Revised

Supporting Information (11 pages)

On the Electronic Character of Localized Singlet 2,2-Dimethoxy-cyclopentene-1,3-Diradicals: Substituent Effects on the Lifetime

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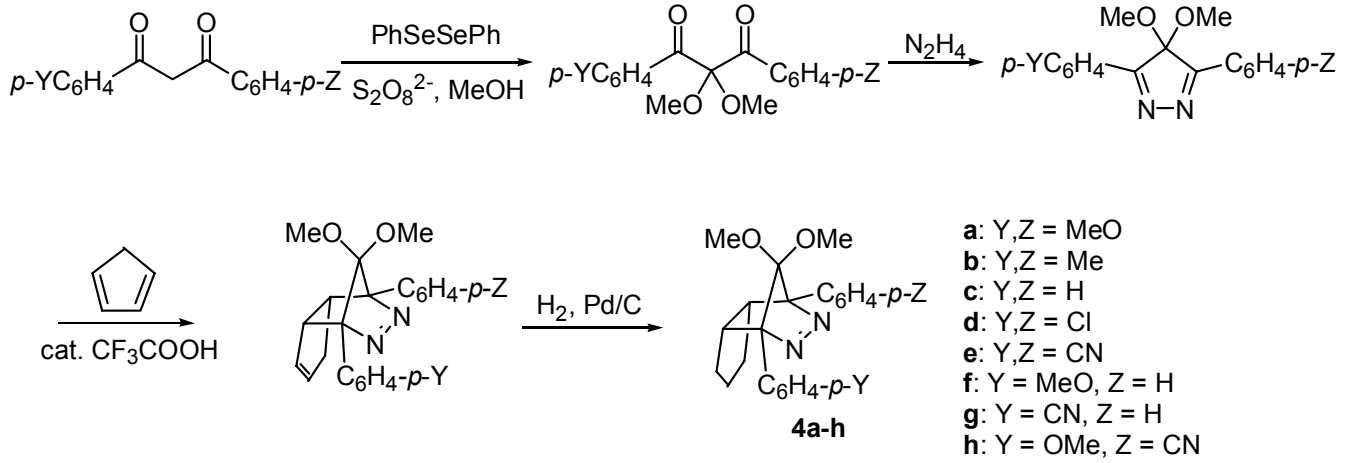
Experimental Section

Preparation of Diazenes 4a-e. The diazenes **4** were prepared according to Scheme S1. 1,3-Diketones were prepared by the reported method.[S1] 2,2-Dimethoxy-1,3-propanediones were synthesized by using the method of Tiecco.[S2] The synthesis of the diazenes **4** followed the Hünig route.[S3]

Scheme S1



The spectroscopic data are as follows:

***endo*-2,3-Diaza-10,10-dimethoxy-1,4-di(4'-methoxyphenyl)tricyclo[5.2.1.05,9]dec-2-ene** (**4a**):

White powder (from MeOH), mp 196-197 °C; IR (KBr): 2993, 2952, 2835, 1612, 1576, 1180, 1034, 1025 cm^{-1}; UV (benzene) λ_{max} 367 (ε 124); ^1H NMR (270 MHz, C_6D_6) δ 1.20-1.58 (m, 6 H), 2.51 (s, 3 H), 2.80 (s, 3 H), 3.35-3.40 (m, 2 H), 3.72 (s, 6 H), 6.68-6.88 (m, 4 H), 7.65-7.71 (m, 4 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 25.7 (2 x t), 27.8 (t), 48.5 (2 x d), 51.4 (q), 51.7 (q), 55.1 (2 x q), 93.9 (s), 113.6 (4 x d), 118.6 (s), 128.6 (2 x s), 129.4 (4 x d), 159.2 (2 x s). Anal. Calcd for $C_{24}H_{28}O_4N_2$: C, 70.57; H, 6.91; N, 6.86. Found: C, 70.50; H, 6.87; N, 6.86.

