Electronic supplementary information for

Preparation and structure of acenaphthylene-1,2-diyldi(9-acridine) derivatives with a long C=C bond

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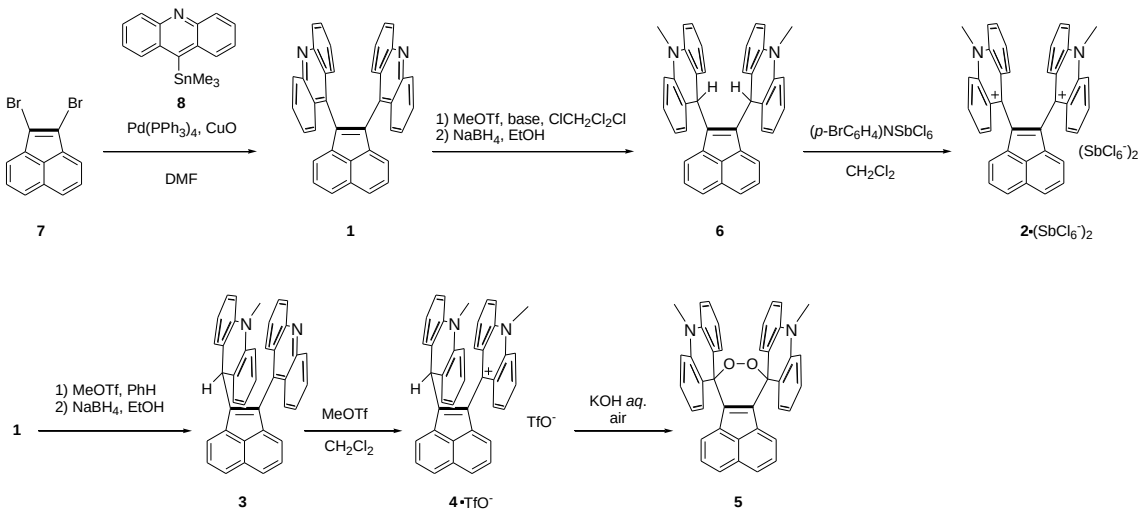
CONTENTS

1. Experimental Detail

General methods

All reactions were performed in argon atmosphere unless otherwise noted. Commercially available reagents and solvents, including dry DMF and CH_2Cl_2, were used as received. Dry 1,2-dichloroethane or benzene were prepared by distillation from CaH_2 prior to use. 1,2-dibromoacenaphthylene[S1] **7** and 9-(trimethylstannyl)acridine[S2] **8** were prepared following the published procedures. Column chromatography was performed using YMC silica gel I-6-40 of particle size 40 - 63 μm or aluminum oxide 90 standardized (Merck 63 - 200 μm). ^{1}H NMR and ^{13}C NMR spectra were taken on a JEOL AL-300, JEOL ECP-300 (^{1}H: 300 MHz, ^{13}C: 75 MHz) or Bruker AVANCE III (^{1}H: 500 MHz, ^{13}C: 125 MHz) spectrometers. Chemical shifts (δ) are expressed in ppm referred to TMS or residual nondeuterated solvent as the internal standard ($CDCl_3$: ^{1}H 7.26 ppm, ^{13}C 77.0 ppm; CD_3CN : ^{1}H 1.93 ppm, ^{13}C 1.3 ppm). IR spectra were measured as a KBr palette on a JASCO FTIR-230 or Thermo Scientific NICOLET 6700 FTIR spectrometer. EI-Mass spectra were taken on a JEOL JMS-600H spectrometer. FAB- or FD-mass spectra were measured on a JEOL JMS-SX102A (FAB) or JMS-01SG-2 (FD) spectrometers at NMR and MS laboratory, Graduate School of Agriculture, Hokkaido University. Elemental Analyses were conducted on a Yanako MT-6 CHN corder at the Center for Instrumental Analysis, Hokkaido University.



Scheme S1 Preparation of acenaphthylene-1,2-diyldi(9-acridine) **1** and its derivatives **2**-**6**

Preparation of acenaphthylene-1,2-diyldi(9-acridine) **1**

To an argon-purged solution of 1,2-dibromoacenaphthylene **7** (1.36 g, 4.40 mmol) in dry DMF (100 mL) were added $Pd(PPh_3)_4$ (1.53 g, 1.32 mmol) and CuO (700 mg, 8.80 mmol). The solution was heated to 140 °C, and then a solution of 9-(trimethylstannyl)acridine **8** (6.02 g, 17.6 mmol) in dry DMF (50 mL) was added via cannula. The mixture was stirred at140 °C for 16 h. After addition of 5% ammonia water at room temperature, the mixture was extracted with $CHCl_3$. Combined organic layer was washed with 5% ammonia water and brine, and then dried over Na_2SO_4. After evaporation of chloroform under reduced pressure, water was added to a resulting DMF solution of crude product. The resulting precipitate was filtered. The solid was subjected to silica gel column chromatography ($PhH/CHCl_3$ = 1/1 → $CHCl_3/Et_3N$ = 100/1) to give acenaphthylene-1,2-diyldi(9-acridine) **1** (749 mg, 34%) as a yellow solid. Mp > 300 °C; ^{1}H NMR ($CDCl_3$) δ 8.18 (d, J = 8.3 Hz, 2H), 8.10-8.02 (m, 6H), 7.66-7.54 (m, 6H), 7.40 (d, 7.0 Hz, 2H), 7.15 (ddd, J = 8.8, 6.6, 1.3 Hz, 4H); ^{13}C NMR ($CDCl_3$) δ 149.0, 141.3, 140.3, 138.5, 130.2, 130.0, 129.1, 129.0, 128.8, 128.5, 127.4, 125.9, 125.6, 125.5; IR 3061, 3010, 2929, 2851, 1629, 1608, 1556, 1540, 1516, 1480, 1459, 1429, 1403, 823, 752, 726 cm^{-1}; HRMS (EI) calcd. for $C_{38}H_{22}N_2$ 506.1783 (M^+), found 506.1764; anal. calcd. for $C_{38}H_{22}N_2$ + 0.3 $CHCl_3$: C, 84.81; H, 4.14, N 5.16 found: C, 84.75; H, 4.40; N 5.11.

Preparation of Acenaphthylene-1,2-diyldi(10-methyl-9-acridan) **6**

To a suspension of acenaphthylene-1,2-diyldi(9-acridine) **1** (52.0 mg, 103 μmol) and 2,6-di-*tert*-butyl-4-methylpyridine (26.7 mg, 130 μmol) in dry 1,2-dichloroethane (4 mL) was added methyl trifrate (900 μl, 7.95 mmol). The mixture was stirred at 60 °C under argon atmosphere for 12 h. After cooling to room temperature, ether was added and the resulting precipitate was collected by filtration to give a mixture of trifrate salts of acenaphthylene-1,2-diyldi(10-methyl-9-acridinium) and 2,6-di-*tert*-4-methylpyridinium, which were used for next reaction without further purification. The single crystals of **2**•$(TfO^-)_2$ for X-ray analyses were obtained by recrystallization from this mixture. The solution of the above mixture in EtOH (20 mL) was added $NaBH_4$ (135 mg, 3.57 mmol). The mixture was stirred at room temperature for 4 h. After evaporation of solvent under reduced pressure, the mixture was dissolved in CH_2Cl_2/water. The aqueous layer was separated and extracted with CH_2Cl_2. Combined organic layer was washed with brined and then dried over Na_2SO_4. After evaporation of solvent under reduced pressure, the crude product was subjected to alumina column chromatography (Hexane/CH_2Cl_2 = 1) to give Acenaphthylene-1,2-diyldi(10-methyl-9-acridan) **6** (53.2 mg, 96%) as a yellow solid.

Mp 212–213 °C (decomp.); ^{1}H NMR ($CDCl_3$) δ 7.65 (d, J = 8.0 Hz, 1H), 7.28-7.15 (m, 5H), 7.09 (d, J = 7.6 Hz, 2H), 6.96 (d, J = 8.0 Hz), 6.76 (td, J = 8.5, 8.0 Hz, 2H), 5.64 (s, 1H), 3.62 (s, 3H); ^{13}C NMR ($CDCl_3$) δ 142.8, 140.7, 138.3, 129.6, 128.7, 128.2, 127.5, 127.2, 126.6, 126.5, 125.2, 120.5, 112.0, 39.1, 33.3; IR 3063, 2040, 2961, 2882, 2874, 2820, 1606, 1591, 1480, 1463, 1431, 1354, 1340,

1287, 1266, 1134, 1050, 900, 819, 776, 754 cm^{-1}; HRMS (EI) calcd. for $C_{40}H_{30}N_2$ 538.2409 (M^+), found 538.2414; anal. calcd. for $C_{40}H_{30}N_2$ + 0.3 EtOH: C, 88.26; H, 5.80, N 5.05 found: C, 88.59; H, 6.13; N 4.99.

