-2.4519
3.8	-0.3324	0.7507	0.6594	-2.4073
3.9	-0.3238	0.7361	0.6602	-2.3676
4.0	-0.3160	0.7221	0.6620	-2.3322
4.1	-0.3090	0.7086	0.6647	-2.3003
4.2	-0.3025	0.6957	0.6679	-2.2711
4.3	-0.2964	0.6834	0.6714	-2.2441
4.4	-0.2908	0.6715	0.6751	-2.2189
4.5	-0.2854	0.6600	0.6787	-2.1948
4.6	-0.2803	0.6488	0.6821	-2.1717
4.7	-0.2753	0.6380	0.6851	-2.1491
4.8	-0.2705	0.6275	0.6878	-2.1267
4.9	-0.2657	0.6173	0.6900	-2.1045
5.0	-0.2611	0.6073	0.6916	-2.0821

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	1.9516	-9.6280	-7.1317	22.6146
0.1	1.8159	-9.8013	-6.9456	22.1945
0.2	1.5543	-9.7817	-6.6372	21.0818
0.3	1.1895	-9.5722	-6.2083	19.3489
0.4	0.7529	-9.1898	-5.6649	17.1134
0.5	0.2811	-8.6637	-5.0205	14.5275
0.6	-0.1893	-8.0317	-4.2971	11.7609
0.7	-0.6255	-7.3347	-3.5226	8.9808
0.8	-1.0021	-6.6119	-2.7271	6.3328
0.9	-1.3028	-5.8969	-1.9394	3.9278
1.0	-1.5212	-5.2160	-1.1835	**1.8360**
1.1	-1.6590	-4.5878	-0.4779	0.0886
1.2	-1.7246	-4.0236	0.1651	-1.3151
1.3	-1.7299	-3.5293	0.7382	-2.3986
1.4	-1.6890	-3.1064	1.2385	-3.1989
1.5	-1.6153	-2.7533	1.6663	-3.7588
1.6	-1.5210	-2.4662	2.0246	-4.1215
1.7	-1.4163	-2.2397	2.3178	-4.3271
1.8	-1.3089	-2.0673	2.5516	-4.4109
1.9	-1.2041	-1.9418	2.7325	-4.4030
2.0	-1.1055	-1.8557	2.8672	-4.3281
2.1	-1.0151	-1.8016	2.9624	-4.2062
2.2	-0.9337	-1.7720	3.0244	-4.0535
2.3	-0.8613	-1.7603	3.0591	-3.8828
2.4	-0.7975	-1.7604	3.0718	-3.7039
2.5	-0.7415	-1.7668	3.0667	-3.5245
2.6	-0.6927	-1.7751	3.0477	-3.3506
2.7	-0.6501	-1.7817	3.0178	-3.1864
2.8	-0.6130	-1.7837	2.9795	-3.0349
2.9	-0.5808	-1.7790	2.9347	-2.8980
3.0	-0.5527	-1.7662	2.8849	-2.7770
3.1	-0.5283	-1.7444	2.8313	-2.6720
3.2	-0.5071	-1.7133	2.7749	-2.5828
3.3	-0.4886	-1.6731	2.7162	-2.5087
3.4	-0.4723	-1.6242	2.6558	-2.4486
3.5	-0.4581	-1.5673	2.5943	-2.4012
3.6	-0.4454	-1.5033	2.5319	-2.3648
3.7	-0.4341	-1.4332	2.4689	-2.3380
3.8	-0.4238	-1.3582	2.4057	-2.3190
3.9	-0.4144	-1.2795	2.3424	-2.3062
4.0	-0.4057	-1.1980	2.2792	-2.2983
4.1	-0.3974	-1.1148	2.2164	-2.2937
4.2	-0.3894	-1.0309	2.1540	-2.2914
4.3	-0.3817	-0.9472	2.0923	-2.2902
4.4	-0.3741	-0.8643	2.0313	-2.2892
4.5	-0.3665	-0.7830	1.9713	-2.2878
4.6	-0.3589	-0.7037	1.9123	-2.2853
4.7	-0.3513	-0.6270	1.8544	-2.2813
4.8	-0.3436	-0.5532	1.7977	-2.2755
4.9	-0.3359	-0.4824	1.7423	-2.2676
5.0	-0.3281	-0.4151	1.6883	-2.2575

Ring D

Top side

NICS@	isotropic	xx	yy	zz
0.0	9.6416	-10.6739	-9.9549	49.5535
0.1	9.6014	-11.1075	-9.3655	49.2771
0.2	9.4735	-11.3484	-8.6327	48.4018
0.3	9.2392	-11.3739	-7.7542	46.8458
0.4	8.8786	-11.1658	-6.7390	44.5405
0.5	8.3817	-10.7249	-5.6189	41.4890
0.6	7.7565	-10.0775	-4.4466	37.7936
0.7	7.0296	-9.2721	-3.2840	33.6449
0.8	6.2413	-8.3693	-2.1878	29.2812
0.9	5.4371	-7.4296	-1.1993	24.9403
1.0	4.6588	-6.5044	-0.3410	**20.8218**
1.1	3.9383	-5.6320	0.3813	17.0657
1.2	3.2952	-4.8375	0.9727	13.7503
1.3	2.7371	-4.1345	1.4449	10.9009
1.4	2.2626	-3.5280	1.8111	8.5047
1.5	1.8642	-3.0172	2.0850	6.5248
1.6	1.5316	-2.5972	2.2791	4.9128
1.7	1.2536	-2.2607	2.4051	3.6165
1.8	1.0201	-1.9984	2.4737	2.5852
1.9	0.8224	-1.8000	2.4950	1.7723
2.0	0.6536	-1.6547	2.4788	1.1366
2.1	0.5082	-1.5514	2.4340	0.6418
2.2	0.3823	-1.4793	2.3690	0.2570
2.3	0.2729	-1.4284	2.2912	-0.0442
2.4	0.1777	-1.3900	2.2069	-0.2838
2.5	0.0950	-1.3565	2.1212	-0.4798
2.6	0.0231	-1.3222	2.0382	-0.6466
2.7	-0.0391	-1.2827	1.9606	-0.7952
2.8	-0.0929	-1.2354	1.8902	-0.9335
2.9	-0.1393	-1.1789	1.8276	-1.0667
3.0	-0.1792	-1.1130	1.7731	-1.1978
3.1	-0.2134	-1.0384	1.7261	-1.3280
3.2	-0.2426	-0.9565	1.6857	-1.4572
3.3	-0.2674	-0.8689	1.6509	-1.5843
3.4	-0.2883	-0.7776	1.6204	-1.7078
3.5	-0.3058	-0.6845	1.5932	-1.8260
3.6	-0.3201	-0.5913	1.5681	-1.9370
3.7	-0.3316	-0.4997	1.5443	-2.0395
3.8	-0.3406	-0.4108	1.5211	-2.1322
3.9	-0.3474	-0.3257	1.4979	-2.2144
4.0	-0.3521	-0.2452	1.4743	-2.2856
4.1	-0.3551	-0.1698	1.4501	-2.3456
4.2	-0.3564	-0.0997	1.4251	-2.3947
4.3	-0.3563	-0.0350	1.3993	-2.4332
4.4	-0.3550	0.0241	1.3727	-2.4618
4.5	-0.3525	0.0780	1.3455	-2.4811
4.6	-0.3491	0.1268	1.3178	-2.4919
4.7	-0.3449	0.1708	1.2896	-2.4951
4.8	-0.3400	0.2103	1.2611	-2.4914
4.9	-0.3345	0.2455	1.2324	-2.4816
5.0	-0.3286	0.2769	1.2038	-2.4666

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	9.6549	-9.3352	-11.2434	49.5432
0.1	9.6150	-9.6089	-10.8079	49.2617
0.2	9.4872	-9.7425	-10.1757	48.3797
0.3	9.2522	-9.6999	-9.3600	46.8166
0.4	8.8898	-9.4462	-8.3894	44.5051
0.5	8.3899	-8.9671	-7.3117	41.4486
0.6	7.7606	-8.2791	-6.1894	37.7504
0.7	7.0290	-7.4267	-5.0871	33.6007
0.8	6.2360	-6.4701	-4.0599	29.2379
0.9	5.4277	-5.4712	-3.1453	24.8997
1.0	4.6464	-4.4833	-2.3625	**20.7849**
1.1	3.9242	-3.5458	-1.7152	17.0335
1.2	3.2806	-2.6842	-1.1970	13.7230
1.3	2.7232	-1.9126	-0.7965	10.8787
1.4	2.2502	-1.2362	-0.5004	8.4872
1.5	1.8539	-0.6548	-0.2952	6.5116
1.6	1.5236	-0.1643	-0.1682	4.9032
1.7	1.2481	0.2416	-0.1072	3.6098
1.8	1.0170	0.5707	-0.1004	2.5807
1.9	0.8215	0.8316	-0.1364	1.7693
2.0	0.6546	1.0334	-0.2042	1.1344
2.1	0.5108	1.1854	-0.2929	0.6400
2.2	0.3863	1.2963	-0.3924	0.2551
2.3	0.2781	1.3744	-0.4938	-0.0464
2.4	0.1838	1.4268	-0.5890	-0.2864
2.5	0.1017	1.4597	-0.6717	-0.4829
2.6	0.0303	1.4782	-0.7372	-0.6501
2.7	-0.0317	1.4863	-0.7823	-0.7989
2.8	-0.0853	1.4868	-0.8055	-0.9373
2.9	-0.1317	1.4819	-0.8066	-1.0703
3.0	-0.1716	1.4730	-0.7868	-1.2010
3.1	-0.2059	1.4611	-0.7481	-1.3307
3.2	-0.2353	1.4466	-0.6930	-1.4593
3.3	-0.2602	1.4298	-0.6248	-1.5857
3.4	-0.2813	1.4111	-0.5465	-1.7084
3.5	-0.2989	1.3903	-0.4613	-1.8258
3.6	-0.3134	1.3678	-0.3720	-1.9361
3.7	-0.3251	1.3435	-0.2811	-2.0379
3.8	-0.3344	1.3177	-0.1909	-2.1300
3.9	-0.3414	1.2905	-0.1030	-2.2117
4.0	-0.3463	1.2622	-0.0188	-2.2824
4.1	-0.3495	1.2330	0.0607	-2.3421
4.2	-0.3510	1.2030	0.1349	-2.3909
4.3	-0.3511	1.1727	0.2033	-2.4293
4.4	-0.3499	1.1421	0.2658	-2.4578
4.5	-0.3477	1.1116	0.3224	-2.4771
4.6	-0.3445	1.0813	0.3733	-2.4880
4.7	-0.3405	1.0513	0.4186	-2.4912
4.8	-0.3357	1.0219	0.4586	-2.4877
4.9	-0.3305	0.9930	0.4936	-2.4780
5.0	-0.3247	0.9649	0.5241	-2.4631