***endo*-2,3-Diaza-10,10-dimethoxy-1,4-di(4'-methylphenyl)tricyclo[5.2.1.05,9]dec-2-ene** (**4b**):

White powder (from MeOH), mp 156-158 °C; IR (KBr): 2947, 2870, 1511, 1450, 1187, 1118 cm^{-1}; UV (benzene) λ_{max} 366 (ε 119); ^1H NMR (270 MHz, $CDCl_3$) δ 1.35-1.72 (m, 6 H), 2.40 (s, 6 H), 2.65 (s, 3 H), 2.94 (s, 3 H), 3.52-3.60 (m, 2 H), 7.24-7.28 (m, 4 H), 7.77-7.82 (m, 4 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 21.3 (2 x q), 25.8 (2 x t), 28.0 (t), 48.6 (2 x d), 51.6 (q), 51.9 (q), 94.2 (2 x s), 118.9 (s), 128.2

(4 x d), 128.9 (4 x d), 133.4 (2 x s), 137.3 (2 x s). Anal. Calcd for $C_{24}H_{28}N_2O_2$: C, 76.56; H, 7.50; N, 7.44. Found: C, 76.65; H, 7.44; N, 7.26.

***endo*-2,3-Diaza-10,10-dimethoxy-1,4-diphenyltricyclo[5.2.1.05,9]dec-2-ene** (**4c**): White powder (from MeOH), mp 142-143 °C; IR (KBr): 2969, 2943, 2837, 1185, 1118 cm^{-1}; UV (benzene) λ_{max} 367 (ε 112); ^1H NMR (270 MHz, C_6D_6) δ 1.05-1.70 (m, 6 H), 2.50 (s, 3 H), 2.67 (s, 3 H), 3.38-3.42 (m, 2 H), 7.20-7.38 (m, 6 H), 7.95-8.03 (m, 4 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 25.7 (2 x t), 27.8 (t), 48.6 (2 x d), 51.6 (q), 51.8 (q), 94.4 (2 x s), 119.0 (s), 127.8 (2 x d), 128.3 (4 x d), 128.4 (4 x d), 136.4 (2 x s). Anal. Calcd for $C_{22}H_{24}O_2N_2$: C, 75.84; H, 6.94; N, 8.04. Found: C, 75.75; H, 6.85; N, 8.12.

***endo*-2,3-Diaza-10,10-dimethoxy-1,4-di(4'-chlorophenyl)tricyclo[5.2.1.05,9]dec-2-ene** (**4d**): White powder (from MeOH), mp 103-104 °C; IR (KBr): 2946, 2869, 2838, 1488, 1180, 1088 cm^{-1}; UV (benzene) λ_{max} 366 (ε 123); ^1H NMR (270 MHz, $CDCl_3$) δ 1.33-1.66 (m, 6 H), 2.63 (s, 3 H), 2.93 (s, 3 H), 3.45-3.54 (m, 2 H), 7.24-7.44 (m, 4 H), 7.76-7.85 (m, 4 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 25.5 (2 x t), 27.8 (t), 48.8 (2 x d), 51.7 (q), 52.0 (q), 93.9 (2 x s), 119.0 (s), 128.6 (4 x d), 129.7 (4 x d), 134.0 (2 x s), 134.9 (2 x s). Anal. Calcd for $C_{22}H_{22}Cl_2N_2O_2$: C, 63.32; H, 5.31; N,6.71. Found: C,63.22; H,5.22; N,6.74.

***endo*-2,3-Diaza-10,10-dimethoxy-1,4-di(4'-cyanophenyl)tricyclo[5.2.1.05,9]dec-2-ene** (**4e**): White powder (from MeOH), mp 209-210 °C; IR (KBr): 2947, 2870, 2839, 1488, 1180, 1126, 1018 cm^{-1}; UV (benzene) λ_{max} 362 (ε 152); ^1H NMR (270 MHz, $CDCl_3$) δ 1.40-1.68 (m, 6 H), 2.64 (s, 3 H), 2.94 (s, 3 H), 3.48-3.62 (m, 2 H), 7.75-7.79 (m, 4 H), 8.03-8.10 (m, 4 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 25.4 (2 x t) 27.8 (t), 49.1 (2 x d), 51.88 (q), 52.4 (q), 94.3 (2 x s), 112.0 (2 x s), 118.8 (s), 119.7 (s), 129.1 (4 x d), 132.2 (4 x d), 141.5 (2 x s). Anal. Calcd for $C_{24}H_{22}N_4O_2$: C, 72.34; H, 5.56; N, 14.06. Found: C, 72.18; H, 5.63; N, 14.08.