Preparation of Acenaphthylene1,2-diyldi(10-methyl-9-acridinium) $(SbCl_6^-)_2$ [**2**•$(SbCl_6^-)_2$]

To a solution of acenaphthylene-1,2-diyldi(10-methyl-9-acridan) **6** (19.4 mg, 36.0 μmol) in dry CH_2Cl_2 (15 mL) was added $(4\text{-}BrC_6H_4)_3NSbCl_6$ (58.8 mg, 72.0 μmol). The mixture was stirred for 17 h and then excess amount of ether was added. The resulting precipitate was filtered to give acenaphthylene-1,2-diyldi(10-methyl-9-acridinium) $(SbCl_6^-)_2$ [**2**•$(SbCl_6^-)_2$] (34.3 mg, 79%) as a yellow solid.

Mp 194-196 °C (decomp.); ^{1}H NMR (CD_3CN) δ 8.58(dd, J = 8.8, 1.3 Hz, 4H), 8.40-8.32 (m, 6H), 8.19 (ddd, J = 9.1, 6.7, 1.3 Hz), 7.81 (dd, J = 8.2, 7.6 Hz, 2H), 7.67-7.57 (m, 6H), 4.59 (s, 6H); ^{13}C NMR (CD_3CN) δ 155.0, 142.3, 141.0, 140.0, 138.6, 132.0, 131.1, 130.32, 130.29, 128.9, 128.5, 127.9, 127.6, 119.6, 39.9; IR 1609, 1579, 1548, 1484, 1360, 1387, 1257, 1191, 1170, 1032, 822, 809, 769, 754, 698, 647, 604 cm^{-1}; HRMS (FAB) calcd. for $C_{40}H_{28}N_2$ 536.2252 (M^+), found 536.2256; anal. calcd. for $C_{40}H_{22}N_2Sb_2Cl_{12}$ + 0.5 CH_2Cl_2: C, 38.97; H, 2.34, N 2.24 found: C, 39.28; H, 2.54; N 2.15.

Preparation of Acenaphthylene-2-(9-acridinyl)-1-(10-methyl-9-acridan) **3**

To a mixture of acenapthylene-1,2-diyldi(9-acridine) **1** (121 mg, 238 μmol) and 2,6-di-*tert*-butyl-4-methylpyridine (34.4 mg, 460 μmol) in PhH (80 mL) was added a solution of methyl trifrate in PhH (238 uL / mL, 1 mL, 238 μmol) at 50 °C. The mixture was stirred at 60 °C. After evaporation of solvent, the product was suspended in EtOH (40 mL) and then $NaBH_4$ (150 mg, 397 mmol) was added. The mixture was stirred at room temperature for 3 h. After evaporation of solvent, the product was dissolved in CH_2Cl_2/water. The aqueous layer was separated and extracted with CH_2Cl_2. Combined organic layer was washed with brined and the dried over Na_2SO_4. After evaporation of solvent under reduced pressure, the crude product was subjected to alumina column chromatography (Hexane / CH_2Cl_2 = 1) to give acenaphthylene-2-(9-acridine)-yl-1-(10-methyl-9-acridan) **3** (86.0 mg, 69 %) as a yellow solid.

Mp 220–222 °C (decomp.); ^{1}H NMR ($CDCl_3$) δ 8.24 (d, J = 8.8 Hz, 2H), 7.90 (d, J = 8.1 Hz, 1H), 7.82 (d, J = 8.1 Hz, 1H), 7.79-7.73 (m, 3H), 7.68 (ddd, J = 8.1, 6.6, 1.3 Hz, 2H), 7.58 (dd, J = 8.1, 6.9 Hz, 1H), 7.35 (dd, J = 8.1, 6.9 Hz, 1H), 7.22-7.11(m, 4H), 7.00-6.92 (m, 2H), 6.88 (d, J = 6.9 Hz, 1H), 6.68 (td, J = 7.4, 0.8 Hz, 2H), 6.48 (d, J = 8.1 Hz, 2H), 5.23 (s, 1H), 2.77 (s, 3H); ^{13}C NMR ($CDCl_3$) δ 148.6, 144.8, 142.2, 141.4, 139.1, 134.9, 130.1, 129.5, 128.8, 128.5, ;128.4, 128.1, 1280, 127.7, 127.6, 127.24, 127.17, 126.0, 125.23, 125.19, 124.8, 123.4, 120.4, 111.8, 40.4, 32.3; IR 3061, 3040, 2879, 2825, 1593, 1517, 1480, 1431, 1351, 1292, 1269, 1132, 900, 821, 771, 741 cm^{-1};

HRMS (EI) calcd. for $C_{39}H_{26}N_2$ 522.2096 (M^+), found 522.2095; anal. calcd. for $C_{39}H_{26}N_2$ + 0.5 EtOH: C, 88.04; H, 5.36, N 5.13 found: C, 88.14; H, 5.30; N 5.16.

Preparation of Acenaphthylene-2-(10-methyl-9-acridan)-yl-1-(10-methyl-9-acridinium) TfO^- [**4**•TfO^-]

To a solution of Acenaphthylene-2-(9-acridine)-yl-1-(10-methyl-9-acridan) **3** (116 mg, 222 μmol) and 2,6-di-*tert*-butyl-4-methylpyridine (22.0 mg, 107 μmol) in dry PhH (20 mL) was added methyl trifrate (250 μL, 2.22 mmol). The mixture was stirred at room temperature for 30 min and then the resulting precipitate was filtered and washed with ether to give acenaphthylene-2-(10-methyl-9-acridan)-yl-1-(10-methyl-9-acridinium) TfO^- [**4**•TfO^-] (160 mg, 95%) as a dark green solid.

Mp 158–160 °C (decomp.); ^{1}H NMR (CD_3CN) δ 8.48 (d, J = 9.1 Hz, 2H), 8.38 (d, J = 7.0 Hz, 1H), 8.22 (ddd, J = 9.1, 6.6, 1.5 Hz, 2H), 8.09 (d, J = 8.5 Hz, 1H), 7.95 (d, J = 8.1 Hz, 1H), 7.85 (dd, J = 8.1, 6.9 Hz, 1H), 7.79-7.72 (m, 2H), 7.50 (ddd, J = 8.9, 6.9, 0.7 Hz, 2H), 7.38 (dd, J = 8.1, 6.9 Hz, 1H), 7.25 (dd, J = 7.5, 1.5 Hz, 2H), 6.90-6.80 (m, 2H), 6.75 (d, J = 6.9 Hz, 1H), 6.53 (td, J = 7.5, 0.8 Hz, 2H), 6.25 (d, J = 8.1 Hz, 2H), 5.86 (s, 1H), 4.79 (s, 3H), 2.20 (s, 3H); ^{13}C NMR could not be taken because disportionation reaction into dication and peroxide occurred in solution ; IR 3069, 3032, 1608, 1591, 1580, 1548, 1481, 1431, 1351, 1263, 1223, 1152, 1029, 822, 776, 748, 689, 636, 516 cm^{-1}; HRMS (FAB) calcd. for $C_{40}H_{29}N_2$ 537.2331 (M^+), found 537.2336; anal. calcd. for $C_{41}H_{29}F_3N_2O_3S$ + PhH: C, 73.81; H, 4.61, N 3.66 found: C, 74.00; H, 4.64; N 3.46.

Preparation of peroxide **5**

To a solution of acenaphthylene-2-(10-methyl-9-acridan)-yl-1-(10-methyl-9-acridinium) TfO^- [**4**•TfO^-] (18.9 mg, 27.5 μmol) in dry THF (3 mL) was added 0.1 M aqueous KOH solution (3 mL). The mixture was stirred under air at room temperature for 16 h and then diluted with ether. Aqueous phase was separated and extracted with ether. The combined organic layer was washed with brine and then dried over Na_2SO_4. After evaporation of solvent under reduced pressure, the crude product was purified by Al_2O_3 column chromatography (CH_2Cl_2), followed by recrystallization from $CHCl_3$/hexane to give peroxide **5** (6.0 mg, 38%) as a yellow crystal.

Mp 158–160 °C (decomp.); ^{1}H NMR ($CDCl_3$) δ 7.83 (d, J = 8.1 Hz, 2H), 7.66-7.55 (br m, 4H), 7.38 (dd, J = 8.1, 7.0 Hz, 6H), 7.12 (d, J =8.1 Hz, 4H), 7.08 (d, J = 7.0 Hz, 2H), 6.95-6.82 (br m, 4H), 3.56 (s, 6H); IR 1481, 1262, 1152, 1030, 748, 690, 637 cm^{-1}; HRMS (FD) calcd. for $C_{40}H_{28}O_2N_2$ 568.2151(M^+), found 568.2178. Due to potential risk of explosion of the peroxide, the author did not conduct large scale synthesis enough to take ^{13}C NMR measurement and elemental analysis.

X-ray crystal structure analyses

Data collection was conducted with a Rigaku Mercury70 diffractometer (Mo-Kα radiation, λ = 0.71075 Å). The structure was solved by the direct method and refined by the full-matrix least-squares method on F^2 with anisotropic temperature factors for non-hydrogen atoms. All the hydrogen atoms are located at the calculated positions. In the subsequent refinement, the function $\Sigma w(F_o^2 - F_c^2)^2$ was minimized, where $|F_o|$ and $|F_c|$ are the observed and calculated structure factor amplitudes, respectively.

