Supporting Information

Ruthenium(II)-Catalyzed Mild and Selective Intramolecular [2 + 2 + 2] Alkyne Cyclotrimerizations

Yoshihiko Yamamoto,[‡] Takayasu Arakawa,[†] Ryuji Ogawa,[†] and Kenji Itoh[†]*

[‡]Department of Applied Chemistry, Graduate School of Engineering, Nagoya University, Chikusa,
Nagoya 464-8603, Japan

[†]Department of Molecular Design and Engineering, Graduate School of Engineering, Nagoya
University, Chikusa, Nagoya 464-8603, Japan

yamamoto@apchem.nagoya-u.ac.jp

Analytical Data for Cycloadducts

4ab: mp. 76-77 °C; IR (CHCl₃) 1737 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, 25 °C): δ 3.37 (s, 3 H), 3.25 (m, 4 H), 3.74 (s, 6 H), 4.40 (s, 2 H), 7.11-7.18 (m, 3 H); ¹³C NMR (75 MHz, CDCl₃, 25 °C): δ 40.38, 40.51, 52.96, 58.11, 60.48, 74.67, 123.59, 123.98, 126.61, 136.97, 139.26, 140.04, 171.83; MS (FAB): *m/z* (%): 279 (63) [MH⁺], 247 (100) [M⁺-OMe], 218 (53) [M⁺-H-CO₂Me], 187 (79) [M⁺-CO₂Me-HOMe]; EA calcd (%) for C₁₅H₁₈O₅ (278.30): C 67.74, H 6.52; found: C 64.62, H 6.55.

4ac: mp. 70-71 °C; IR (CHCl₃) 3396, 1732 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, 25 °C): δ 1.77 (br s, 1 H), 3.58 (s, 4 H), 3.74 (s, 6 H), 4.63 (s, 2 H), 7.16-7.21 (m, 3 H); ¹³C NMR (75 MHz, CDCl₃, 25 °C): δ 40.35, 40.51, 52.99, 60.48, 65.29, 122.90, 124.16, 125.90, 139.24, 139.75, 140.19, 171.83; MS (FAB): *m/z* (%): 265 (88) [MH⁺], 247 (100) [M⁺-OH], 204 (69) [M⁺-H-CO₂Me], 187 (77) [M⁺-CO₂Me-H₂O]; EA calcd (%) for C₁₄H₁₆O₅ (264.27): C 63.63, H 6.10; found: C 63.51, H 6.08.

4ad: IR (CHCl₃) 1732 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, 25 °C): δ 2.26 (s, 6 H), 3.42 (s, 2 H), 3.58 (s, 4 H), 3.74 (s, 6 H), 7.09-7.17 (m, 3 H); ¹³C NMR (75 MHz, CDCl₃, 25 °C): δ 40.32, 40.48, 45.30, 52.91, 60.41, 64.18, 123.73, 124.77, 127.85, 137.46, 138.58, 139.88, 171.84; MS (FAB): *m/z* (%): 292 (100) [MH⁺], 247 (94) [M⁺-NMe₂], 187 (100) [M⁺-CO₂Me-HNMe₂]; EA calcd (%) for C₁₆H₂₁NO₄ (291.34): C 65.96, H 7.27, N 4.81; found: C 65.93, H 7.35, N 4.76.

4ae: IR (CHCl₃) 1732, 1210 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, 25 °C): δ 2.01-2.10 (m, 2 H), 2.73 (t, *J* = 7.5 Hz, 2 H), 3.52 (t, *J* = 6.6 Hz, 2 H), 3.57 (s, 4 H), 3.75 (s, 6 H), 7.00 (d, *J* = 7.5 Hz, 1 H), 7.03 (s, 1 H), 7.11 (d, *J* = 7.5 Hz, 1 H); ¹³C NMR (75 MHz, CDCl₃, 25 °C): δ 32.65, 34.22, 40.32, 40.57, 44.30, 52.97, 60.43, 124.05, 124.22, 127.24, 137.54, 139.44, 140.09, 171.93; MS (FAB): *m/z* (%): 311 (61) [MH⁺], 251 (100) [M⁺-CO₂Me], 187 (57) [M⁺-CO₂Me-CH₃CH₂Cl]; EA calcd (%) for C₁₆H₁₉ClO₄ (310.77): C 61.84, H 6.16; found: C 61.83, H 6.17.

4af: mp. 55.0-55.5 °C; IR (CHCl₃) 1732 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, 25 °C): δ 1.30 (s, 9 H), 3.58 (s, 2 H), 3.60 (s, 2 H), 3.75 (s, 6 H), 7.12 (d, *J* = 8.4 Hz, 1 H), 7.21 (d, *J* = 8.4 Hz, 1 H), 7.22 (s, 1 H); ¹³C NMR (75 MHz, CDCl₃, 25 °C): δ 31.58, 34.63, 40.29, 40.79, 52.93, 60.42, 120.95, 123.53, 124.04, 136.66, 139.52, 150.00, 172.04; MS (FAB): *m/z* (%): 291 (100) [MH⁺], 231 (71) [M⁺-CO₂Me]; EA calcd (%) for C₁₇H₂₂O₄ (290.35): C 70.32, H 7.64; found: C 70.20, H 7.56.