***endo*-2,3-Diaza-10,10-dimethoxy-1-(4'-methoxyphenyl)-4-phenyltricyclo[5.2.1.05,9]dec-2-ene** (**4f**): White powder (from MeOH), mp 139-140 °C; IR (KBr): 2943, 2838, 1516, 1464, 1179, 1126, 1025 cm^{-1}; UV (benzene) λ_{max} 366 (ε 120); ^1H NMR (270 MHz, $CDCl_3$) δ 1.38-1.75 (m, 6 H), 2.65 (s, 3

H), 2.94 (s, 3 H), 3.48-3.62 (m, 2 H), 3.86 (s, 3 H), 6.88-7.05 (m, 2 H), 7.36-7.59 (m, 3 H), 7.78-7.84 (m, 2 H), 7.90-7.97 (m, 2 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 25.7 (t), 25.8 (t), 27.8 (t), 48.4 (d), 48.9 (d), 51.6 (q), 51.8 (q), 55.2 (q), 94.1 (s), 94.2 (s), 113.6 (2 x d), 118.8 (s), 127.6 (d), 128.2 (2 x d), 128.2 (2 x d), 128.4 (s), 129.5 (2 x d), 136.5 (s), 159.1 (s). Anal. Calcd for $C_{23}H_{26}N_2O_3$: C, 72.99; H, 6.92; N, 7.40. Found: C, 72.81; H, 6.89; N, 7.42.

***endo*-2,3-Diaza-10,10-dimethoxy-1-(4'-cyanophenyl)-4-phenyltricyclo[5.2.1.05,9]dec-2-ene** (**4g**): White powder (from MeOH), mp 120-121 °C; IR (KBr): 2943, 2859, 2226, 1212, 1081 cm^{-1}; UV (benzene) λ_{max} 363 (ε 112); ^{1}H NMR (270 MHz, $CDCl_3$) δ 1.40-1.68 (m, 6 H), 2.64 (s, 3 H), 2.94 (s, 3 H), 3.52-3.64 (m, 2 H), 7.38-7.52 (m, 3), 7.72-7.78 (m, 2 H), 7.85-7.90 (m, 2 H), 8.05-8.12 (m, 2 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 25.5 (t), 25.6 (t), 27.8 (t), 48.6 (d), 49.1 (d), 51.7 (q), 52.1 (q), 93.7 (s), 95.0 (s), 111.6 (d), 118.8 (s), 119.4 (s), 128.1 (s), 128.4 (2 x d), 128.5 (2 x d), 129.1 (2 x d), 132.1 (2 x d), 135.8 (s), 142.2 (s). Anal. Calcd for $C_{23}H_{23}N_3O_2$: C, 73.97; H, 6.21; N, 11.25. Found: C, 73.88; H, 6.16; N, 11.18.

***endo*-2,3-diaza-10,10-dimethoxy-1-(4'-cyanophenyl)-4-(4'-methoxyphenyl)tricyclo[5.2.1.05,9]-dec-2-ene** (**4h**): White powder (from MeOH), mp 160-161 °C; IR (KBr): 2950, 2837, 2228, 1517, 1299, 1183, 1082 cm^{-1}; UV (benzene) λ_{max} 364 (ε 129); ^{1}H NMR (270 MHz, $CDCl_3$) δ 1.42-1.68 (m, 6 H), 2.64 (s, 3 H), 2.94 (s, 3 H), 3.48-3.60 (m, 2 H), 3.86 (s, 3 H), 6.96-7.10 (m, 2 H), 7.72-7.81 (m, 4 H), 8.04-8.16 (m, 2 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 25.5 (t), 25.6 (t), 27.8 (t), 48.3 (d), 49.4 (d), 51.6 (q), 52.0 (q), 55.2 (q), 93.4 (s), 94.8 (s), 111.6 (s), 113.8 (2 x d), 118.9 (s), 119.2 (s), 127.8 (s), 129.0 (2 x d), 129.6 (2 x d), 132.1 (2 x d), 142.3 (s), 159.5 (s). Anal. Calcd for $C_{24}H_{25}N_3O_3$: C, 71.44; H, 6.25; N, 10.41. Found: C, 71.35; H, 6.25; N, 10.40.