Crystal data of 1: Single-crystalline sample was obtained by recrystallization from CH_2Cl_2 / hexane. $C_{38}H_{22}N_2$, M = 506.61, monoclinic C2/c, a = 16.181(9) Å, b = 10.378(5) Å, c = 17.045(9) Å, β = 117.095(6)°, V = 2548(3) Å^3, Z = 4, Dc = 1.320 g cm^{-3}. Independent reflection 2769 (all), T = 150 K, μ = 0.768 cm^{-1}, R = 5.6%. CCDC 975883.

Crystal data of 1•$CHCl_3$: Single-crystalline sample was obtained by recrystallization from $CHCl_3$ / hexane. $C_{39}H_{23}Cl_3N_2$, M = 625.98, monoclinic $P2_1/c$, a = 21.8437(16) Å, b = 13.9673(9) Å, c = 9.6149(11) Å, β = 94.127(4)°, V = 2925.9(5) Å^3, Z = 4, Dc = 1.421 g cm^{-3}. Independent reflection 6265 (all), T = 150 K, μ = 3.462 cm^{-1}, R = 5.2%. CCDC 975884.

Crystal data of 2•$(TfO^-)_2$•MeCN: Single-crystalline sample was obtained by recrystallization from MeCN / ether. $C_{42}H_{30}F_6N_2O_6S_2$, M = 836.82, triclinic P1 bar, a = 12.972(3) Å, b = 13.438(3) Å, c = 13.490(3) Å, α = 67.715(13)°, β = 67.100(12)°, γ = 82.25(2)°, V = 2004.1(8) Å^3, Z = 2, Dc = 1.387 g cm^{-3}. Independent reflection 8496 (all), T = 153 K, μ = 2.103 cm^{-1}, R = 5.0%. CCDC 975886.

Crystal data of 2•$(TfO^-)_2$•$CHCl_3$: Single-crystalline sample was obtained by recrystallization from $CHCl_3$. $C_{43}H_{29}Cl_3F_6N_2O_6S_2$, M = 954.18, triclinic P1 bar, a = 13.040(3) Å, b = 13.546(3) Å, c = 13.7353(13) Å, α = 67.07(2)°, β = 66.22(2)°, γ = 81.35(2)°, V = 2044.7(7) Å^3, Z = 2, Dc = 1.550 g cm^{-3}. Independent reflection 8694 (all), T = 153 K, μ = 4.058 cm^{-1}, R = 7.6%. CCDC 975885.

Crystal data of 3: Single-crystalline sample was obtained by recrystallization from CH_2Cl_2/hexane. $C_{39}H_{26}N_2$, M = 522.65, triclinic P1 bar, a = 9.848(6) Å, b = 11.966(6) Å, c = 12.247(7) Å, α = 97.850(6)°, β = 111.742(10)°, γ = 95.696(8)°, V = 1309.7(12) Å^3, Z = 2, Dc = 1.325 g cm^{-3}. Independent reflection 5557 (all), T = 153 K, μ = 0.769 cm^{-1}, R = 5.8%. CCDC 975887.

Crystal data of 4•TfO^-•$CHCl_3$: Single-crystalline sample was obtained by recrystallization from $CHCl_3$. $C_{42}H_{30}Cl_3F_3N_2O_3S$, M = 806.12, monoclinic $P2_1/n$, a = 14.643(4) Å, b = 31.409(8) Å, c = 16.869(5) Å, β = 105.429(6)°, V = 7479(4) Å^3, Z = 8, Dc = 1.432 g cm^{-3}. Independent reflection 16776 (all), T = 295 K, μ = 3.588 cm^{-1}, R = 9.1%. CCDC 975888.

Crystal data of 5•CH_2Cl_2: Single-crystalline sample was obtained by recrystallization from CH_2Cl_2/hexane.$C_{41}H_{30}Cl_2N_2O_2$, M = 653.61, monoclinic C2/c, a = 33.64(2) Å, b = 11.993(6) Å, c = 15.904(8) Å, β = 97.925(9)°, V = 6355(6) Å^3, Z = 8, Dc = 1.366 g cm^{-3}. Independent reflection 6973 (all), T = 150 K, μ = 2.452 cm^{-1}, R = 7.6%. CCDC 975889.

Crystal data of 6$_6$•$(C_6H_{14})_3$•$CHCl_3$: Single-crystalline sample was obtained by recrystallization from $CHCl_3$ / hexane. $C_{247}H_{178}Cl_3N_{12}$, M = 3437.70, trigonal R-3, a = 36.2356, c = 11.6336 Å, V = 13228.6540 Å^3, Z = 3, Dc = 1.294 g cm^{-3}. Independent reflection 6700 (all), T = 100 K, μ = 1.185 cm^{-1}, R = 5.7%. CCDC 975890.

Computational Methods

DFT calculations were performed with the Gaussian 09 program package.[S5] The geometries of the compound were optimized using the B3LYP method with the 6-31G* basis set. The natures of the stationary points were assessed by means of vibration frequency analysis.

2. ORTEP drawings of 1-6

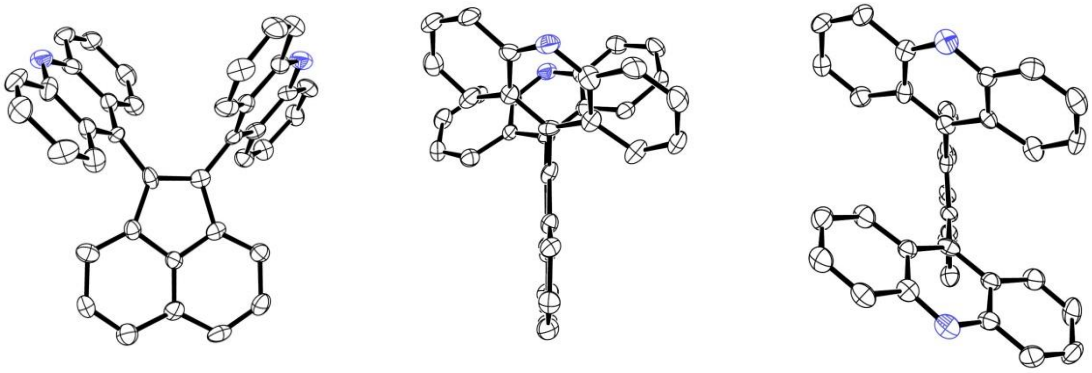


Figure S1 ORTEP drawing of **1** in **1**•$CHCl_3$ solvate determined by X-ray analysis at 150 K: (a) front view, (b) side view and (c) top view.

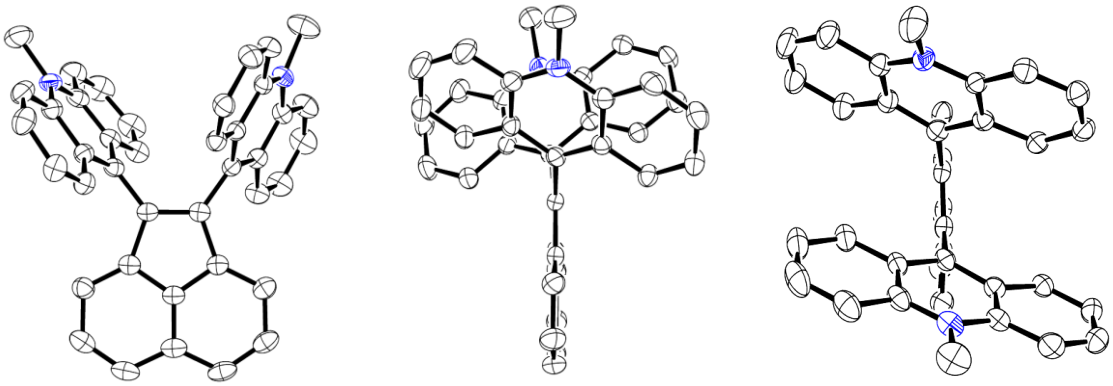


Figure S2 ORTEP drawing of **2** in **2**•$(TfO^-)_2$•MeCN solvate determined by X-ray analysis at 153 K: (a) front view, (b) side view and (c) top view.

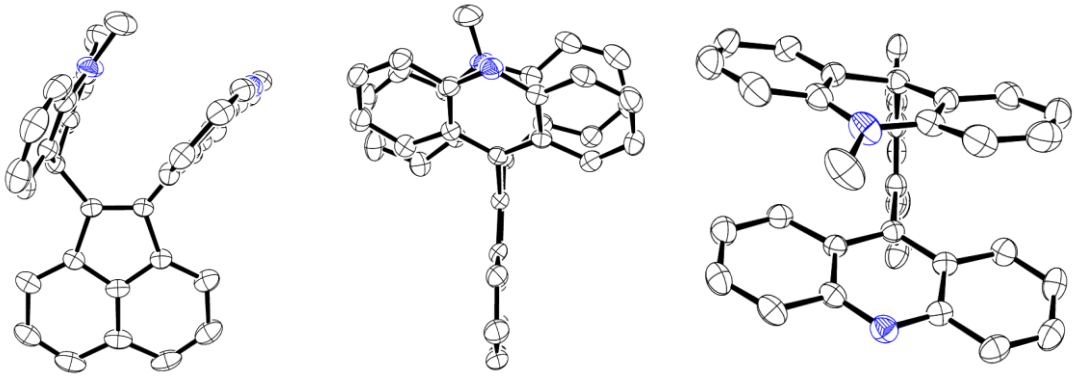


Figure S3 ORTEP drawing of **3** determined by X-ray analysis at 153 K: (a) front view, (b) side view and (c) top view.