Ring E

Top side

NICS@	isotropic	xx	yy	zz
0.0	1.9517	-7.6649	-9.0969	22.6169
0.1	1.8169	-7.8105	-8.9354	22.1968
0.2	1.5568	-7.8017	-8.6125	21.0845
0.3	1.1936	-7.6264	-8.1453	19.3524
0.4	0.7587	-7.2819	-7.5599	17.1178
0.5	0.2883	-6.7786	-6.8893	14.5329
0.6	-0.1809	-6.1405	-6.1695	11.7673
0.7	-0.6163	-5.4014	-5.4356	8.9882
0.8	-0.9923	-4.6006	-4.7177	6.3413
0.9	-1.2929	-3.7768	-4.0391	3.9373
1.0	-1.5112	-2.9644	-3.4157	**1.8464**
1.1	-1.6492	-2.1906	-2.8570	0.0998
1.2	-1.7151	-1.4749	-2.3669	-1.3033
1.3	-1.7208	-0.8300	-1.9460	-2.3864
1.4	-1.6803	-0.2622	-1.5920	-3.1865
1.5	-1.6070	0.2267	-1.3013	-3.7464
1.6	-1.5132	0.6384	-1.0689	-4.1092
1.7	-1.4089	0.9774	-0.8891	-4.3150
1.8	-1.3018	1.2495	-0.7558	-4.3992
1.9	-1.1973	1.4618	-0.6623	-4.3915
2.0	-1.0991	1.6219	-0.6022	-4.3169
2.1	-1.0089	1.7375	-0.5689	-4.1953
2.2	-0.9277	1.8160	-0.5561	-4.0429
2.3	-0.8555	1.8642	-0.5583	-3.8723
2.4	-0.7918	1.8885	-0.5703	-3.6936
2.5	-0.7359	1.8943	-0.5878	-3.5144
2.6	-0.6872	1.8861	-0.6072	-3.3405
2.7	-0.6447	1.8679	-0.6255	-3.1764
2.8	-0.6077	1.8425	-0.6406	-3.0249
2.9	-0.5755	1.8126	-0.6509	-2.8881
3.0	-0.5475	1.7799	-0.6552	-2.7671
3.1	-0.5231	1.7458	-0.6529	-2.6622
3.2	-0.5019	1.7113	-0.6439	-2.5731
3.3	-0.4834	1.6772	-0.6281	-2.4992
3.4	-0.4672	1.6439	-0.6061	-2.4393
3.5	-0.4529	1.6115	-0.5782	-2.3920
3.6	-0.4402	1.5803	-0.5452	-2.3559
3.7	-0.4289	1.5503	-0.5078	-2.3292
3.8	-0.4187	1.5213	-0.4668	-2.3105
3.9	-0.4092	1.4933	-0.4230	-2.2980
4.0	-0.4005	1.4662	-0.3772	-2.2904
4.1	-0.3922	1.4398	-0.3301	-2.2861
4.2	-0.3842	1.4139	-0.2824	-2.2841
4.3	-0.3764	1.3885	-0.2346	-2.2832
4.4	-0.3688	1.3635	-0.1873	-2.2825
4.5	-0.3612	1.3388	-0.1410	-2.2814
4.6	-0.3536	1.3143	-0.0959	-2.2792
4.7	-0.3460	1.2900	-0.0524	-2.2754
4.8	-0.3383	1.2658	-0.0108	-2.2698
4.9	-0.3305	1.2418	0.0288	-2.2621
5.0	-0.3227	1.2180	0.0663	-2.2522

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	1.9633	-9.6186	-7.1255	22.6339
0.1	1.9623	-9.2744	-7.1767	22.3381
0.2	1.8268	-8.7707	-7.1030	21.3541
0.3	1.5715	-8.1394	-6.9017	19.7556
0.4	1.2218	-7.4180	-6.5729	17.6563
0.5	0.8104	-6.6457	-6.1230	15.2000
0.6	0.3731	-5.8595	-5.5672	12.5461
0.7	-0.0556	-5.0906	-4.9285	9.8523
0.8	-0.4465	-4.3624	-4.2350	7.2580
0.9	-0.7781	-3.6900	-3.5163	4.8721
1.0	-1.0382	-3.0816	-2.7997	**2.7667**
1.1	-1.2235	-2.5398	-2.1085	0.9780
1.2	-1.3376	-2.0640	-1.4605	-0.4884
1.3	-1.3897	-1.6515	-0.8684	-1.6492
1.4	-1.3914	-1.2988	-0.3400	-2.5356
1.5	-1.3554	-1.0018	0.1209	-3.1853
1.6	-1.2935	-0.7564	0.5139	-3.6380
1.7	-1.2160	-0.5578	0.8409	-3.9312
1.8	-1.1312	-0.4010	1.1059	-4.0984
1.9	-1.0451	-0.2809	1.3143	-4.1687
2.0	-0.9619	-0.1918	1.4723	-4.1662
2.1	-0.8842	-0.1283	1.5867	-4.1109
2.2	-0.8132	-0.0852	1.6642	-4.0185
2.3	-0.7494	-0.0576	1.7114	-3.9019
2.4	-0.6927	-0.0410	1.7341	-3.7710
2.5	-0.6425	-0.0319	1.7376	-3.6333
2.6	-0.5984	-0.0272	1.7265	-3.4946
2.7	-0.5597	-0.0244	1.7045	-3.3592
2.8	-0.5256	-0.0217	1.6747	-3.2299
2.9	-0.4958	-0.0178	1.6394	-3.1088
3.0	-0.4695	-0.0120	1.6004	-2.9970
3.1	-0.4464	-0.0037	1.5593	-2.8949
3.2	-0.4262	0.0072	1.5170	-2.8027
3.3	-0.4083	0.0208	1.4744	-2.7201
3.4	-0.3926	0.0370	1.4319	-2.6466
3.5	-0.3787	0.0553	1.3900	-2.5813
3.6	-0.3663	0.0756	1.3490	-2.5236
3.7	-0.3554	0.0974	1.3090	-2.4725
3.8	-0.3456	0.1204	1.2701	-2.4273
3.9	-0.3368	0.1442	1.2325	-2.3870
4.0	-0.3288	0.1684	1.1962	-2.3509
4.1	-0.3215	0.1927	1.1612	-2.3183
4.2	-0.3147	0.2168	1.1275	-2.2885
4.3	-0.3085	0.2405	1.0950	-2.2609
4.4	-0.3025	0.2635	1.0639	-2.2350
4.5	-0.2969	0.2857	1.0339	-2.2104
4.6	-0.2916	0.3069	1.0051	-2.1866
4.7	-0.2863	0.3270	0.9774	-2.1634
4.8	-0.2813	0.3458	0.9509	-2.1406
4.9	-0.2763	0.3635	0.9254	-2.1178
5.0	-0.2714	0.3798	0.9009	-2.0949

Ring F

Top side

NICS@	isotropic	xx	yy	zz
0.0	7.2882	-10.4238	-9.4137	41.7020
0.1	7.2323	-10.5717	-9.1859	41.4545
0.2	7.0532	-10.5884	-8.7183	40.4664
0.3	6.7451	-10.4261	-8.0440	38.7055
0.4	6.3075	-10.0433	-7.2115	36.1773
0.5	5.7502	-9.4266	-6.2807	32.9580
0.6	5.0961	-8.6001	-5.3155	29.2040
0.7	4.3794	-7.6184	-4.3739	25.1305
0.8	3.6406	-6.5520	-3.4999	20.9736
0.9	2.9199	-5.4700	-2.7202	16.9500
1.0	2.2511	-4.4295	-2.0456	**13.2285**
1.1	1.6573	-3.4706	-1.4752	9.9176
1.2	1.1500	-2.6167	-1.0011	7.0678
1.3	0.7307	-1.8783	-0.6130	4.6834
1.4	0.3933	-1.2561	-0.3002	2.7364
1.5	0.1275	-0.7453	-0.0533	1.1811
1.6	-0.0790	-0.3373	0.1361	-0.0359
1.7	-0.2381	-0.0214	0.2757	-0.9685
1.8	-0.3602	0.2139	0.3723	-1.6670
1.9	-0.4542	0.3808	0.4328	-2.1763
2.0	-0.5268	0.4916	0.4638	-2.5358
2.1	-0.5829	0.5582	0.4719	-2.7789
2.2	-0.6263	0.5918	0.4632	-2.9339
2.3	-0.6595	0.6026	0.4436	-3.0247
2.4	-0.6843	0.5997	0.4181	-3.0707
2.5	-0.7022	0.5904	0.3910	-3.0879
2.6	-0.7142	0.5805	0.3654	-3.0886
2.7	-0.7213	0.5744	0.3438	-3.0820
2.8	-0.7241	0.5748	0.3276	-3.0747
2.9	-0.7234	0.5831	0.3174	-3.0706
3.0	-0.7197	0.5998	0.3132	-3.0719
3.1	-0.7134	0.6243	0.3145	-3.0791
3.2	-0.7051	0.6556	0.3206	-3.0915
3.3	-0.6951	0.6922	0.3303	-3.1078
3.4	-0.6836	0.7326	0.3427	-3.1260
3.5	-0.6708	0.7750	0.3568	-3.1443
3.6	-0.6571	0.8179	0.3715	-3.1608
3.7	-0.6425	0.8601	0.3862	-3.1738
3.8	-0.6272	0.9003	0.4001	-3.1821
3.9	-0.6114	0.9377	0.4130	-3.1848
4.0	-0.5951	0.9716	0.4244	-3.1812
4.1	-0.5784	1.0016	0.4343	-3.1711
4.2	-0.5615	1.0274	0.4425	-3.1545
4.3	-0.5445	1.0490	0.4490	-3.1315
4.4	-0.5274	1.0665	0.4541	-3.1026
4.5	-0.5103	1.0798	0.4576	-3.0684
4.6	-0.4933	1.0893	0.4600	-3.0292
4.7	-0.4765	1.0952	0.4611	-2.9859
4.8	-0.4599	1.0978	0.4613	-2.9389
4.9	-0.4436	1.0973	0.4607	-2.8890
5.0	-0.4277	1.0942	0.4593	-2.8366