General Photolysis Procedure. A sample (30.0 mg) of the diazenes **4** was dissolved in 1.0 mL of C_6D_6. The photolysis was performed by using a high-pressure Hg lamp (300 W) and a band-path filter (320-380 nm) at room temperature (ca. 20 ^{o}C). The photolysate was directly analyzed by NMR spectroscopy (^{1}H: 270 MHz, ^{13}C: 68 MHz), which indicated the quantitative formation of the housanes **5**.

The housanes **5b-h** were isolated by using flash chromatography on silica gel, and assigned on the basis of the spectral data; however, the housane **5a** (Ar = *p*-$MeOC_6H_4$) was quite labile to silica gel (acidic conditions) and, thus, the structure was assigned by direct NMR measurements (^1H and ^{13}C), which were quite similar to those of the housanes **5b-h**. The spectroscopic data are as follows:

2,4-Di(4'-methoxyphenyl)-3,3-dimethoxytricyclo[3.3.0.^{1,5}0^{2,4}]octane (5a): ^1H NMR (270 MHz, C_6D_6) δ 1.38-1.59 (m, 3 H), 1.85-2.02 (m, 3 H), 2.88 (s, 3 H), 2.92-2.98 (m, 2 H), 3.27 (s, 6 H), 3.52 (s, 3 H), 6.78-6.84 (m, 4 H), 7.25-7.34 (m, 4 H); ^{13}C NMR (68 MHz, C_6D_6) δ 25.5 (t), 28.5 (2 x t), 41.6 (2 x d), 46.7 (2 x s), 52.3 (q), 54.2 (q), 54.8 (2 x q), 98.5 (s), 113.7 (4 x d), 127.2 (2 x s), 131.5 (4 x d), 158.5 (2 x s).

2,4-Di(4'-methylphenyl)-3,3-dimethoxytricyclo[3.3.0.^{1,5}0^{2,4}]octane (5b): White powder (from *n*-hexane), mp 135-136 °C; IR (KBr): 3956, 1496, 1444, 1397, 1276, 1206, 1119, 1067 cm^{-1}; ^1H NMR (270 MHz, $CDCl_3$) δ 1.35-1.78 (m, 6 H), 2.23 (s, 6 H), 2.70 (s, 3 H), 2.70-2.73 (m, 2 H), 3.57 (s, 3 H), 6.97-7.05 (m, 8 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 21.3 (2 x q), 24.9 (t), 28.0 (2 x t), 41.0 (2 x d), 46.8 (2 x s), 52.5 (q), 54.3 (q), 98.3 (s), 128.3 (4 x d), 129.6 (4 x d), 131.6 (2 x s), 135.4 (2 x d). Anal. Calcd for $C_{24}H_{28}O_2$: C, 82.72; H, 8.10. Found: C, 82.99; H, 8.11.

2,4-Diphenyl-3,3-dimethoxytricyclo[3.3.0^{1,5}0^{2,4}]octane (5c): White powder (from *n*-hexane), mp 107-109 °C; IR (KBr): 2954, 1496, 1442, 1118 cm^{-1}; ^1H NMR (270 MHz, $CDCl_3$) δ 1.35-1.78 (m, 6 H), 2.71 (s, 3 H), 2.74-2.79 (m, 2 H), 3.61 (s, 3 H), 7.10-7.29 (m, 8 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 24.9 (t), 28.0 (2 x t), 41.1 (2 x d), 47.2 (2 x s), 52.5 (q), 54.4 (q), 98.2 (s), 125.9 (2 x d), 127.6 (4 x d), 129.8 (4 x d), 134.6 (2 x s). Anal. Calcd for $C_{22}H_{24}O_2$: C, 82.46; H, 7.55. Found: C, 82.55; H, 7.49.