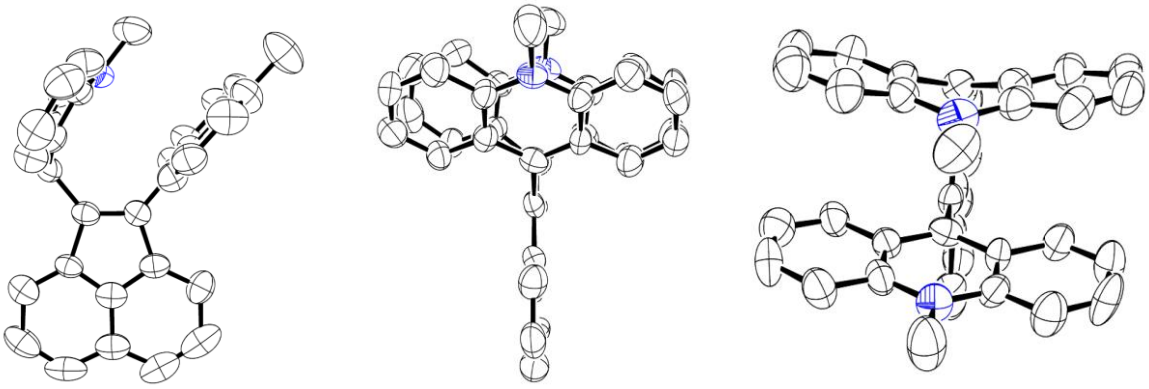


Figure S4 ORTEP drawing of $\mathbf{4}_{Mol1}$ in $\mathbf{4}$•TfO^-•$CHCl_3$ solvate determined by X-ray analysis at 295 K: (a) front view, (b) side view and (c) top view.

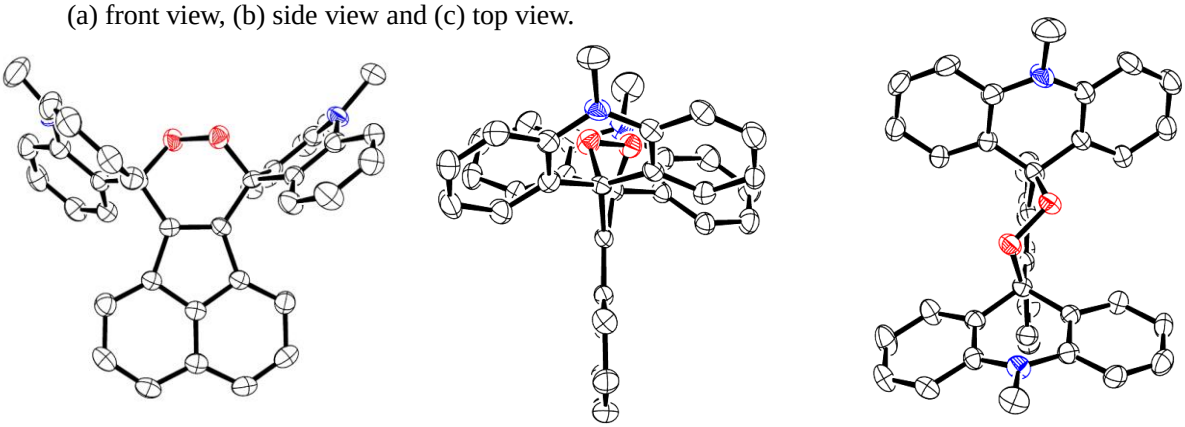


Figure S5 ORTEP drawing of **5** in **5**•$CHCl_3$ solvate determined by X-ray analysis at 150 K: (a) front view, (b) side view and (c) top view.

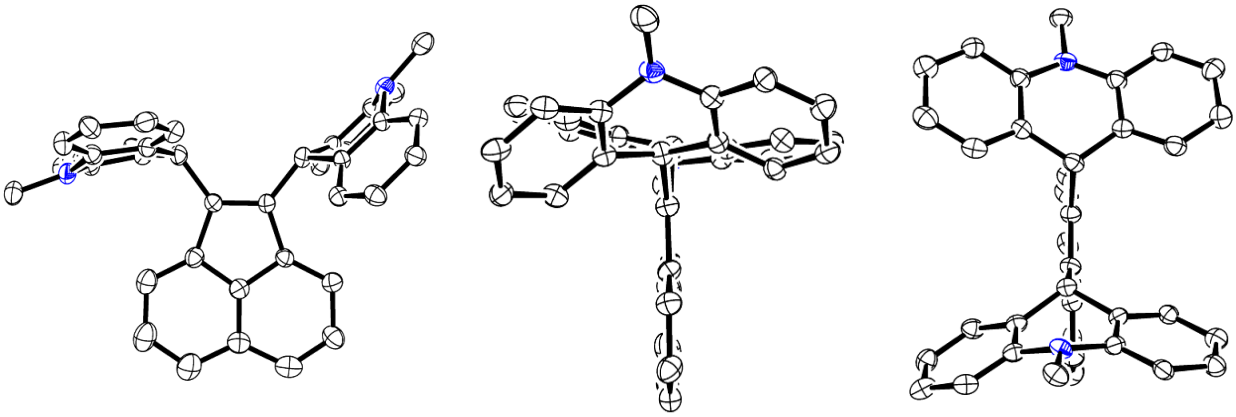


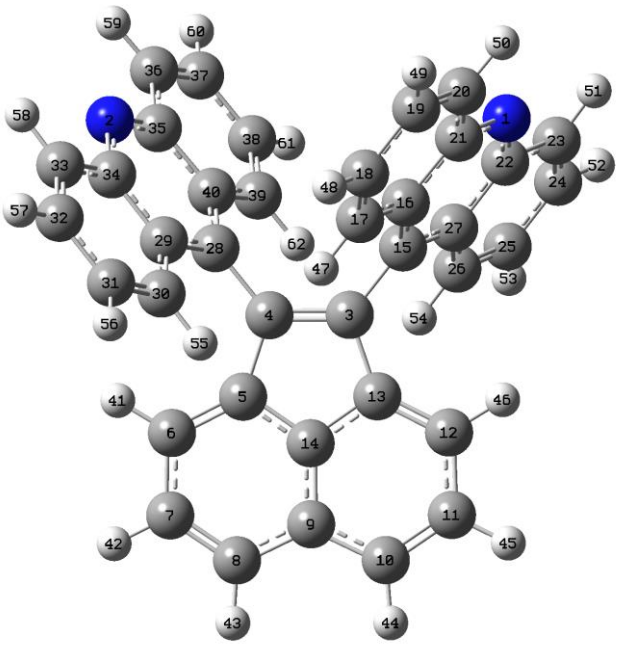
Figure S6 ORTEP drawing of **6** in $\mathbf{6}_6$•$(C_6H_{14})_3$•$CHCl_3$ solvate determined by X-ray analysis at 100 K: (a) front view, (b) side view and (c) top view.

3. Cartesian coordinates of optimized structures

Optimized structure of **1**

SCF Done: E(RB3LYP) = -1570.83592445 A.U. after 9 cycles

Number of imaginary frequencies: 0



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.174806	-2.461579	1.260533
2	7	0	3.176496	-2.459267	-1.260722
3	6	0	-0.640373	0.921628	0.261582
4	6	0	0.639951	0.922239	-0.261515
5	6	0	1.065762	2.329579	-0.449117
6	6	0	2.191256	2.956851	-0.949183
7	6	0	2.223874	4.380582	-0.972776
8	6	0	1.172812	5.158375	-0.514020
9	6	0	-0.001884	4.535891	0.000244
10	6	0	-1.177119	5.157216	0.514710
11	6	0	-2.227437	4.378412	0.973371
12	6	0	-2.193550	2.954697	0.949504
13	6	0	-1.067496	2.328520	0.449321
14	6	0	-0.001249	3.137082	0.000123