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	7.3104	-8.4662	-11.3225	41.7199
0.1	7.2481	-8.2720	-11.2387	41.2549
0.2	7.0709	-7.8809	-10.9920	40.0855
0.3	6.7790	-7.2973	-10.5743	38.2087
0.4	6.3744	-6.5367	-9.9845	35.6443
0.5	5.8658	-5.6306	-9.2397	32.4677
0.6	5.2723	-4.6265	-8.3785	28.8218
0.7	4.6229	-3.5791	-7.4541	24.9019
0.8	3.9531	-2.5411	-6.5230	20.9234
0.9	3.2986	-1.5549	-5.6347	17.0853
1.0	2.6899	-0.6487	-4.8253	**13.5438**
1.1	2.1483	0.1621	-4.1170	10.3998
1.2	1.6845	0.8726	-3.5198	7.7009
1.3	1.2999	1.4840	-3.0350	5.4508
1.4	0.9889	2.0014	-2.6579	3.6231
1.5	0.7417	2.4318	-2.3805	2.1738
1.6	0.5471	2.7825	-2.1925	1.0513
1.7	0.3940	3.0614	-2.0824	0.2031
1.8	0.2729	3.2766	-2.0378	-0.4202
1.9	0.1757	3.4362	-2.0458	-0.8632
2.0	0.0967	3.5483	-2.0932	-1.1651
2.1	0.0314	3.6208	-2.1670	-1.3596
2.2	-0.0231	3.6611	-2.2551	-1.4754
2.3	-0.0689	3.6760	-2.3463	-1.5365
2.4	-0.1075	3.6714	-2.4310	-1.5628
2.5	-0.1398	3.6521	-2.5014	-1.5703
2.6	-0.1669	3.6222	-2.5516	-1.5712
2.7	-0.1893	3.5845	-2.5779	-1.5745
2.8	-0.2078	3.5411	-2.5784	-1.5862
2.9	-0.2230	3.4935	-2.5529	-1.6096
3.0	-0.2354	3.4425	-2.5027	-1.6460
3.1	-0.2455	3.3885	-2.4302	-1.6949
3.2	-0.2537	3.3319	-2.3384	-1.7545
3.3	-0.2602	3.2725	-2.2309	-1.8223
3.4	-0.2654	3.2106	-2.1113	-1.8955
3.5	-0.2694	3.1462	-1.9833	-1.9712
3.6	-0.2724	3.0794	-1.8502	-2.0465
3.7	-0.2745	3.0103	-1.7149	-2.1190
3.8	-0.2758	2.9393	-1.5798	-2.1868
3.9	-0.2762	2.8667	-1.4471	-2.2483
4.0	-0.2760	2.7928	-1.3182	-2.3025
4.1	-0.2750	2.7181	-1.1944	-2.3488
4.2	-0.2735	2.6429	-1.0765	-2.3869
4.3	-0.2714	2.5677	-0.9650	-2.4167
4.4	-0.2687	2.4928	-0.8602	-2.4387
4.5	-0.2656	2.4185	-0.7622	-2.4531
4.6	-0.2621	2.3451	-0.6709	-2.4604
4.7	-0.2582	2.2729	-0.5861	-2.4614
4.8	-0.2540	2.2021	-0.5076	-2.4565
4.9	-0.2496	2.1328	-0.4352	-2.4463
5.0	-0.2449	2.0652	-0.3684	-2.4316

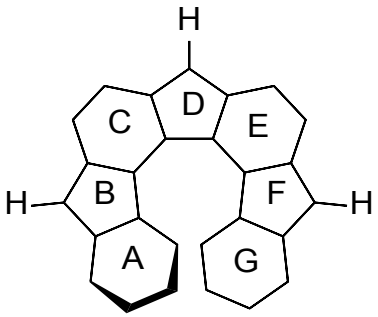
Ring G

Top side

NICS@	isotropic	xx	yy	zz
0.0	-4.3184	-7.0136	-7.0594	1.1177
0.1	-4.4792	-7.0843	-6.9043	0.5511
0.2	-4.8119	-7.0004	-6.5977	-0.8377
0.3	-5.2709	-6.7689	-6.1590	-2.8849
0.4	-5.7929	-6.4054	-5.6157	-5.3575
0.5	-6.3100	-5.9336	-4.9998	-7.9965
0.6	-6.7615	-5.3822	-4.3440	-10.5582
0.7	-7.1020	-4.7820	-3.6774	-12.8465
0.8	-7.3049	-4.1621	-3.0237	-14.7288
0.9	-7.3622	-3.5477	-2.4000	-16.1389
1.0	-7.2811	-2.9584	-1.8176	**-17.0674**
1.1	-7.0796	-2.4085	-1.2829	-17.5473
1.2	-6.7815	-1.9075	-0.7993	-17.6378
1.3	-6.4130	-1.4608	-0.3678	-17.4103
1.4	-5.9990	-1.0709	0.0116	-16.9379
1.5	-5.5618	-0.7378	0.3403	-16.2879
1.6	-5.1195	-0.4600	0.6202	-15.5188
1.7	-4.6864	-0.2343	0.8538	-14.6787
1.8	-4.2726	-0.0568	1.0444	-13.8054
1.9	-3.8848	0.0776	1.1956	-12.9276
2.0	-3.5269	0.1741	1.3116	-12.0665
2.1	-3.2005	0.2386	1.3966	-11.2366
2.2	-2.9054	0.2767	1.4549	-10.4478
2.3	-2.6404	0.2940	1.4908	-9.7061
2.4	-2.4037	0.2956	1.5080	-9.0146
2.5	-2.1927	0.2860	1.5103	-8.3744
2.6	-2.0051	0.2692	1.5007	-7.7851
2.7	-1.8383	0.2484	1.4818	-7.2452
2.8	-1.6900	0.2264	1.4560	-6.7525
2.9	-1.5580	0.2051	1.4250	-6.3043
3.0	-1.4404	0.1861	1.3904	-5.8977
3.1	-1.3353	0.1703	1.3533	-5.5296
3.2	-1.2413	0.1583	1.3146	-5.1968
3.3	-1.1569	0.1505	1.2751	-4.8964
3.4	-1.0811	0.1468	1.2352	-4.6252
3.5	-1.0126	0.1471	1.1955	-4.3804
3.6	-0.9507	0.1511	1.1561	-4.1592
3.7	-0.8945	0.1584	1.1173	-3.9592
3.8	-0.8433	0.1686	1.0793	-3.7779
3.9	-0.7966	0.1812	1.0423	-3.6133
4.0	-0.7538	0.1958	1.0062	-3.4634
4.1	-0.7145	0.2118	0.9712	-3.3264
4.2	-0.6782	0.2289	0.9373	-3.2007
4.3	-0.6446	0.2468	0.9045	-3.0850
4.4	-0.6134	0.2649	0.8729	-2.9781
4.5	-0.5844	0.2831	0.8425	-2.8788
4.6	-0.5574	0.3010	0.8132	-2.7863
4.7	-0.5320	0.3186	0.7851	-2.6997
4.8	-0.5082	0.3355	0.7581	-2.6183
4.9	-0.4859	0.3516	0.7322	-2.5415
5.0	-0.4648	0.3668	0.7075	-2.4689

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	-4.3364	-6.6192	-7.4929	1.1027
0.1	-4.3643	-6.5992	-7.2823	0.7886
0.2	-4.5690	-6.4267	-6.9217	-0.3585
0.3	-4.9098	-6.1093	-6.4347	-2.1853
0.4	-5.3278	-5.6628	-5.8528	-4.4676
0.5	-5.7582	-5.1108	-5.2115	-6.9522
0.6	-6.1420	-4.4820	-4.5458	-9.3982
0.7	-6.4339	-3.8072	-3.8866	-11.6080
0.8	-6.6061	-3.1161	-3.2578	-13.4446
0.9	-6.6482	-2.4344	-2.6758	-14.8345
1.0	-6.5644	-1.7826	-2.1502	**-15.7603**
1.1	-6.3693	-1.1757	-1.6855	-16.2468
1.2	-6.0840	-0.6234	-1.2826	-16.3459
1.3	-5.7317	-0.1310	-0.9406	-16.1235
1.4	-5.3354	0.2994	-0.6573	-15.6485
1.5	-4.9157	0.6687	-0.4298	-14.9861
1.6	-4.4898	0.9797	-0.2549	-14.1942
1.7	-4.0709	1.2368	-0.1284	-13.3211
1.8	-3.6689	1.4455	-0.0461	-12.4060
1.9	-3.2901	1.6122	-0.0031	-11.4793
2.0	-2.9383	1.7434	0.0058	-10.5642
2.1	-2.6152	1.8460	-0.0142	-9.6774
2.2	-2.3208	1.9263	-0.0580	-8.8307
2.3	-2.0542	1.9900	-0.1207	-8.0318
2.4	-1.8137	2.0421	-0.1979	-7.2852
2.5	-1.5974	2.0866	-0.2857	-6.5930
2.6	-1.4032	2.1265	-0.3808	-5.9553
2.7	-1.2291	2.1639	-0.4803	-5.3709
2.8	-1.0733	2.1999	-0.5820	-4.8377
2.9	-0.9339	2.2351	-0.6838	-4.3529
3.0	-0.8093	2.2694	-0.7840	-3.9134
3.1	-0.6983	2.3024	-0.8809	-3.5164
3.2	-0.5995	2.3335	-0.9729	-3.1590
3.3	-0.5117	2.3619	-1.0582	-2.8388
3.4	-0.4340	2.3869	-1.1350	-2.5538
3.5	-0.3653	2.4078	-1.2013	-2.3025
3.6	-0.3049	2.4242	-1.2552	-2.0837
3.7	-0.2518	2.4357	-1.2948	-1.8964
3.8	-0.2055	2.4421	-1.3188	-1.7396
3.9	-0.1651	2.4431	-1.3260	-1.6125
4.0	-0.1303	2.4388	-1.3161	-1.5136
4.1	-0.1003	2.4292	-1.2892	-1.4411
4.2	-0.0749	2.4145	-1.2464	-1.3928
4.3	-0.0536	2.3946	-1.1894	-1.3660
4.4	-0.0361	2.3698	-1.1203	-1.3577
4.5	-0.0219	2.3403	-1.0417	-1.3644
4.6	-0.0109	2.3064	-0.9563	-1.3828
4.7	-0.0027	2.2684	-0.8669	-1.4097
4.8	0.0029	2.2267	-0.7759	-1.4420
4.9	0.0064	2.1817	-0.6855	-1.4770
5.0	0.0080	2.1340	-0.5976	-1.5125