2,4-Di(4'-chlorophenyl)-3,3-dimethoxytricyclo[3.3.0.^{1,5}0^{2,4}]octane (5d): White powder (from *n*-hexane), mp 132-133 °C;IR (KBr): 2939, 1496, 1257, 1087, 1064, 1025 cm^{-1}; ^1H NMR (270 MHz, $CDCl_3$) δ 1.41-1.65 (m, 6 H), 2.70 (s, 3 H), 2.71-2.75 (m, 2 H), 3.56 (s, 3 H), 6.96-7.03 (m, 4 H), 7.13-7.21 (m, 4 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 24.9 (t), 27.9 (2 x t), 41.0 (2 x d), 46.6 (2 x s), 52.6 (q),

54.4 (q), 98.0 (s), 127.9 (4 x d), 131.0 (4 x d), 132.0 (2 x s). 132.8 (2 x s). Anal. Calcd for $C_{22}H_{22}Cl_2O_2$: C, 67.87; H, 5.70. Found: C, 67.94; H, 5.67.

2,4-Di(4'-cyanophenyl)-3,3-dimethoxytricyclo[3.3.0.^{1,5}0^{2,4}]octane (5e): White powder (from *n*-hexane), mp 146-148 °C; IR (KBr): 2939, 2869, 2222, 1604, 1504, 1450, 1396, 1265, 1126, 1025 cm^{-1}; ^{1}H NMR (270 MHz, $CDCl_3$) δ 1.41-1.68 (m, 6 H), 2.67 (s, 3 H), 2.78-2.83 (m, 2 H), 3.58 (s, 3 H), 7.11-7.18 (m, 4 H), 7.46-7.53 (m, 4 H); ^{13}C NMR (68 MHz, $CDCl_3$) δ 24.9 (t), 27.8 (2 x t), 41.2 (2 x d), 47.9 (2 x s), 52.8 (q), 54.6 (q), 98.2 (s), 110.1 (2 x s), 118.8 (2 x s), 130.2 (4 x d), 131.6 (4 x d), 139.8 (2 x s). Anal. Calcd for $C_{24}H_{22}N_2O_2$: C, 77.81; H, 5.99; N, 7.56. Found: C, 77.42; H, 6.03; N, 7.26.

2-(4'-Methoxyphenyl)-4-phenyl-3,3-dimethoxytricyclo[3.3.0.^{1,5}0^{2,4}]octane (5f): White powder (from *n*-hexane), mp 132-133 °C; IR (KBr): 3062, 2947, 2862, 1604, 1511, 1442, 1241, 1118, 1056 cm^{-1}; ^{1}H NMR (270 MHz, C_6D_6) δ 1.40-1.56 (m, 3 H), 1.85-1.98 (m, 3 H), 2.83 (s, 3 H), 2.88-2.94 (m, 1 H), 2.97-3.02 (m, 1 H), 3.31 (s, 3 H), 3.49 (s, 3 H), 6.60-6.82 (m, 2 H), 7.03-7.38 (m, 7 H); ^{13}C NMR (68 MHz, C_6D_6) δ 25.4 (t), 28.5 (t), 28.5 (t), 41.6 (d), 41.8 (d), 47.1 (s), 47.3 (s), 52.3 (q), 54.2 (q), 54.8 (q), 98.6 (s), 113.7 (2 x d), 126.2 (d), 126.9 (s), 127.9 (2 x d), 130.2 (2 x d), 131.7 (2 x d), 135.7 (s), 158.6 (s). Anal. Calcd for $C_{23}H_{26}O_3$: C, 78.83; H, 7.48. Found: C, 78.55; H, 7.52.