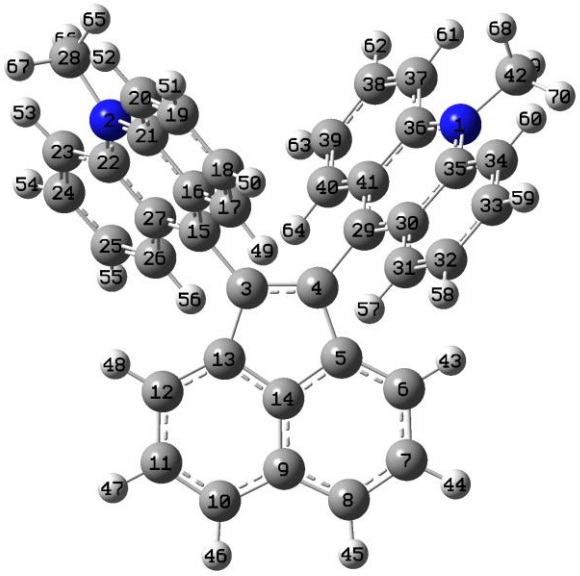
15	6	0	-1.496852	-0.240914	0.607867
16	6	0	-1.163960	-1.113730	1.669767
17	6	0	-0.017790	-0.940715	2.506065
18	6	0	0.257282	-1.819652	3.520310
19	6	0	-0.597544	-2.931306	3.771338
20	6	0	-1.717426	-3.125112	3.009162
21	6	0	-2.046377	-2.225741	1.946175
22	6	0	-3.503777	-1.617705	0.270944
23	6	0	-4.714515	-1.879283	-0.445512
24	6	0	-5.111982	-1.070764	-1.475744
25	6	0	-4.316998	0.048979	-1.853948
26	6	0	-3.150190	0.334157	-1.192908
27	6	0	-2.698764	-0.477694	-0.103411
28	6	0	1.497230	-0.239625	-0.607911
29	6	0	2.699228	-0.475794	0.103436
30	6	0	3.150148	0.336136	1.193085
31	6	0	4.317161	0.051651	1.854056
32	6	0	5.112863	-1.067507	1.475688
33	6	0	4.715868	-1.876205	0.445401
34	6	0	3.504970	-1.615282	-0.271059
35	6	0	2.047951	-2.224007	-1.946409
36	6	0	1.719525	-3.123471	-3.009491
37	6	0	0.599646	-2.930111	-3.771799
38	6	0	-0.255694	-1.818878	-3.520798
39	6	0	0.018817	-0.939908	-2.506421
40	6	0	1.164948	-1.112485	-1.669964
41	1	0	3.045825	2.393721	-1.313994
42	1	0	3.111570	4.869703	-1.364449
43	1	0	1.243717	6.242787	-0.547656
44	1	0	-1.249019	6.241555	0.548508
45	1	0	-3.115559	4.866663	1.365171
46	1	0	-3.047573	2.390758	1.314355
47	1	0	0.634145	-0.094199	2.330294
48	1	0	1.136111	-1.668440	4.140909
49	1	0	-0.357924	-3.619493	4.577539
50	1	0	-2.397128	-3.953869	3.180070
51	1	0	-5.292239	-2.743635	-0.133547
52	1	0	-6.033301	-1.279648	-2.012845
53	1	0	-4.639962	0.681476	-2.676474
54	1	0	-2.557906	1.192059	-1.492500
55	1	0	2.557320	1.193562	1.492931
56	1	0	4.639709	0.684247	2.676668
57	1	0	6.034334	-1.275861	2.012740

58	1	0	5.294143	-2.740152	0.133341
59	1	0	2.399673	-3.951856	-3.180415
60	1	0	0.360398	-3.618386	-4.578037
61	1	0	-1.134462	-1.667962	-4.141554
62	1	0	-0.633600	-0.093750	-2.330717

Optimized structure of **2**

SCF Done: E(RB3LYP) = -1650.17494509 A.U. after 7 cycles

Number of imaginary frequencies: 0



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.383894	-2.197296	0.970595
2	7	0	-3.306715	-2.210023	-0.905385
3	6	0	-0.659793	1.108593	-0.155019
4	6	0	0.685880	1.079804	0.217472
5	6	0	1.150748	2.469912	0.375745
6	6	0	2.336898	3.078140	0.767954
7	6	0	2.394465	4.494476	0.805843
8	6	0	1.308151	5.292750	0.468396
9	6	0	0.078341	4.695219	0.073942
10	6	0	-1.127712	5.345982	-0.309121
11	6	0	-2.241683	4.595745	-0.666663
12	6	0	-2.236231	3.177908	-0.660632

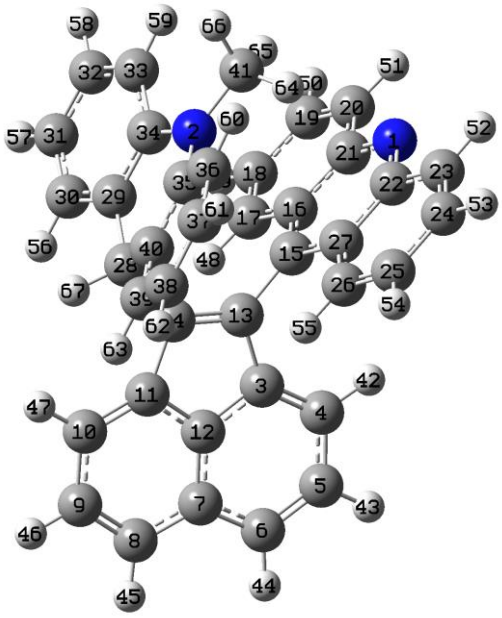
13	6	0	-1.074394	2.517760	-0.278918
14	6	0	0.052495	3.293805	0.058807
15	6	0	-1.575827	-0.022117	-0.433567
16	6	0	-1.384684	-0.864345	-1.558020
17	6	0	-0.354141	-0.618036	-2.514272
18	6	0	-0.197041	-1.412277	-3.620518
19	6	0	-1.081062	-2.495404	-3.832616
20	6	0	-2.099134	-2.769662	-2.945119
21	6	0	-2.278939	-1.967221	-1.790963
22	6	0	-3.607817	-1.324892	0.107680
23	6	0	-4.780005	-1.478995	0.890293
24	6	0	-5.043911	-0.612520	1.928587
25	6	0	-4.151096	0.436605	2.249970
26	6	0	-3.023845	0.622655	1.491637
27	6	0	-2.722104	-0.224170	0.379830
28	6	0	-4.110652	-3.444501	-1.049864
29	6	0	1.569578	-0.085030	0.451657
30	6	0	2.704097	-0.285730	-0.379209
31	6	0	2.975594	0.553734	-1.503989
32	6	0	4.056205	0.335212	-2.319214
33	6	0	4.915696	-0.757771	-2.060524
34	6	0	4.698176	-1.596836	-0.989541
35	6	0	3.603973	-1.376373	-0.115272
36	6	0	2.247642	-2.083494	1.741693
37	6	0	1.958051	-3.020536	2.765930
38	6	0	0.865160	-2.842009	3.585629
39	6	0	0.016512	-1.720242	3.437934
40	6	0	0.249166	-0.825778	2.425621
41	6	0	1.338634	-0.990461	1.517832
42	6	0	4.413934	-3.194955	1.340948
43	1	0	3.218684	2.504739	1.040212
44	1	0	3.323094	4.967225	1.109650
45	1	0	1.398748	6.374512	0.510873
46	1	0	-1.178362	6.431008	-0.328453
47	1	0	-3.151348	5.108917	-0.962164
48	1	0	-3.137445	2.643580	-0.948402
49	1	0	0.285315	0.241128	-2.362812
50	1	0	0.580221	-1.197458	-4.346308
51	1	0	-0.978193	-3.108519	-4.722703
52	1	0	-2.783710	-3.574008	-3.175155
53	1	0	-5.503017	-2.249356	0.660966
54	1	0	-5.956408	-0.738694	2.503162
55	1	0	-4.368511	1.098063	3.082086

56	1	0	-2.351859	1.441533	1.714573
57	1	0	2.309100	1.383718	-1.700723
58	1	0	4.247374	0.987416	-3.164973
59	1	0	5.756318	-0.950366	-2.720050
60	1	0	5.358838	-2.441009	-0.850642
61	1	0	2.573231	-3.898344	2.906016
62	1	0	0.664235	-3.572153	4.363664
63	1	0	-0.810203	-1.571308	4.124585
64	1	0	-0.386411	0.040940	2.306206
65	1	0	-3.483235	-4.237459	-1.449145
66	1	0	-4.453474	-3.766602	-0.069794
67	1	0	-4.967252	-3.278574	-1.709624
68	1	0	4.244045	-4.143984	0.824388
69	1	0	4.396787	-3.348020	2.416707
70	1	0	5.397223	-2.805371	1.089250

Optimized structure of **3**

SCF Done: E(RB3LYP) = -1611.33996539 A.U. after 7 cycles

Number of Imaginary frequencies: 0



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.699889	-1.822709	-1.986718
2	7	0	-2.344673	1.285738	0.966292