Ring A

Top side

NICS@	isotropic	xx	yy	zz
0.0	-4.3805	-7.7650	-6.7445	1.3680
0.1	-4.4052	-7.7509	-6.5349	1.0702
0.2	-4.6021	-7.5838	-6.1738	-0.0488
0.3	-4.9317	-7.2695	-5.6837	-1.8418
0.4	-5.3368	-6.8225	-5.0954	-4.0926
0.5	-5.7548	-6.2653	-4.4439	-6.5552
0.6	-6.1283	-5.6264	-3.7644	-8.9940
0.7	-6.4133	-4.9374	-3.0885	-11.2140
0.8	-6.5826	-4.2287	-2.4410	-13.0779
0.9	-6.6258	-3.5276	-1.8396	-14.5100
1.0	-6.5466	-2.8556	-1.2948	**-15.4894**
1.1	-6.3592	-2.2287	-0.8118	-16.0370
1.2	-6.0836	-1.6573	-0.3923	-16.2012
1.3	-5.7424	-1.1470	-0.0356	-16.0445
1.4	-5.3578	-0.7000	0.2600	-15.6336
1.5	-4.9499	-0.3154	0.4973	-15.0317
1.6	-4.5353	0.0098	0.6795	-14.2952
1.7	-4.1271	0.2802	0.8104	-13.4719
1.8	-3.7347	0.5017	0.8943	-12.6001
1.9	-3.3645	0.6808	0.9361	-11.7103
2.0	-3.0200	0.8245	0.9407	-10.8254
2.1	-2.7030	0.9398	0.9134	-9.9624
2.2	-2.4136	1.0332	0.8593	-9.1332
2.3	-2.1507	1.1107	0.7832	-8.3459
2.4	-1.9128	1.1773	0.6896	-7.6052
2.5	-1.6981	1.2373	0.5823	-6.9138
2.6	-1.5046	1.2935	0.4647	-6.2720
2.7	-1.3304	1.3481	0.3397	-5.6790
2.8	-1.1737	1.4023	0.2096	-5.1331
2.9	-1.0330	1.4563	0.0766	-4.6317
3.0	-0.9066	1.5100	-0.0576	-4.1723
3.1	-0.7934	1.5628	-0.1909	-3.7520
3.2	-0.6921	1.6139	-0.3216	-3.3685
3.3	-0.6017	1.6622	-0.4475	-3.0199
3.4	-0.5212	1.7071	-0.5662	-2.7046
3.5	-0.4497	1.7476	-0.6750	-2.4217
3.6	-0.3863	1.7833	-0.7714	-2.1709
3.7	-0.3303	1.8137	-0.8526	-1.9519
3.8	-0.2808	1.8385	-0.9163	-1.7646
3.9	-0.2373	1.8576	-0.9606	-1.6089
4.0	-0.1991	1.8711	-0.9845	-1.4840
4.1	-0.1658	1.8789	-0.9876	-1.3886
4.2	-0.1369	1.8811	-0.9709	-1.3208
4.3	-0.1120	1.8778	-0.9360	-1.2779
4.4	-0.0910	1.8690	-0.8854	-1.2567
4.5	-0.0736	1.8548	-0.8222	-1.2533
4.6	-0.0594	1.8356	-0.7497	-1.2640
4.7	-0.0483	1.8114	-0.6713	-1.2849
4.8	-0.0399	1.7827	-0.5900	-1.3125
4.9	-0.0341	1.7499	-0.5087	-1.3435
5.0	-0.0305	1.7134	-0.4295	-1.3753

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	-4.3606	-6.3852	-8.0828	1.3861
0.1	-4.5212	-6.4618	-7.9167	0.8147
0.2	-4.8496	-6.3842	-7.5989	-0.5655
0.3	-5.3015	-6.1592	-7.1493	-2.5958
0.4	-5.8158	-5.8015	-6.5957	-5.0503
0.5	-6.3269	-5.3336	-5.9703	-7.6769
0.6	-6.7756	-4.7832	-5.3058	-10.2376
0.7	-7.1172	-4.1803	-4.6319	-12.5395
0.8	-7.3255	-3.5534	-3.9723	-14.4507
0.9	-7.3917	-2.9275	-3.3440	-15.9036
1.0	-7.3222	-2.3224	-2.7578	**-16.8863**
1.1	-7.1339	-1.7526	-2.2199	-17.4291
1.2	-6.8496	-1.2279	-1.7327	-17.5881
1.3	-6.4946	-0.7543	-1.2972	-17.4323
1.4	-6.0932	-0.3346	-0.9125	-17.0324
1.5	-5.6671	0.0303	-0.5773	-16.4542
1.6	-5.2344	0.3413	-0.2895	-15.7549
1.7	-4.8091	0.6009	-0.0467	-14.9815
1.8	-4.4015	0.8122	0.1544	-14.1709
1.9	-4.0183	0.9793	0.3171	-13.3513
2.0	-3.6636	1.1069	0.4453	-12.5430
2.1	-3.3390	1.1999	0.5433	-11.7603
2.2	-3.0447	1.2633	0.6150	-11.0126
2.3	-2.7796	1.3020	0.6647	-10.3055
2.4	-2.5418	1.3204	0.6960	-9.6419
2.5	-2.3291	1.3226	0.7126	-9.0226
2.6	-2.1391	1.3123	0.7175	-8.4473
2.7	-1.9694	1.2926	0.7134	-7.9142
2.8	-1.8176	1.2659	0.7026	-7.4215
2.9	-1.6817	1.2344	0.6870	-6.9666
3.0	-1.5598	1.1996	0.6680	-6.5469
3.1	-1.4501	1.1629	0.6468	-6.1599
3.2	-1.3511	1.1252	0.6243	-5.8029
3.3	-1.2616	1.0872	0.6013	-5.4734
3.4	-1.1805	1.0494	0.5782	-5.1691
3.5	-1.1067	1.0123	0.5554	-4.8878
3.6	-1.0394	0.9761	0.5332	-4.6275
3.7	-0.9779	0.9410	0.5117	-4.3864
3.8	-0.9215	0.9070	0.4910	-4.1627
3.9	-0.8698	0.8743	0.4713	-3.9549
4.0	-0.8221	0.8428	0.4525	-3.7616
4.1	-0.7781	0.8126	0.4347	-3.5816
4.2	-0.7374	0.7837	0.4178	-3.4137
4.3	-0.6997	0.7560	0.4018	-3.2569
4.4	-0.6647	0.7294	0.3866	-3.1102
4.5	-0.6322	0.7040	0.3723	-2.9729
4.6	-0.6019	0.6797	0.3588	-2.8441
4.7	-0.5736	0.6565	0.3460	-2.7233
4.8	-0.5471	0.6343	0.3339	-2.6096
4.9	-0.5224	0.6130	0.3225	-2.5027
5.0	-0.4992	0.5926	0.3116	-2.4019

Ring B

Top side

NICS@	isotropic	xx	yy	zz
0.0	7.0641	-11.0725	-11.4745	43.7392
0.1	6.9956	-11.1760	-11.0866	43.2494
0.2	6.8190	-10.9556	-10.6238	42.0365
0.3	6.5316	-10.4391	-10.0641	40.0980
0.4	6.1311	-9.6797	-9.3802	37.4533
0.5	5.6225	-8.7485	-8.5610	34.1770
0.6	5.0220	-7.7225	-7.6232	30.4117
0.7	4.3579	-6.6728	-6.6070	26.3535
0.8	3.6664	-5.6555	-5.5643	22.2189
0.9	2.9853	-4.7080	-4.5453	18.2094
1.0	2.3481	-3.8501	-3.5896	**14.4839**
1.1	1.7786	-3.0881	-2.7226	11.1466
1.2	1.2901	-2.4199	-1.9576	8.2479
1.3	0.8856	-1.8393	-1.2982	5.7944
1.4	0.5606	-1.3387	-0.7419	3.7623
1.5	0.3057	-0.9104	-0.2827	2.1101
1.6	0.1095	-0.5472	0.0873	0.7885
1.7	-0.0393	-0.2425	0.3769	-0.2525
1.8	-0.1513	0.0102	0.5955	-1.0596
1.9	-0.2351	0.2169	0.7526	-1.6747
2.0	-0.2976	0.3836	0.8575	-2.1338
2.1	-0.3439	0.5164	0.9196	-2.4675
2.2	-0.3778	0.6207	0.9473	-2.7014
2.3	-0.4021	0.7018	0.9486	-2.8567
2.4	-0.4188	0.7643	0.9302	-2.9510
2.5	-0.4295	0.8122	0.8980	-2.9986
2.6	-0.4352	0.8488	0.8568	-3.0111
2.7	-0.4370	0.8768	0.8101	-2.9978
2.8	-0.4356	0.8983	0.7608	-2.9659
2.9	-0.4319	0.9146	0.7109	-2.9211
3.0	-0.4263	0.9270	0.6618	-2.8678
3.1	-0.4194	0.9363	0.6145	-2.8091
3.2	-0.4117	0.9428	0.5696	-2.7475
3.3	-0.4034	0.9471	0.5273	-2.6848
3.4	-0.3949	0.9493	0.4880	-2.6220
3.5	-0.3863	0.9497	0.4515	-2.5601
3.6	-0.3777	0.9484	0.4181	-2.4996
3.7	-0.3693	0.9454	0.3875	-2.4409
3.8	-0.3612	0.9410	0.3597	-2.3841
3.9	-0.3533	0.9351	0.3346	-2.3295
4.0	-0.3457	0.9280	0.3121	-2.2770
4.1	-0.3383	0.9196	0.2921	-2.2266
4.2	-0.3313	0.9101	0.2744	-2.1782
4.3	-0.3244	0.8996	0.2589	-2.1319
4.4	-0.3179	0.8882	0.2455	-2.0873
4.5	-0.3115	0.8760	0.2339	-2.0445
4.6	-0.3054	0.8631	0.2241	-2.0034
4.7	-0.2994	0.8495	0.2159	-1.9637
4.8	-0.2936	0.8353	0.2091	-1.9253
4.9	-0.2880	0.8206	0.2036	-1.8882
5.0	-0.2825	0.8056	0.1992	-1.8521