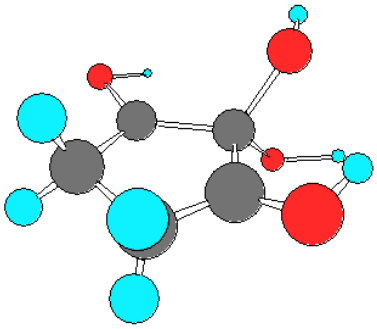
2-(4'-Cyanophenyl)-4-phenyl-3,3-dimethoxytricyclo[3.3.0.^{1,5}0^{2,4}]octane (5g): White powder (from *n*-hexane), mp 144-145 °C; IR (KBr): 2947, 2861, 2221, 1604, 1504, 1442, 1396, 1257, 1126, 1064, 1033 cm^{-1}; ^{1}H NMR (270 MHz, C_6D_6) δ 1.24-1.50 (m, 3 H), 1.56-1.72 (m, 3), 2.63 (s, 3 H), 2.74-2.78 (m, 1 H), 2.81-2.88 (m, 1 H), 3.36 (s, 3 H), 6.91-7.02 (m, 4 H), 7.08-7.22 (m, 5 H); ^{13}C NMR (68 MHz, C_6D_6) δ 25.2 (t), 28.2 (t), 28.2 (t), 41.3 (d), 41.9 (d), 47.2 (s), 48.8 (s), 52.4 (q), 54.3 (q), 98.7 (s), 110.1 (s), 119.1 (s), 126.9 (d), 128.2 (2 x d), 130.2 (2 x d), 130.6 (2 x d), 131.3 (2 x d), 134.0 (s), 140.9 (s). Anal. Calcd for $C_{23}H_{23}NO_2$: C, 79.97; H, 6.71; N, 4.05. Found: C, 79.97; H, 6.78; N, 4.03.

2-(4'-Cyanophenyl)-4-(4'-methoxyphenyl)-3,3-dimethoxytricyclo[3.3.0.^{1,5}0^{2,4}]octane (5h):

White powder (from *n*-hexane), mp 68-69 °C; IR (KBr): 2947, 2861, 2229, 1604, 1511, 1450, 1396, 1249, 1180, 1126, 1033 cm^{-1}; ^{1}H NMR (270 MHz, C_6D_6) δ 1.31-1.58 (m, 3 H), 1.61-1.82 (m, 3 H), 2.67 (s, 3 H), 2.70-2.78 (m, 1 H), 2.85-2.92 (m, 1 H), 3.33 (s, 3 H), 3.39 (s, 3 H), 6.78-6.84 (2 H), 6.92-7.04 (m, 4 H), 7.12-7.18 (m, 2 H); ^{13}C NMR (68 MHz, C_6D_6) δ 25.3 (t), 28.2 (t), 28.3 (t), 41.2 (d), 42.0 (d), 47.0 (s), 48.3 (d), 52.4 (q), 54.3 (q), 54.9 (q), 98.9 (s), 110.0 (s), 113.9 (2 x d), 119.2 (s), 125.6 (s), 130.0 (2 x d), 131.3 (2 x d), 131.9 (2 x d), 141.3 (s), 159.0 (s). Anal. Calcd for $C_{24}H_{25}NO_3$: C, 76.78; H, 6.71; N, 3.73. Found: C, 76.55; H, 6.59; N, 3.44.

Transient Absorption Measurement. Benzene was purchased from Nacalai Tesque (spectrophotometric grade) and used without further purification. Since degassing did not affect the transient kinetics in several control experiments, all measurements were performed in aerated solutions. Solutions of the diazenes **4** in benzene (ca. 0.1 mM) were transferred into the thermostated Quartz cells (10 mm x 10mm) and the temperature was adjusted at 20 ^{o}C (± 0.1 ^{o}C). The THG (355 nm) of a *Q*-switched Nd:YAG laser (Continuum Surelite, 5-ns pulse width, pulse energy ca. 50 mJ) was used for the excitation source. For the measurement of transient absorption spectra and decay traces, the light from a Xe lamp was used as the monitor light and detected with a PMT (photomultiplier; Hamamatau Photonix R928). The decay traces were analyzed by nonlinear least-square fitting of monoexponential functions.