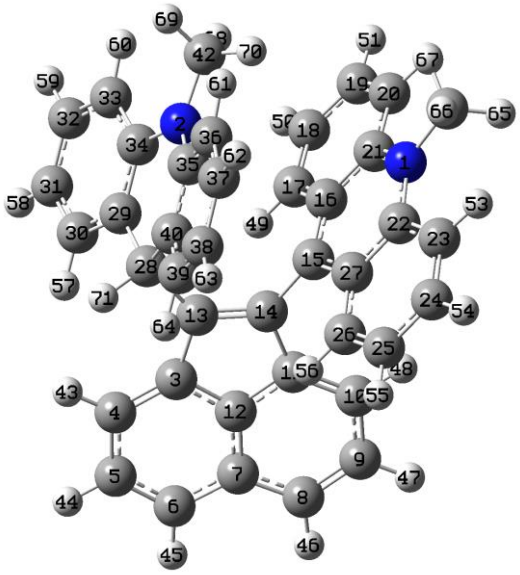
3	6	0	2.328413	-0.934813	-0.921114
4	6	0	2.654521	-1.814300	-1.934457
5	6	0	4.032306	-2.057874	-2.207223
6	6	0	5.052773	-1.448845	-1.495880
7	6	0	4.740513	-0.537399	-0.444276
8	6	0	5.638915	0.179665	0.399027
9	6	0	5.141330	1.022906	1.378398
10	6	0	3.744393	1.214789	1.588130
11	6	0	2.850247	0.535256	0.782124
12	6	0	3.380055	-0.321295	-0.207782
13	6	0	1.064749	-0.424502	-0.337579
14	6	0	1.372309	0.453207	0.677940
15	6	0	-0.253453	-0.870110	-0.862076
16	6	0	-0.848011	-2.062055	-0.393291
17	6	0	-0.279857	-2.865162	0.644411
18	6	0	-0.893649	-4.018507	1.056272
19	6	0	-2.117736	-4.442118	0.461870
20	6	0	-2.698699	-3.700680	-0.531587
21	6	0	-2.088064	-2.493630	-0.997217
22	6	0	-2.119698	-0.702020	-2.445704
23	6	0	-2.764929	-0.006144	-3.516715
24	6	0	-2.218101	1.134260	-4.042599
25	6	0	-0.995409	1.652610	-3.525598
26	6	0	-0.348968	1.020230	-2.496198
27	6	0	-0.881771	-0.174488	-1.918237
28	6	0	0.470934	1.273000	1.598246
29	6	0	-0.544293	0.449883	2.376096
30	6	0	-0.127382	-0.333495	3.453940
31	6	0	-1.022532	-1.116394	4.180723
32	6	0	-2.370859	-1.099630	3.825466
33	6	0	-2.814508	-0.308124	2.769264
34	6	0	-1.909567	0.473380	2.026227
35	6	0	-1.578688	2.398591	0.584489
36	6	0	-2.160274	3.492930	-0.083365
37	6	0	-1.390049	4.591291	-0.456698
38	6	0	-0.028748	4.636318	-0.157496
39	6	0	0.545626	3.561193	0.518927
40	6	0	-0.201811	2.440536	0.886357
41	6	0	-3.682659	1.110411	0.424160
42	1	0	1.892718	-2.319722	-2.522130
43	1	0	4.285317	-2.750274	-3.005679
44	1	0	6.090222	-1.665890	-1.738214
45	1	0	6.712924	0.064013	0.275116

46	1	0	5.837338	1.561971	2.015539
47	1	0	3.418751	1.889056	2.376880
48	1	0	0.644379	-2.538291	1.108123
49	1	0	-0.448807	-4.615976	1.847211
50	1	0	-2.588080	-5.360169	0.804416
51	1	0	-3.629126	-3.997954	-1.005342
52	1	0	-3.692259	-0.428036	-3.891883
53	1	0	-2.714457	1.651309	-4.859783
54	1	0	-0.577759	2.561562	-3.949283
55	1	0	0.573087	1.427336	-2.095589
56	1	0	0.928890	-0.333942	3.716240
57	1	0	-0.673959	-1.723588	5.011016
58	1	0	-3.092315	-1.692234	4.381802
59	1	0	-3.873343	-0.282977	2.540328
60	1	0	-3.222912	3.499910	-0.295524
61	1	0	-1.866803	5.421918	-0.970653
62	1	0	0.574573	5.494400	-0.439034
63	1	0	1.606649	3.578751	0.759050
64	1	0	-3.696877	1.441837	-0.615901
65	1	0	-3.938112	0.049180	0.428459
66	1	0	-4.452339	1.663491	0.984055
67	1	0	1.150033	1.709886	2.341909

Optimized structure of **4**

SCF Done: E(RB3LYP) = -1651.05166109 A.U. after 7 cycles

Number of imaginary frequencies: 0



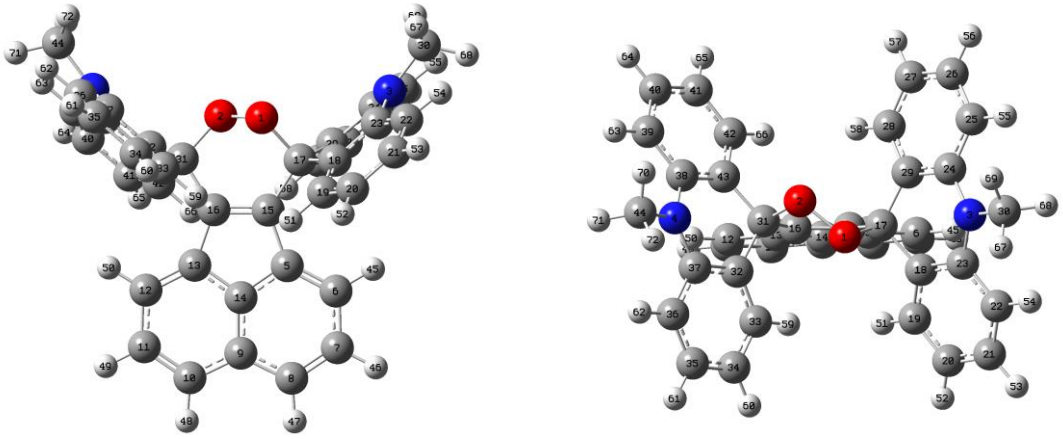
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.100928	1.566325	1.086179
2	7	0	1.660721	-2.413163	-0.591910
3	6	0	-3.058581	-0.074277	-0.561142
4	6	0	-4.143225	-0.663930	-1.188917
5	6	0	-5.447312	-0.163007	-0.919754
6	6	0	-5.672579	0.900677	-0.060001
7	6	0	-4.574954	1.541349	0.583557
8	6	0	-4.605187	2.657080	1.469605
9	6	0	-3.422645	3.166907	1.980990
10	6	0	-2.149651	2.619969	1.653504
11	6	0	-2.096066	1.535256	0.797573
12	6	0	-3.309318	1.019609	0.294476
13	6	0	-1.593406	-0.278492	-0.580243
14	6	0	-1.023093	0.691929	0.218694
15	6	0	0.402111	0.968559	0.498241
16	6	0	1.101577	0.241298	1.494089
17	6	0	0.463835	-0.792550	2.239769
18	6	0	1.120822	-1.455893	3.246181
19	6	0	2.452303	-1.102063	3.555816
20	6	0	3.116137	-0.115993	2.853445
21	6	0	2.464157	0.571670	1.801270
22	6	0	2.408648	2.380776	0.210771
23	6	0	3.014755	3.521983	-0.367141
24	6	0	2.305156	4.316405	-1.244807
25	6	0	0.975020	4.006772	-1.601833
26	6	0	0.364344	2.909741	-1.047100
27	6	0	1.043529	2.078892	-0.108143
28	6	0	-0.928334	-1.371974	-1.410750
29	6	0	-0.769266	-2.686715	-0.646833
30	6	0	-1.895261	-3.449241	-0.323277
31	6	0	-1.796051	-4.657291	0.362771
32	6	0	-0.532888	-5.126872	0.717638
33	6	0	0.606205	-4.394818	0.394359
34	6	0	0.506607	-3.161603	-0.277791
35	6	0	1.618392	-1.465573	-1.623570
36	6	0	2.795839	-1.026231	-2.266916
37	6	0	2.742569	-0.082676	-3.287496
38	6	0	1.517096	0.433740	-3.714135
39	6	0	0.352320	-0.012920	-3.096954

40	6	0	0.379348	-0.937538	-2.049016
41	6	0	4.550002	1.774535	1.261593
42	6	0	2.946078	-2.839106	-0.057622
43	1	0	-4.032306	-1.492807	-1.883258
44	1	0	-6.293263	-0.634502	-1.410948
45	1	0	-6.686145	1.251594	0.114707
46	1	0	-5.554490	3.110450	1.741705
47	1	0	-3.460911	4.017588	2.655070
48	1	0	-1.254905	3.066733	2.079820
49	1	0	-0.562899	-1.036376	1.996215
50	1	0	0.618647	-2.235431	3.809057
51	1	0	2.965603	-1.600251	4.373116
52	1	0	4.120386	0.149048	3.155068
53	1	0	4.022179	3.812133	-0.101672
54	1	0	2.783950	5.197359	-1.661772
55	1	0	0.440692	4.635790	-2.306072
56	1	0	-0.657025	2.658092	-1.303554
57	1	0	-2.875748	-3.081943	-0.610875
58	1	0	-2.688747	-5.226208	0.602763
59	1	0	-0.423650	-6.077201	1.232291
60	1	0	1.575670	-4.808934	0.642125
61	1	0	3.755689	-1.455219	-2.006672
62	1	0	3.664919	0.224840	-3.772500
63	1	0	1.470104	1.153550	-4.525279
64	1	0	-0.612956	0.364929	-3.427200
65	1	0	4.753448	2.524494	2.032383
66	1	0	4.982493	2.092208	0.314916
67	1	0	5.020407	0.832761	1.533297
68	1	0	2.815034	-3.182525	0.969811
69	1	0	3.409935	-3.645302	-0.643610
70	1	0	3.629278	-1.988987	-0.031939
71	1	0	-1.631132	-1.568311	-2.232290