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	7.0636	-10.9201	-11.6039	43.7148
0.1	7.0230	-11.2493	-11.1598	43.4783
0.2	6.8644	-11.4645	-10.4189	42.4766
0.3	6.5776	-11.5061	-9.4362	40.6751
0.4	6.1568	-11.3201	-8.2869	38.0774
0.5	5.6073	-10.8818	-7.0564	34.7602
0.6	4.9493	-10.2061	-5.8275	30.8813
0.7	4.2166	-9.3415	-4.6681	26.6595
0.8	3.4520	-8.3547	-3.6238	22.3345
0.9	2.6992	-7.3137	-2.7162	18.1274
1.0	1.9956	-6.2765	-1.9475	**14.2108**
1.1	1.3682	-5.2851	-1.3071	10.6968
1.2	0.8313	-4.3665	-0.7787	7.6389
1.3	0.3880	-3.5352	-0.3446	5.0437
1.4	0.0332	-2.7968	0.0107	2.8858
1.5	-0.2433	-2.1511	0.2999	1.1213
1.6	-0.4540	-1.5944	0.5333	-0.3008
1.7	-0.6115	-1.1211	0.7188	-1.4321
1.8	-0.7272	-0.7242	0.8629	-2.3203
1.9	-0.8108	-0.3961	0.9711	-3.0073
2.0	-0.8699	-0.1288	1.0484	-3.5293
2.1	-0.9104	0.0859	1.0996	-3.9166
2.2	-0.9365	0.2557	1.1290	-4.1942
2.3	-0.9516	0.3881	1.1406	-4.3834
2.4	-0.9578	0.4899	1.1381	-4.5013
2.5	-0.9569	0.5669	1.1248	-4.5623
2.6	-0.9502	0.6243	1.1033	-4.5783
2.7	-0.9389	0.6662	1.0761	-4.5589
2.8	-0.9238	0.6960	1.0449	-4.5122
2.9	-0.9056	0.7164	1.0112	-4.4445
3.0	-0.8851	0.7296	0.9762	-4.3612
3.1	-0.8628	0.7370	0.9407	-4.2662
3.2	-0.8393	0.7401	0.9052	-4.1631
3.3	-0.8148	0.7396	0.8704	-4.0544
3.4	-0.7898	0.7363	0.8364	-3.9422
3.5	-0.7646	0.7308	0.8035	-3.8281
3.6	-0.7394	0.7235	0.7718	-3.7135
3.7	-0.7144	0.7148	0.7414	-3.5994
3.8	-0.6897	0.7049	0.7123	-3.4864
3.9	-0.6656	0.6941	0.6845	-3.3752
4.0	-0.6419	0.6825	0.6579	-3.2662
4.1	-0.6189	0.6703	0.6326	-3.1597
4.2	-0.5966	0.6577	0.6085	-3.0560
4.3	-0.5750	0.6447	0.5856	-2.9551
4.4	-0.5541	0.6314	0.5637	-2.8573
4.5	-0.5339	0.6180	0.5429	-2.7626
4.6	-0.5144	0.6045	0.5231	-2.6710
4.7	-0.4957	0.5910	0.5043	-2.5824
4.8	-0.4777	0.5775	0.4864	-2.4969
4.9	-0.4604	0.5640	0.4693	-2.4144
5.0	-0.4438	0.5506	0.4530	-2.3349

Ring C

Top side

NICS@	isotropic	xx	yy	zz
0.0	2.1323	-9.0627	-8.4551	23.9148
0.1	2.1256	-9.2748	-7.9540	23.6055
0.2	1.9919	-9.3429	-7.3186	22.6374
0.3	1.7449	-9.2567	-6.5831	21.0745
0.4	1.4072	-9.0119	-5.7831	19.0167
0.5	1.0084	-8.6142	-4.9534	16.5928
0.6	0.5811	-8.0807	-4.1258	13.9498
0.7	0.1573	-7.4386	-3.3269	11.2375
0.8	-0.2349	-6.7212	-2.5764	8.5929
0.9	-0.5747	-5.9635	-1.8872	6.1265
1.0	-0.8492	-5.1976	-1.2657	**3.9155**
1.1	-1.0539	-4.4506	-0.7137	2.0024
1.2	-1.1913	-3.7434	-0.2301	0.3996
1.3	-1.2688	-3.0906	0.1879	-0.9036
1.4	-1.2968	-2.5013	0.5437	-1.9328
1.5	-1.2869	-1.9800	0.8411	-2.7218
1.6	-1.2501	-1.5278	1.0842	-3.3069
1.7	-1.1962	-1.1427	1.2773	-3.7231
1.8	-1.1328	-0.8211	1.4252	-4.0026
1.9	-1.0660	-0.5575	1.5328	-4.1733
2.0	-0.9998	-0.3458	1.6053	-4.2590
2.1	-0.9368	-0.1791	1.6481	-4.2793
2.2	-0.8782	-0.0507	1.6662	-4.2502
2.3	-0.8248	0.0459	1.6645	-4.1849
2.4	-0.7765	0.1169	1.6473	-4.0937
2.5	-0.7331	0.1674	1.6183	-3.9849
2.6	-0.6940	0.2022	1.5808	-3.8650
2.7	-0.6589	0.2250	1.5373	-3.7389
2.8	-0.6272	0.2389	1.4900	-3.6104
2.9	-0.5985	0.2464	1.4404	-3.4823
3.0	-0.5725	0.2493	1.3899	-3.3566
3.1	-0.5488	0.2491	1.3394	-3.2348
3.2	-0.5271	0.2469	1.2894	-3.1177
3.3	-0.5073	0.2433	1.2405	-3.0058
3.4	-0.4891	0.2390	1.1931	-2.8995
3.5	-0.4724	0.2343	1.1472	-2.7987
3.6	-0.4569	0.2296	1.1030	-2.7033
3.7	-0.4426	0.2250	1.0607	-2.6133
3.8	-0.4292	0.2206	1.0201	-2.5284
3.9	-0.4168	0.2164	0.9813	-2.4481
4.0	-0.4052	0.2126	0.9443	-2.3724
4.1	-0.3942	0.2091	0.9090	-2.3007
4.2	-0.3839	0.2059	0.8753	-2.2330
4.3	-0.3742	0.2030	0.8432	-2.1687
4.4	-0.3649	0.2004	0.8127	-2.1077
4.5	-0.3561	0.1980	0.7835	-2.0497
4.6	-0.3476	0.1958	0.7558	-1.9944
4.7	-0.3395	0.1938	0.7293	-1.9417
4.8	-0.3318	0.1920	0.7041	-1.8913
4.9	-0.3242	0.1903	0.6800	-1.8430
5.0	-0.3170	0.1887	0.6571	-1.7967

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	2.1209	-8.0631	-9.4922	23.9181
0.1	2.0006	-8.2167	-9.3236	23.5421
0.2	1.7598	-8.1798	-9.0381	22.4972
0.3	1.4176	-7.9549	-8.6342	20.8420
0.4	1.0018	-7.5580	-8.1140	18.6774
0.5	0.5449	-7.0169	-7.4879	16.1394
0.6	0.0808	-6.3679	-6.7756	13.3860
0.7	-0.3590	-5.6508	-6.0043	10.5782
0.8	-0.7491	-4.9039	-5.2049	7.8615
0.9	-1.0723	-4.1604	-4.4073	5.3507
1.0	-1.3202	-3.4463	-3.6370	**3.1228**
1.1	-1.4922	-2.7797	-2.9137	1.2168
1.2	-1.5944	-2.1721	-2.2509	-0.3603
1.3	-1.6371	-1.6297	-1.6564	-1.6252
1.4	-1.6325	-1.1544	-1.1337	-2.6095
1.5	-1.5931	-0.7453	-0.6826	-3.3514
1.6	-1.5303	-0.3993	-0.3008	-3.8909
1.7	-1.4539	-0.1123	0.0163	-4.2656
1.8	-1.3712	0.1212	0.2741	-4.5090
1.9	-1.2879	0.3071	0.4790	-4.6497
2.0	-1.2075	0.4514	0.6376	-4.7114
2.1	-1.1322	0.5604	0.7566	-4.7135
2.2	-1.0630	0.6400	0.8425	-4.6714
2.3	-1.0002	0.6955	0.9012	-4.5974
2.4	-0.9437	0.7319	0.9380	-4.5009
2.5	-0.8928	0.7533	0.9577	-4.3894
2.6	-0.8470	0.7633	0.9642	-4.2686
2.7	-0.8057	0.7648	0.9606	-4.1426
2.8	-0.7683	0.7600	0.9498	-4.0147
2.9	-0.7343	0.7507	0.9336	-3.8871
3.0	-0.7031	0.7383	0.9137	-3.7614
3.1	-0.6744	0.7238	0.8915	-3.6386
3.2	-0.6479	0.7080	0.8677	-3.5195
3.3	-0.6233	0.6913	0.8431	-3.4045
3.4	-0.6004	0.6743	0.8183	-3.2937
3.5	-0.5789	0.6571	0.7934	-3.1873
3.6	-0.5587	0.6399	0.7690	-3.0850
3.7	-0.5397	0.6230	0.7450	-2.9870
3.8	-0.5216	0.6063	0.7216	-2.8929
3.9	-0.5045	0.5900	0.6989	-2.8025
4.0	-0.4883	0.5741	0.6770	-2.7158
4.1	-0.4727	0.5585	0.6559	-2.6326
4.2	-0.4579	0.5434	0.6355	-2.5525
4.3	-0.4437	0.5287	0.6158	-2.4755
4.4	-0.4300	0.5144	0.5969	-2.4014
4.5	-0.4169	0.5006	0.5788	-2.3301
4.6	-0.4043	0.4871	0.5613	-2.2614
4.7	-0.3922	0.4741	0.5445	-2.1951
4.8	-0.3805	0.4614	0.5283	-2.1312
4.9	-0.3692	0.4491	0.5128	-2.0694
5.0	-0.3583	0.4372	0.4978	-2.0099