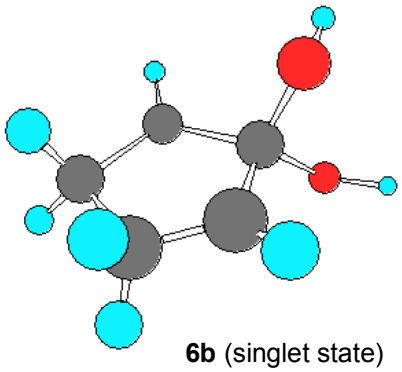
Computational Study. The UB3LYP/6-31G* level of theory was used throughout this work. Optimization of the geometry of singlet diradicals **6a-c** was carried out by using the keyword "guess=mix" within Gaussian 98[S4] suite programs. The bond orders were calculated for the optimized geometry at the same level of theory within SPARTAN 02. Optimized geometries and their Cartesian coordinates are as follows:



6a (singlet state)

SCF Done: E(UB+HF-LYP) = -496.110713301, S**2 = 0.5596

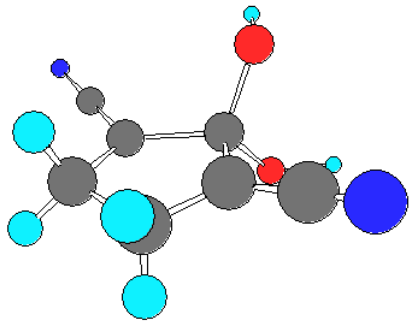
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.000000	1.154621	1.508421
2	6	0.000000	0.000000	0.595705
3	6	-1.097722	0.197269	-0.350121
4	6	-0.775380	0.042750	-1.790720
5	6	0.775380	-0.042750	-1.790720
6	6	1.097722	-0.197269	-0.350121
7	8	0.000000	-1.154621	1.508421
8	1	2.232533	-0.944235	0.950593
9	8	-2.334783	0.572244	0.054551
10	1	-1.206928	-0.867352	-2.236794
11	1	-1.159474	0.886911	-2.381482
12	1	1.206928	0.867352	-2.236794
13	1	1.159474	-0.886911	-2.381482
14	8	2.334783	-0.572244	0.054551
15	1	-2.232533	0.944235	0.950593
16	1	0.630810	0.959989	2.221841
17	1	-0.630810	-0.959989	2.221841



6b (singlet state)

SCF Done: E(UB+HF-LYP) = -345.663286693, S**2 = 0.8685

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.666840	0.000005	-0.000026
2	6	0	0.271456	1.159581	0.030222
3	6	0	1.709877	0.776359	-0.020648
4	6	0	1.709857	-0.776373	0.020696
5	6	0	0.271447	-1.159567	-0.030667
6	8	0	-1.517727	-0.054046	-1.155242
7	8	0	-1.517294	0.054061	1.155536
8	1	0	-0.083956	2.184254	0.087875
9	1	0	2.202988	1.148142	-0.933681
10	1	0	2.281598	1.209223	0.814887
11	1	0	2.202667	-1.148170	0.933892
12	1	0	2.281838	-1.209236	-0.814654
13	1	0	-0.083974	-2.184207	-0.088832
14	1	0	-2.148172	0.681327	-1.058108
15	1	0	-2.147595	-0.681490	1.058806



6c (singlet state)

SCF Done: E(UB+HF-LYP) = -530.172034318, S**2 = 0.9614

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	1.155109	0.095733	1.366017
2	6	0.000000	0.000000	0.561300
3	6	-0.017065	1.176744	-0.397473
4	6	-0.138738	0.761779	-1.834302
5	6	0.138738	-0.761779	-1.834302
6	6	0.017065	-1.176744	-0.397473
7	8	-1.155109	-0.095733	1.366017
8	6	0.000000	2.491022	0.055767
9	1	1.130173	-0.651745	1.990687
10	1	-1.151116	0.971926	-2.209724
11	1	0.550417	1.318321	-2.480133
12	1	1.151116	-0.971926	-2.209724
13	1	-0.550417	-1.318321	-2.480133
14	1	-1.130173	0.651745	1.990687
15	6	0.000000	-2.491022	0.055767
16	7	0.001731	3.597293	0.449026
17	7	-0.001731	-3.597293	0.449026

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