Optimized structure of **5**

SCF Done: E(RB3LYP) = -1800.99248254 A.U. after 7 cycles

Number of imaginary frequencies: 0



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.598740	-1.463820	-0.416166
2	8	0	-0.598529	-1.463631	0.417093
3	7	0	3.732086	-2.134503	0.297890
4	7	0	-3.732515	-2.134362	-0.297172
5	6	0	1.158738	2.278021	0.111886
6	6	0	2.380384	2.909772	0.242220
7	6	0	2.415417	4.334268	0.255139
8	6	0	1.274094	5.108904	0.135584
9	6	0	-0.000200	4.483584	-0.000930
10	6	0	-1.274547	5.108735	-0.137716
11	6	0	-2.415805	4.333939	-0.256924
12	6	0	-2.380651	2.909455	-0.243364
13	6	0	-1.158950	2.277859	-0.112774
14	6	0	-0.000146	3.085318	-0.000629
15	6	0	0.682646	0.880925	0.048275
16	6	0	-0.682710	0.880842	-0.048618
17	6	0	1.493392	-0.392339	0.049923
18	6	0	2.579866	-0.438119	-1.012684
19	6	0	2.497840	0.317270	-2.186962
20	6	0	3.426488	0.176520	-3.214074
21	6	0	4.462093	-0.747216	-3.067449

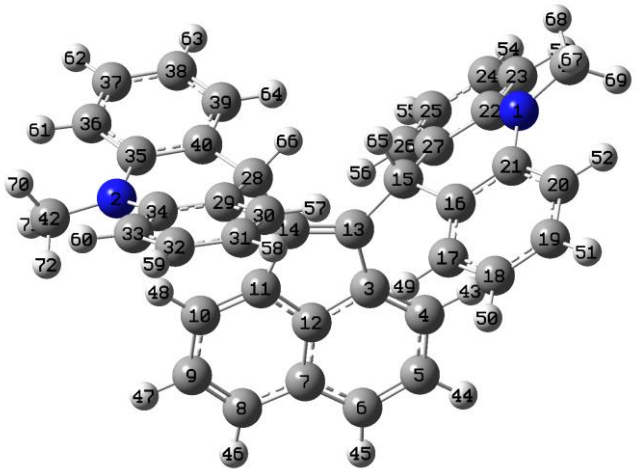
22	6	0	4.568684	-1.511671	-1.910850
23	6	0	3.627111	-1.377212	-0.871381
24	6	0	3.139634	-1.669273	1.478662
25	6	0	3.611459	-2.083376	2.737802
26	6	0	3.032144	-1.595951	3.905602
27	6	0	1.984544	-0.678027	3.844525
28	6	0	1.519565	-0.263419	2.598728
29	6	0	2.073357	-0.744775	1.409856
30	6	0	4.605954	-3.296095	0.334337
31	6	0	-1.493315	-0.392529	-0.049667
32	6	0	-2.073086	-0.745759	-1.409492
33	6	0	-1.518848	-0.265312	-2.598545
34	6	0	-1.983583	-0.680610	-3.844195
35	6	0	-3.031393	-1.598331	-3.904960
36	6	0	-3.611136	-2.084851	-2.737008
37	6	0	-3.139542	-1.670049	-1.478012
38	6	0	-3.627373	-1.376660	0.871788
39	6	0	-4.569102	-1.510516	1.911208
40	6	0	-4.462351	-0.745803	3.067609
41	6	0	-3.426431	0.177618	3.214062
42	6	0	-2.497699	0.317822	2.186968
43	6	0	-2.579886	-0.437830	1.012856
44	6	0	-4.606454	-3.295910	-0.333043
45	1	0	3.306717	2.350030	0.332037
46	1	0	3.379236	4.825165	0.360264
47	1	0	1.348543	6.193673	0.146696
48	1	0	-1.349100	6.193492	-0.149301
49	1	0	-3.379670	4.824699	-0.362263
50	1	0	-3.306947	2.349614	-0.332948
51	1	0	1.683714	1.025458	-2.295134
52	1	0	3.339272	0.774149	-4.116431
53	1	0	5.204447	-0.867732	-3.852255
54	1	0	5.403676	-2.194382	-1.805449
55	1	0	4.453034	-2.762547	2.810421
56	1	0	3.416816	-1.927693	4.866600
57	1	0	1.529420	-0.294852	4.752978
58	1	0	0.695787	0.438542	2.540688
59	1	0	-0.694903	0.436463	-2.540723
60	1	0	-1.528178	-0.298090	-4.752785
61	1	0	-3.415882	-1.930601	-4.865849
62	1	0	-4.452824	-2.763905	-2.809406
63	1	0	-5.404322	-2.192968	1.805842
64	1	0	-5.204820	-0.865839	3.852379

65	1	0	-3.339029	0.775414	4.116293
66	1	0	-1.683351	1.025772	2.295008
67	1	0	4.584216	-3.794000	-0.637281
68	1	0	5.649187	-3.047009	0.579900
69	1	0	4.231254	-4.003037	1.077218
70	1	0	-4.584894	-3.793190	0.638886
71	1	0	-5.649629	-3.046926	-0.578951
72	1	0	-4.231667	-4.003350	-1.075421

Optimized structure of **6**

SCF Done: E(RB3LYP) = -1651.84856478 A.U. after 8 cycles

Number of imaginary frequencies: 0



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.278003	0.002672	1.670845
2	7	0	-4.315249	0.001785	1.022394
3	6	0	0.858720	-0.003256	-2.021020
4	6	0	1.968005	-0.004745	-2.845208
5	6	0	1.772667	-0.007032	-4.256379
6	6	0	0.514331	-0.007853	-4.833597
7	6	0	-0.646785	-0.006405	-4.006786
8	6	0	-2.012424	-0.007020	-4.413990
9	6	0	-3.014663	-0.005443	-3.459713
10	6	0	-2.743591	-0.003213	-2.060725
11	6	0	-1.428721	-0.002562	-1.636509

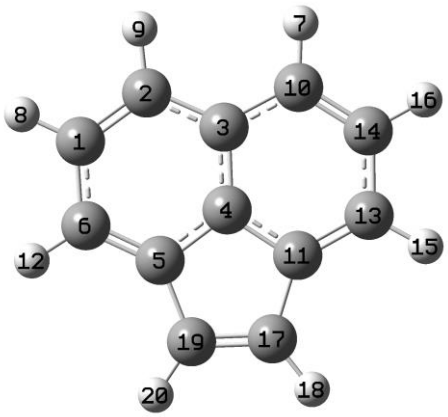
12	6	0	-0.418170	-0.004137	-2.626377
13	6	0	0.627322	-0.000946	-0.556640
14	6	0	-0.730659	-0.000551	-0.327466
15	6	0	1.739470	0.000686	0.464141
16	6	0	2.617421	-1.251698	0.419474
17	6	0	2.197942	-2.451104	-0.156435
18	6	0	2.978095	-3.607710	-0.082299
19	6	0	4.205411	-3.559082	0.573304
20	6	0	4.652348	-2.368234	1.145839
21	6	0	3.862238	-1.208885	1.084279
22	6	0	3.862135	1.212342	1.080465
23	6	0	4.652183	2.371920	1.138376
24	6	0	4.205184	3.560934	0.562092
25	6	0	2.977862	3.607425	-0.093657
26	6	0	2.197755	2.450558	-0.164126
27	6	0	2.617310	1.252993	0.415542
28	6	0	-1.417638	0.001550	1.029260
29	6	0	-2.242158	-1.256148	1.279131
30	6	0	-1.596950	-2.469528	1.525526
31	6	0	-2.308220	-3.647112	1.750239
32	6	0	-3.701229	-3.603116	1.744052
33	6	0	-4.368453	-2.401443	1.517182
34	6	0	-3.651360	-1.215782	1.270572
35	6	0	-3.651154	1.219992	1.266847
36	6	0	-4.368008	2.406566	1.509834
37	6	0	-3.700546	3.608794	1.733005
38	6	0	-2.307525	3.652539	1.739046
39	6	0	-1.596494	2.474133	1.517952
40	6	0	-2.241945	1.260125	1.275301
41	6	0	5.412349	0.004159	2.576759
42	6	0	-5.749750	0.001511	0.790743
43	1	0	2.977582	-0.004206	-2.445616
44	1	0	2.649636	-0.008159	-4.898410
45	1	0	0.410753	-0.009628	-5.916112
46	1	0	-2.265048	-0.008731	-5.471729
47	1	0	-4.052396	-0.005956	-3.783375
48	1	0	-3.570506	-0.002107	-1.358036
49	1	0	1.236928	-2.481856	-0.660145
50	1	0	2.625472	-4.531717	-0.531123
51	1	0	4.831970	-4.445132	0.634493
52	1	0	5.626317	-2.343600	1.621486
53	1	0	5.626141	2.348846	1.614133
54	1	0	4.831726	4.447188	0.620439