Ring D

Top side

NICS@	isotropic	xx	yy	zz
0.0	9.2065	-11.9712	-11.4691	51.0598
0.1	9.1697	-12.3583	-10.9020	50.7694
0.2	9.0511	-12.5253	-10.1798	49.8583
0.3	8.8284	-12.4583	-9.3019	48.2456
0.4	8.4775	-12.1498	-8.2814	45.8637
0.5	7.9848	-11.6092	-7.1538	42.7173
0.6	7.3561	-10.8685	-5.9744	38.9111
0.7	6.6181	-9.9780	-4.8052	34.6376
0.8	5.8131	-8.9970	-3.7013	30.1374
0.9	4.9892	-7.9821	-2.7008	25.6503
1.0	4.1912	-6.9806	-1.8231	**21.3773**
1.1	3.4538	-6.0268	-1.0717	17.4599
1.2	2.7983	-5.1429	-0.4396	13.9775
1.3	2.2336	-4.3408	0.0848	10.9569
1.4	1.7586	-3.6253	0.5145	8.3864
1.5	1.3654	-2.9964	0.8616	6.2310
1.6	1.0433	-2.4510	1.1369	4.4440
1.7	0.7804	-1.9841	1.3498	2.9756
1.8	0.5655	-1.5897	1.5086	1.7778
1.9	0.3892	-1.2608	1.6210	0.8073
2.0	0.2434	-0.9901	1.6943	0.0261
2.1	0.1223	-0.7699	1.7350	-0.5983
2.2	0.0211	-0.5929	1.7495	-1.0934
2.3	-0.0637	-0.4519	1.7434	-1.4824
2.4	-0.1345	-0.3405	1.7215	-1.7845
2.5	-0.1936	-0.2529	1.6881	-2.0160
2.6	-0.2426	-0.1841	1.6466	-2.1902
2.7	-0.2828	-0.1299	1.5998	-2.3184
2.8	-0.3156	-0.0871	1.5497	-2.4095
2.9	-0.3420	-0.0530	1.4981	-2.4710
3.0	-0.3629	-0.0255	1.4460	-2.5091
3.1	-0.3791	-0.0031	1.3943	-2.5285
3.2	-0.3914	0.0155	1.3436	-2.5332
3.3	-0.4004	0.0312	1.2941	-2.5264
3.4	-0.4065	0.0446	1.2462	-2.5104
3.5	-0.4104	0.0561	1.2001	-2.4874
3.6	-0.4123	0.0663	1.1556	-2.4589
3.7	-0.4126	0.0753	1.1130	-2.4261
3.8	-0.4116	0.0833	1.0721	-2.3901
3.9	-0.4094	0.0905	1.0329	-2.3516
4.0	-0.4063	0.0971	0.9954	-2.3113
4.1	-0.4024	0.1030	0.9595	-2.2697
4.2	-0.3978	0.1084	0.9252	-2.2271
4.3	-0.3928	0.1134	0.8923	-2.1840
4.4	-0.3872	0.1179	0.8609	-2.1405
4.5	-0.3814	0.1220	0.8308	-2.0969
4.6	-0.3752	0.1257	0.8020	-2.0534
4.7	-0.3688	0.1292	0.7744	-2.0100
4.8	-0.3623	0.1322	0.7479	-1.9670
4.9	-0.3556	0.1350	0.7226	-1.9243
5.0	-0.3488	0.1375	0.6983	-1.8821

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	9.2024	-11.0513	-12.3803	51.0388
0.1	9.1656	-11.3136	-11.9376	50.7479
0.2	9.0468	-11.4454	-11.2493	49.8353
0.3	8.8238	-11.4131	-10.3359	48.2205
0.4	8.4721	-11.1828	-9.2374	45.8366
0.5	7.9781	-10.7393	-8.0147	42.6884
0.6	7.3478	-10.0961	-6.7414	38.8808
0.7	6.6080	-9.2928	-5.4901	34.6068
0.8	5.8011	-8.3838	-4.3198	30.1068
0.9	4.9755	-7.4255	-3.2686	25.6206
1.0	4.1764	-6.4666	-2.3533	**21.3492**
1.1	3.4384	-5.5439	-1.5748	17.4339
1.2	2.7828	-4.6819	-0.9237	13.9541
1.3	2.2185	-3.8945	-0.3861	10.9362
1.4	1.7442	-3.1886	0.0525	8.3685
1.5	1.3520	-2.5655	0.4058	6.2158
1.6	1.0311	-2.0234	0.6854	4.4313
1.7	0.7694	-1.5584	0.9015	2.9651
1.8	0.5557	-1.1651	1.0630	1.7692
1.9	0.3805	-0.8369	1.1779	0.8003
2.0	0.2358	-0.5667	1.2536	0.0204
2.1	0.1156	-0.3471	1.2967	-0.6029
2.2	0.0152	-0.1708	1.3137	-1.0973
2.3	-0.0688	-0.0307	1.3100	-1.4856
2.4	-0.1391	0.0796	1.2906	-1.7874
2.5	-0.1976	0.1658	1.2599	-2.0186
2.6	-0.2462	0.2328	1.2212	-2.1927
2.7	-0.2862	0.2848	1.1776	-2.3208
2.8	-0.3187	0.3248	1.1311	-2.4119
2.9	-0.3448	0.3557	1.0834	-2.4735
3.0	-0.3655	0.3793	1.0358	-2.5117
3.1	-0.3816	0.3972	0.9892	-2.5312
3.2	-0.3938	0.4106	0.9440	-2.5360
3.3	-0.4027	0.4204	0.9008	-2.5293
3.4	-0.4088	0.4274	0.8596	-2.5135
3.5	-0.4126	0.4320	0.8207	-2.4906
3.6	-0.4145	0.4346	0.7840	-2.4622
3.7	-0.4148	0.4357	0.7495	-2.4295
3.8	-0.4137	0.4354	0.7172	-2.3935
3.9	-0.4114	0.4339	0.6868	-2.3551
4.0	-0.4083	0.4315	0.6584	-2.3148
4.1	-0.4044	0.4283	0.6318	-2.2732
4.2	-0.3998	0.4245	0.6068	-2.2306
4.3	-0.3947	0.4200	0.5835	-2.1875
4.4	-0.3891	0.4151	0.5616	-2.1440
4.5	-0.3832	0.4097	0.5410	-2.1004
4.6	-0.3770	0.4041	0.5217	-2.0568
4.7	-0.3706	0.3981	0.5035	-2.0134
4.8	-0.3640	0.3919	0.4865	-1.9704
4.9	-0.3573	0.3856	0.4703	-1.9277
5.0	-0.3504	0.3790	0.4551	-1.8854

Ring E

Top side

NICS@	isotropic	xx	yy	zz
0.0	2.1069	-9.2831	-8.2933	23.8971
0.1	1.9880	-9.4432	-8.1144	23.5215
0.2	1.7485	-9.4535	-7.7778	22.4767
0.3	1.4075	-9.2990	-7.3000	20.8216
0.4	0.9926	-8.9736	-6.7059	18.6572
0.5	0.5362	-8.4848	-6.0265	16.1197
0.6	0.0723	-7.8544	-5.2960	13.3673
0.7	-0.3677	-7.1162	-4.5478	10.5610
0.8	-0.7583	-6.3097	-3.8112	7.8461
0.9	-1.0821	-5.4747	-3.1088	5.3373
1.0	-1.3305	-4.6467	-2.4564	**3.1115**
1.1	-1.5032	-3.8538	-1.8631	1.2075
1.2	-1.6059	-3.1164	-1.3335	-0.3679
1.3	-1.6490	-2.4474	-0.8683	-1.6314
1.4	-1.6446	-1.8534	-0.4661	-2.6144
1.5	-1.6053	-1.3364	-0.1241	-3.3554
1.6	-1.5425	-0.8948	0.1616	-3.8942
1.7	-1.4658	-0.5247	0.3956	-4.2683
1.8	-1.3828	-0.2202	0.5830	-4.5113
1.9	-1.2991	0.0254	0.7290	-4.6517
2.0	-1.2183	0.2193	0.8391	-4.7132
2.1	-1.1425	0.3690	0.9187	-4.7151
2.2	-1.0728	0.4816	0.9729	-4.6728
2.3	-1.0095	0.5637	1.0063	-4.5986
2.4	-0.9524	0.6214	1.0233	-4.5020
2.5	-0.9011	0.6597	1.0274	-4.3903
2.6	-0.8548	0.6831	1.0218	-4.2693
2.7	-0.8131	0.6951	1.0089	-4.1432
2.8	-0.7752	0.6987	0.9907	-4.0151
2.9	-0.7408	0.6962	0.9689	-3.8874
3.0	-0.7092	0.6892	0.9447	-3.7615
3.1	-0.6802	0.6791	0.9189	-3.6386
3.2	-0.6534	0.6669	0.8923	-3.5194
3.3	-0.6285	0.6534	0.8654	-3.4042
3.4	-0.6052	0.6391	0.8386	-3.2933
3.5	-0.5835	0.6243	0.8121	-3.1868
3.6	-0.5630	0.6093	0.7860	-3.0845
3.7	-0.5437	0.5944	0.7606	-2.9863
3.8	-0.5255	0.5797	0.7359	-2.8921
3.9	-0.5082	0.5652	0.7120	-2.8017
4.0	-0.4917	0.5510	0.6888	-2.7149
4.1	-0.4760	0.5372	0.6664	-2.6316
4.2	-0.4610	0.5238	0.6448	-2.5515
4.3	-0.4466	0.5107	0.6240	-2.4745
4.4	-0.4328	0.4980	0.6039	-2.4004
4.5	-0.4196	0.4857	0.5845	-2.3290
4.6	-0.4068	0.4738	0.5659	-2.2603
4.7	-0.3946	0.4622	0.5480	-2.1940
4.8	-0.3828	0.4510	0.5307	-2.1300
4.9	-0.3714	0.4401	0.5141	-2.0683
5.0	-0.3604	0.4295	0.4981	-2.0087

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	2.1182	-8.0602	-9.5008	23.9155
0.1	2.1089	-7.7394	-9.5400	23.6062
0.2	1.9731	-7.2586	-9.4595	22.6374
0.3	1.7243	-6.6466	-9.2538	21.0733
0.4	1.3854	-5.9383	-8.9189	19.0135
0.5	0.9860	-5.1711	-8.4579	16.5871
0.6	0.5588	-4.3812	-7.8838	13.9413
0.7	0.1357	-3.5999	-7.2191	11.2263
0.8	-0.2553	-2.8522	-6.4931	8.5792
0.9	-0.5935	-2.1548	-5.7367	6.1109
1.0	-0.8662	-1.5177	-4.9796	**3.8986**
1.1	-1.0691	-0.9455	-4.2466	1.9848
1.2	-1.2046	-0.4388	-3.5568	0.3818
1.3	-1.2804	0.0037	-2.9239	-0.9211
1.4	-1.3070	0.3847	-2.3559	-1.9498
1.5	-1.2959	0.7074	-1.8570	-2.7380
1.6	-1.2581	0.9755	-1.4276	-3.3222
1.7	-1.2034	1.1931	-1.0656	-3.7377
1.8	-1.1395	1.3648	-0.7668	-4.0165
1.9	-1.0723	1.4954	-0.5257	-4.1866
2.0	-1.0058	1.5901	-0.3358	-4.2717
2.1	-0.9426	1.6540	-0.1902	-4.2915
2.2	-0.8839	1.6922	-0.0819	-4.2621
2.3	-0.8305	1.7094	-0.0042	-4.1965
2.4	-0.7821	1.7099	0.0488	-4.1051
2.5	-0.7386	1.6975	0.0828	-3.9962
2.6	-0.6996	1.6753	0.1021	-3.8761
2.7	-0.6644	1.6459	0.1108	-3.7499
2.8	-0.6327	1.6114	0.1119	-3.6213
2.9	-0.6039	1.5734	0.1079	-3.4931
3.0	-0.5779	1.5332	0.1006	-3.3674
3.1	-0.5541	1.4917	0.0914	-3.2454
3.2	-0.5324	1.4497	0.0813	-3.1282
3.3	-0.5125	1.4075	0.0711	-3.0162
3.4	-0.4942	1.3657	0.0613	-2.9097
3.5	-0.4774	1.3245	0.0521	-2.8087
3.6	-0.4618	1.2841	0.0439	-2.7132
3.7	-0.4473	1.2445	0.0366	-2.6230
3.8	-0.4338	1.2059	0.0304	-2.5379
3.9	-0.4213	1.1683	0.0253	-2.4574
4.0	-0.4095	1.1318	0.0211	-2.3815
4.1	-0.3985	1.0963	0.0179	-2.3096
4.2	-0.3880	1.0620	0.0156	-2.2416
4.3	-0.3781	1.0286	0.0141	-2.1772
4.4	-0.3687	0.9964	0.0134	-2.1159
4.5	-0.3598	0.9651	0.0133	-2.0577
4.6	-0.3512	0.9349	0.0137	-2.0023
4.7	-0.3430	0.9057	0.0147	-1.9493
4.8	-0.3351	0.8774	0.0161	-1.8987
4.9	-0.3275	0.8501	0.0178	-1.8502
5.0	-0.3201	0.8236	0.0199	-1.8037

Ring F

Top side

NICS@	isotropic	xx	yy	zz
0.0	7.0666	-11.9554	-10.5773	43.7324
0.1	7.0250	-12.1144	-10.3024	43.4918
0.2	6.8651	-12.1157	-9.7735	42.4846
0.3	6.5769	-11.9148	-9.0306	40.6762
0.4	6.1547	-11.4762	-8.1307	38.0709
0.5	5.6038	-10.7932	-7.1413	34.7460
0.6	4.9447	-9.8955	-6.1306	30.8603
0.7	4.2116	-8.8416	-5.1568	26.6331
0.8	3.4470	-7.7027	-4.2609	22.3047
0.9	2.6947	-6.5474	-3.4645	18.0960
1.0	1.9922	-5.4307	-2.7725	**14.1798**
1.1	1.3660	-4.3904	-2.1790	10.6676
1.2	0.8305	-3.4484	-1.6726	7.6125
1.3	0.3887	-2.6141	-1.2408	5.0209
1.4	0.0353	-1.8885	-0.8725	2.8668
1.5	-0.2400	-1.2672	-0.5590	1.1061
1.6	-0.4497	-0.7434	-0.2934	-0.3124
1.7	-0.6064	-0.3085	-0.0704	-1.4404
1.8	-0.7216	0.0465	0.1144	-2.3257
1.9	-0.8048	0.3310	0.2649	-3.0103
2.0	-0.8637	0.5543	0.3850	-3.5303
2.1	-0.9040	0.7253	0.4785	-3.9159
2.2	-0.9302	0.8525	0.5491	-4.1922
2.3	-0.9453	0.9439	0.6006	-4.3803
2.4	-0.9516	1.0064	0.6362	-4.4975
2.5	-0.9509	1.0461	0.6591	-4.5579
2.6	-0.9445	1.0681	0.6719	-4.5735
2.7	-0.9334	1.0768	0.6770	-4.5540
2.8	-0.9185	1.0754	0.6762	-4.5071
2.9	-0.9006	1.0667	0.6709	-4.4394
3.0	-0.8803	1.0525	0.6625	-4.3560
3.1	-0.8582	1.0346	0.6518	-4.2611
3.2	-0.8349	1.0140	0.6394	-4.1580
3.3	-0.8106	0.9916	0.6260	-4.0494
3.4	-0.7858	0.9681	0.6119	-3.9374
3.5	-0.7608	0.9438	0.5974	-3.8235
3.6	-0.7357	0.9191	0.5827	-3.7090
3.7	-0.7109	0.8944	0.5680	-3.5950
3.8	-0.6864	0.8697	0.5533	-3.4822
3.9	-0.6623	0.8452	0.5388	-3.3711
4.0	-0.6389	0.8211	0.5246	-3.2623
4.1	-0.6160	0.7974	0.5106	-3.1559
4.2	-0.5938	0.7741	0.4969	-3.0523
4.3	-0.5722	0.7514	0.4836	-2.9517
4.4	-0.5514	0.7291	0.4706	-2.8540
4.5	-0.5313	0.7075	0.4579	-2.7594
4.6	-0.5120	0.6864	0.4455	-2.6679
4.7	-0.4933	0.6659	0.4335	-2.5794
4.8	-0.4754	0.6460	0.4218	-2.4940
4.9	-0.4582	0.6266	0.4105	-2.4117
5.0	-0.4416	0.6078	0.3995	-2.3322

Bottom side

NICS@	isotropic	xx	yy	zz
0.0	7.0706	-10.3184	-12.2043	43.7345
0.1	6.9994	-10.1530	-12.0856	43.2369
0.2	6.8193	-9.7951	-11.7618	42.0149
0.3	6.5275	-9.2506	-11.2333	40.0663
0.4	6.1218	-8.5358	-10.5097	37.4110
0.5	5.6077	-7.6820	-9.6193	34.1244
0.6	5.0018	-6.7346	-8.6099	30.3498
0.7	4.3328	-5.7449	-7.5407	26.2841
0.8	3.6375	-4.7614	-6.4704	22.1444
0.9	2.9541	-3.8221	-5.4481	18.1323
1.0	2.3158	-2.9522	-4.5074	**14.4068**
1.1	1.7466	-2.1646	-3.6674	11.0716
1.2	1.2593	-1.4636	-2.9352	8.1768
1.3	0.8569	-0.8478	-2.3099	5.7283
1.4	0.5343	-0.3131	-1.7859	3.7019
1.5	0.2822	0.1460	-1.3552	2.0557
1.6	0.0888	0.5352	-1.0089	0.7400
1.7	-0.0574	0.8606	-0.7375	-0.2953
1.8	-0.1669	1.1281	-0.5317	-1.0973
1.9	-0.2485	1.3440	-0.3819	-1.7077
2.0	-0.3090	1.5146	-0.2791	-2.1627
2.1	-0.3537	1.6459	-0.2143	-2.4927
2.2	-0.3862	1.7440	-0.1792	-2.7235
2.3	-0.4094	1.8144	-0.1665	-2.8762
2.4	-0.4252	1.8621	-0.1694	-2.9683
2.5	-0.4350	1.8913	-0.1824	-3.0140
2.6	-0.4401	1.9058	-0.2012	-3.0249
2.7	-0.4414	1.9084	-0.2224	-3.0102
2.8	-0.4397	1.9016	-0.2434	-2.9772
2.9	-0.4356	1.8873	-0.2627	-2.9314
3.0	-0.4298	1.8671	-0.2791	-2.8773
3.1	-0.4227	1.8420	-0.2922	-2.8179
3.2	-0.4148	1.8130	-0.3017	-2.7557
3.3	-0.4064	1.7810	-0.3077	-2.6924
3.4	-0.3977	1.7465	-0.3104	-2.6292
3.5	-0.3890	1.7101	-0.3102	-2.5669
3.6	-0.3803	1.6722	-0.3072	-2.5060
3.7	-0.3719	1.6332	-0.3018	-2.4470
3.8	-0.3636	1.5935	-0.2944	-2.3900
3.9	-0.3557	1.5533	-0.2852	-2.3351
4.0	-0.3480	1.5130	-0.2746	-2.2824
4.1	-0.3406	1.4726	-0.2626	-2.2318
4.2	-0.3335	1.4324	-0.2496	-2.1833
4.3	-0.3266	1.3925	-0.2357	-2.1367
4.4	-0.3200	1.3532	-0.2212	-2.0920
4.5	-0.3136	1.3143	-0.2061	-2.0491
4.6	-0.3074	1.2761	-0.1907	-2.0078
4.7	-0.3014	1.2387	-0.1750	-1.9679
4.8	-0.2956	1.2020	-0.1593	-1.9295
4.9	-0.2899	1.1661	-0.1436	-1.8922
5.0	-0.2843	1.1310	-0.1280	-1.8560