55	1	0	2.625172	4.529987	-0.545391
56	1	0	1.236725	2.479682	-0.667899
57	1	0	-0.509236	-2.488047	1.527178
58	1	0	-1.782250	-4.579699	1.931915
59	1	0	-4.280746	-4.503359	1.931087
60	1	0	-5.451240	-2.388279	1.558261
61	1	0	-5.450793	2.393743	1.551029
62	1	0	-4.279876	4.509729	1.917279
63	1	0	-1.781398	4.585586	1.917881
64	1	0	-0.508775	2.492428	1.519522
65	1	0	1.279021	0.002236	1.465678
66	1	0	-0.617147	0.002586	1.778460
67	1	0	5.358994	-0.878031	3.219070
68	1	0	5.359044	0.888494	3.216104
69	1	0	6.386403	0.003261	2.062472
70	1	0	-6.341610	0.003007	1.719099
71	1	0	-6.021939	0.881740	0.204305
72	1	0	-6.022037	-0.880548	0.207089

Optimized structure of acenaphthylene

SCF Done: E(RB3LYP) = -462.08819555 A.U. after 9 cycles

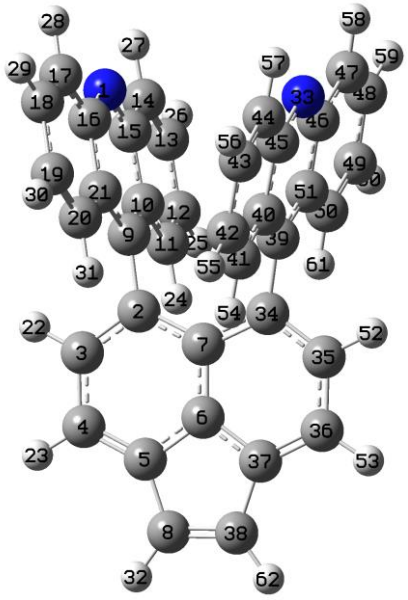
Number of imaginary frequencies: 0



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.429124	1.104046
2	6	0	0.000000	1.282367	1.880437

3	6	0	0.000000	0.000000	1.255871
4	6	0	0.000000	0.000000	-0.141179
5	6	0	-0.000001	1.161464	-0.952137
6	6	0	0.000000	2.390067	-0.321186
7	1	0	0.000000	-1.359383	2.965093
8	1	0	0.000000	3.399139	1.594157
9	1	0	0.000000	1.359383	2.965093
10	6	0	0.000000	-1.282367	1.880437
11	6	0	0.000001	-1.161464	-0.952137
12	1	0	-0.000001	3.323246	-0.879530
13	6	0	0.000000	-2.390067	-0.321186
14	6	0	0.000000	-2.429124	1.104046
15	1	0	0.000001	-3.323246	-0.879530
16	1	0	0.000000	-3.399139	1.594157
17	6	0	0.000003	-0.681869	-2.344802
18	1	0	0.000006	-1.319051	-3.221940
19	6	0	-0.000003	0.681869	-2.344802
20	1	0	-0.000006	1.319051	-3.221940

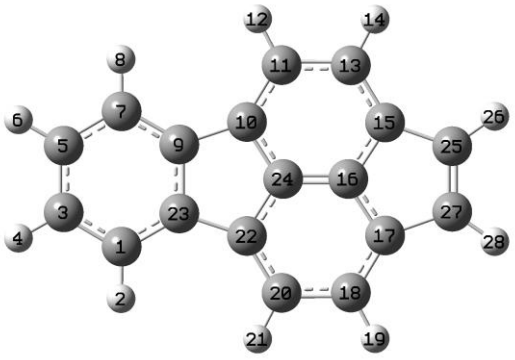
Optimized structure of acenaphthylene-5,6-diyldi(9-acridine)
SCF Done: E(RB3LYP) = -1570.82257871 A.U. after 7 cycles
Number of imaginary frequencies: 0



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.749909	-1.458187	1.774127
2	6	0	1.464224	-0.548130	1.190299
3	6	0	2.282795	-0.957355	2.240465
4	6	0	3.700003	-0.901876	2.212374
5	6	0	4.310417	-0.435422	1.069694
6	6	0	3.483985	0.000005	0.000002
7	6	0	2.077598	0.000004	0.000001
8	6	0	5.701554	-0.254369	0.631386
9	6	0	-0.000929	-0.823624	1.356009
10	6	0	-0.516481	-2.081853	0.973064
11	6	0	0.281150	-3.120918	0.396773
12	6	0	-0.270718	-4.330053	0.062496
13	6	0	-1.658475	-4.577096	0.268137
14	6	0	-2.457979	-3.611171	0.817697
15	6	0	-1.919258	-2.342579	1.200966
16	6	0	-2.245229	-0.282072	2.176601
17	6	0	-3.129677	0.636814	2.824313
18	6	0	-2.672875	1.840693	3.288355
19	6	0	-1.303600	2.201659	3.129506
20	6	0	-0.425688	1.355931	2.504170
21	6	0	-0.858822	0.089649	2.001649
22	1	0	1.801950	-1.369399	3.123295
23	1	0	4.266440	-1.244662	3.074693
24	1	0	1.339479	-2.943327	0.237116
25	1	0	0.353629	-5.110035	-0.365192
26	1	0	-2.077115	-5.540909	-0.009326
27	1	0	-3.516945	-3.769983	0.995127
28	1	0	-4.165270	0.330795	2.933057
29	1	0	-3.352572	2.529658	3.782622
30	1	0	-0.957137	3.160886	3.503788
31	1	0	0.614941	1.637666	2.383708
32	1	0	6.574742	-0.491973	1.227911
33	7	0	-2.749911	1.458177	-1.774128
34	6	0	1.464225	0.548137	-1.190298
35	6	0	2.282797	0.957361	-2.240464
36	6	0	3.700005	0.901884	-2.212370
37	6	0	4.310419	0.435432	-1.069689
38	6	0	5.701555	0.254383	-0.631377
39	6	0	-0.000928	0.823626	-1.356010

40	6	0	-0.516486	2.081853	-0.973063
41	6	0	0.281139	3.120921	-0.396771
42	6	0	-0.270735	4.330054	-0.062494
43	6	0	-1.658492	4.577090	-0.268136
44	6	0	-2.457991	3.611162	-0.817698
45	6	0	-1.919265	2.342573	-1.200966
46	6	0	-2.245226	0.282064	-2.176603
47	6	0	-3.129669	-0.636825	-2.824316
48	6	0	-2.672861	-1.840701	-3.288360
49	6	0	-1.303584	-2.201660	-3.129514
50	6	0	-0.425676	-1.355928	-2.504176
51	6	0	-0.858817	-0.089650	-2.001651
52	1	0	1.801953	1.369402	-3.123296
53	1	0	4.266443	1.244670	-3.074688
54	1	0	1.339469	2.943335	-0.237113
55	1	0	0.353609	5.110038	0.365195
56	1	0	-2.077137	5.540902	0.009327
57	1	0	-3.516958	3.769969	-0.995129
58	1	0	-4.165264	-0.330811	-2.933059
59	1	0	-3.352556	-2.529669	-3.782627
60	1	0	-0.957116	-3.160884	-3.503798
61	1	0	0.614955	-1.637656	-2.383717
62	1	0	6.574744	0.491989	-1.227900

Optimized structure of acefluoranthylene
SCF Done: E(RB3LYP) = -691.92747845 A.U. after 16 cycles
Number of imaginary frequencies: 0



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.994297	-1.413441	-0.000095
2	1	0	-3.006261	-2.500396	-0.000132
3	6	0	-4.202663	-0.696538	0.000001
4	1	0	-5.145416	-1.236692	0.000016
5	6	0	-4.202655	0.696543	0.000097
6	1	0	-5.145400	1.236714	0.000156
7	6	0	-2.994282	1.413437	0.000107
8	1	0	-3.006241	2.500393	0.000193
9	6	0	-1.792803	0.720150	0.000019
10	6	0	-0.380639	1.190705	-0.000087
11	6	0	0.341148	2.379047	-0.000021
12	1	0	-0.159322	3.344151	0.000096
13	6	0	1.784869	2.373506	0.000024
14	1	0	2.291689	3.335714	0.000235
15	6	0	2.498792	1.179385	-0.000087
16	6	0	1.731781	0.000007	-0.000246
17	6	0	2.498809	-1.179380	-0.000090
18	6	0	1.784917	-2.373490	-0.000005
19	1	0	2.291722	-3.335713	0.000207
20	6	0	0.341162	-2.379048	0.000240
21	1	0	-0.159256	-3.344172	0.000366
22	6	0	-0.380635	-1.190741	-0.000041
23	6	0	-1.792810	-0.720169	-0.000076
24	6	0	0.373191	-0.000003	-0.000210
25	6	0	3.898631	0.684668	0.000180
26	1	0	4.785733	1.307779	0.000311
27	6	0	3.898648	-0.684644	0.000040
28	1	0	4.785769	-1.307738	0.000062

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