Ring G

Top side

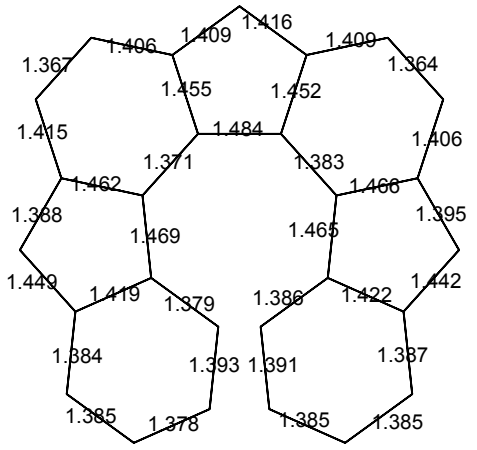
NICS@	isotropic	xx	yy	zz
0.0	-4.3604	-7.5988	-6.8794	1.3968
0.1	-4.5203	-7.5202	-6.8667	0.8261
0.2	-4.8477	-7.2770	-6.7131	-0.5530
0.3	-5.2986	-6.8852	-6.4288	-2.5818
0.4	-5.8120	-6.3705	-6.0309	-5.0344
0.5	-6.3221	-5.7650	-5.5420	-7.6593
0.6	-6.7700	-5.1027	-4.9887	-10.2187
0.7	-7.1113	-4.4154	-4.3986	-12.5198
0.8	-7.3194	-3.7303	-3.7970	-14.4310
0.9	-7.3859	-3.0683	-3.2048	-15.8846
1.0	-7.3170	-2.4441	-2.6381	**-16.8687**
1.1	-7.1294	-1.8672	-2.1078	-17.4132
1.2	-6.8461	-1.3430	-1.6208	-17.5745
1.3	-6.4921	-0.8741	-1.1811	-17.4210
1.4	-6.0916	-0.4611	-0.7904	-17.0234
1.5	-5.6665	-0.1033	-0.4487	-16.4475
1.6	-5.2347	0.2014	-0.1551	-15.7503
1.7	-4.8101	0.4557	0.0926	-14.9787
1.8	-4.4031	0.6631	0.2973	-14.1696
1.9	-4.0204	0.8276	0.4625	-13.3513
2.0	-3.6660	0.9538	0.5921	-12.5441
2.1	-3.3418	1.0464	0.6905	-11.7622
2.2	-3.0477	1.1101	0.7621	-11.0151
2.3	-2.7826	1.1495	0.8111	-10.3085
2.4	-2.5449	1.1689	0.8415	-9.6452
2.5	-2.3322	1.1724	0.8571	-9.0261
2.6	-2.1422	1.1633	0.8610	-8.4508
2.7	-1.9724	1.1447	0.8560	-7.9178
2.8	-1.8206	1.1190	0.8444	-7.4251
2.9	-1.6846	1.0884	0.8280	-6.9701
3.0	-1.5625	1.0545	0.8083	-6.5504
3.1	-1.4527	1.0185	0.7866	-6.1632
3.2	-1.3537	0.9815	0.7635	-5.8061
3.3	-1.2641	0.9442	0.7399	-5.4764
3.4	-1.1828	0.9073	0.7162	-5.1720
3.5	-1.1089	0.8710	0.6927	-4.8906
3.6	-1.0416	0.8357	0.6697	-4.6301
3.7	-0.9800	0.8016	0.6474	-4.3888
3.8	-0.9235	0.7687	0.6257	-4.1650
3.9	-0.8716	0.7372	0.6049	-3.9570
4.0	-0.8239	0.7071	0.5849	-3.7636
4.1	-0.7798	0.6784	0.5657	-3.5835
4.2	-0.7391	0.6510	0.5473	-3.4155
4.3	-0.7013	0.6249	0.5298	-3.2585
4.4	-0.6662	0.6001	0.5130	-3.1118
4.5	-0.6336	0.5766	0.4969	-2.9744
4.6	-0.6033	0.5542	0.4816	-2.8455
4.7	-0.5749	0.5329	0.4669	-2.7245
4.8	-0.5484	0.5127	0.4528	-2.6108
4.9	-0.5236	0.4935	0.4394	-2.5037
5.0	-0.5004	0.4752	0.4265	-2.4029

Bottom side

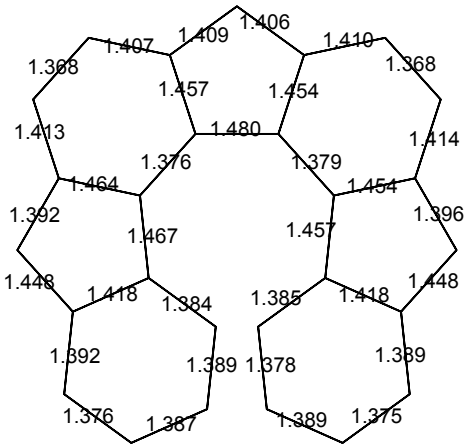
NICS@	isotropic	xx	yy	zz
0.0	-4.3610	-6.3880	-8.0823	1.3875
0.1	-4.3858	-6.1601	-8.0861	1.0888
0.2	-4.5834	-5.7894	-7.9291	-0.0315
0.3	-4.9140	-5.2929	-7.6234	-1.8259
0.4	-5.3207	-4.6940	-7.1904	-4.0777
0.5	-5.7405	-4.0217	-6.6587	-6.5412
0.6	-6.1161	-3.3068	-6.0609	-8.9806
0.7	-6.4032	-2.5794	-5.4293	-11.2009
0.8	-6.5745	-1.8652	-4.7933	-13.0648
0.9	-6.6193	-1.1843	-4.1769	-14.4969
1.0	-6.5415	-0.5506	-3.5978	**-15.4761**
1.1	-6.3550	0.0272	-3.0685	-16.0235
1.2	-6.0798	0.5444	-2.5963	-16.1875
1.3	-5.7387	0.9994	-2.1847	-16.0308
1.4	-5.3540	1.3922	-1.8342	-15.6198
1.5	-4.9456	1.7244	-1.5431	-15.0180
1.6	-4.5303	1.9986	-1.3079	-14.2817
1.7	-4.1213	2.2181	-1.1236	-13.4585
1.8	-3.7281	2.3870	-0.9844	-12.5869
1.9	-3.3570	2.5099	-0.8836	-11.6974
2.0	-3.0118	2.5916	-0.8143	-10.8128
2.1	-2.6941	2.6372	-0.7693	-9.9501
2.2	-2.4039	2.6516	-0.7421	-9.1212
2.3	-2.1403	2.6396	-0.7265	-8.3341
2.4	-1.9019	2.6054	-0.7172	-7.5937
2.5	-1.6866	2.5527	-0.7101	-6.9025
2.6	-1.4927	2.4848	-0.7019	-6.2609
2.7	-1.3181	2.4044	-0.6906	-5.6681
2.8	-1.1611	2.3139	-0.6748	-5.1223
2.9	-1.0200	2.2152	-0.6541	-4.6211
3.0	-0.8934	2.1101	-0.6284	-4.1618
3.1	-0.7799	2.0002	-0.5983	-3.7416
3.2	-0.6785	1.8872	-0.5643	-3.3583
3.3	-0.5879	1.7727	-0.5267	-3.0098
3.4	-0.5074	1.6585	-0.4859	-2.6947
3.5	-0.4359	1.5466	-0.4421	-2.4121
3.6	-0.3726	1.4389	-0.3950	-2.1615
3.7	-0.3166	1.3373	-0.3445	-1.9427
3.8	-0.2674	1.2438	-0.2901	-1.7558
3.9	-0.2241	1.1597	-0.2317	-1.6003
4.0	-0.1863	1.0862	-0.1693	-1.4757
4.1	-0.1533	1.0238	-0.1030	-1.3806
4.2	-0.1248	0.9723	-0.0336	-1.3131
4.3	-0.1004	0.9313	0.0379	-1.2705
4.4	-0.0799	0.8995	0.1103	-1.2494
4.5	-0.0628	0.8756	0.1821	-1.2462
4.6	-0.0491	0.8578	0.2519	-1.2571
4.7	-0.0384	0.8445	0.3183	-1.2781
4.8	-0.0305	0.8341	0.3800	-1.3057
4.9	-0.0251	0.8253	0.4363	-1.3368
5.0	-0.0218	0.8169	0.4864	-1.3687

28. XRD Structural Data Summary

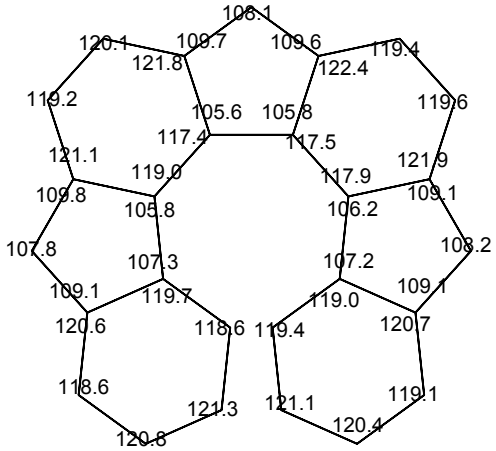
bond lengths [Å], molecule 1

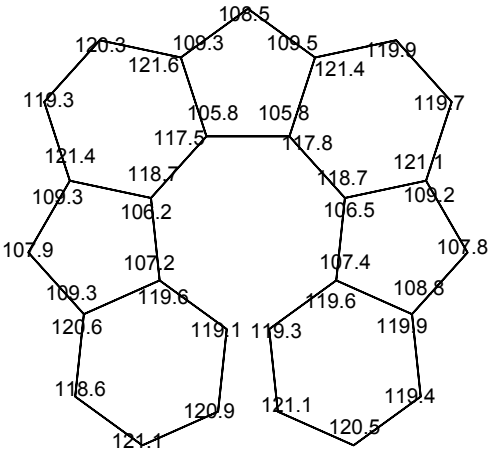


bond lengths [Å], molecule 2

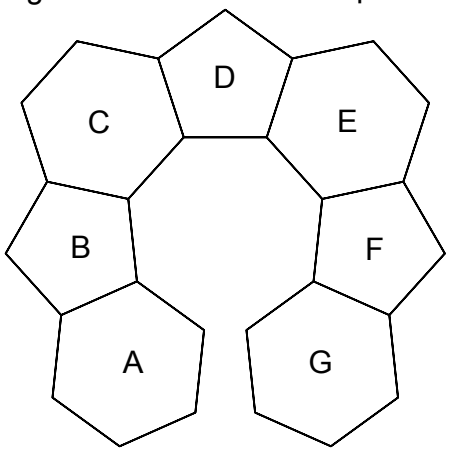


internal angles [°]





angles between the mean planes of the rings



AB 6.4° AC 14.4° AG 39.1°
BC 9.2° CE 19.3°
CD 10.5° EG 9.3°
DE 9.6°
EF 6.1°
FG 4.4°

AB 7.8° AC 18.3° AG 50.1°
BC 11.1° CE 19.4°
CD 10.6° EG 14.7°
DE 9.5°
EF 9.1°
FG 6.3°