4ag: mp. 70.0-70.5 °C; IR (CHCl₃) 1733 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, 25 °C): δ 3.64 (s, 2 H), 3.66 (s, 2 H), 3.77 (s, 6 H), 7.24-7.57 (m, 9 H); ¹³C NMR (75 MHz, CDCl₃, 25 °C): δ 40.38,

40.65, 53.02, 60.51, 122.91, 124.36, 126.08, 126.98, 127.01, 128.57, 138.87, 140.27, 140.42, 141.11, 171.87; MS (FAB): m/z (%): 310 (100) [M^+], 250 (94) [$M^+ - H - CO_2Me$], 191 (92) [$M^+ - H - 2CO_2Me$]; EA calcd (%) for $C_{19}H_{18}O_4$ (310.34): C 73.53, H 5.85; found: C 73.30, H 5.92.

4ah: mp. 65-66 °C; IR ($CHCl_3$) 1732 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$, 25 °C): δ 3.60 (s, 4 H), 3.75 (s, 6 H), 7.14-7.22 (m, 4 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C) δ 40.64, 52.97, 60.29, 124.10, 126.84, 139.59, 171.90; MS (FAB): m/z (%): 235 (100) [M^+], 203 (45) [$M^+ - OMe$], 174 (48) [$M^+ - H - CO_2Me$]; EA calcd (%) for $C_{13}H_{14}O_4$ (234.25): C 66.66, H 6.02; found: C 66.58, H 6.03.

4ba: mp. 84.5-85.9 °C; IR ($CHCl_3$) 1740 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$, 25 °C): δ 0.92 (t, $J = 7.2$ Hz, 3 H), 1.29-1.42 (m, 2 H), 1.52-1.63 (m, 2 H), 1.82 (s, 6 H), 2.59 (t, $J = 7.8$ Hz, 2 H), 3.69 (s, 2 H), 3.70 (s, 2 H), 7.03 (s, 1 H), 7.04 (d, $J = 7.5$ Hz, 1 H), 7.10 (d, $J = 7.5$ Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ 13.93, 22.32, 28.87, 33.70, 35.38, 45.30, 45.34, 52.54, 104.89, 123.43, 123.68, 127.60, 135.78, 138.78, 142.15, 170.24; MS (FAB): m/z (%): 301 (20) [$M^+ - H$], 245 (98) [$MH^+ - Me_2CO$], 217 (100) [$MH^+ - Me_2CO - CO$]; EA calcd (%) for $C_{18}H_{22}O_4$ (302.36): C 71.50, H 7.33; found: C 70.51, H 7.32.

4ca: IR ($CHCl_3$) 1699 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$, 25 °C): δ 0.92 (t, $J = 7.2$ Hz, 3 H), 1.27-1.40 (m, 2 H), 1.50-1.63 (m, 2 H), 2.17 (s, 6 H), 2.55 (t, $J = 7.8$ Hz, 2 H), 3.47 (s, 4 H), 6.98 (d, $J = 7.8$ Hz, 1 H), 7.01 (s, 1 H), 7.09 (d, $J = 7.8$ Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ 13.83, 22.22, 26.33, 33.68, 35.31, 37.16, 34.41, 74.56, 123.78, 124.04, 126.98, 136.56, 139.46, 141.51, 204.39; MS (FAB): m/z (%): 259 (85) [$M^+ - H$], 215 (100) [$M^+ - MeCO$]; EA calcd (%) for $C_{17}H_{22}O_2$ (258.36): C 79.03, H 8.58; found: C 78.86, H 8.75.

4da: IR ($CHCl_3$) 1698 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$, 25 °C): δ 0.91 (t, $J = 7.2$ Hz, 3 H), 1.27-1.40 (m, 2 H), 1.50-1.61 (m, 2 H), 1.97-2.07 (m, 2 H), 2.55 (t, $J = 7.8$ Hz, 2 H), 2.74-2.79 (m, 4 H), 3.43 (s, 2 H), 3.45 (s, 2 H), 6.97 (d, $J = 7.8$ Hz, 1 H), 6.98 (s, 1 H), 7.05 (d, $J = 7.8$ Hz, 1 H); ^{13}C

NMR (75 MHz, CDCl₃, 25 °C): δ 13.94, 17.72, 22.32, 33.77, 35.40, 37.46, 38.09, 38.63, 72.48, 123.61, 123.92, 127.03, 136.14, 139.39, 141.57, 206.37; MS (FAB): m/z (%): 269 (100) [M⁺-H], 242 (72) [M⁺-CO]; EA calcd (%) for C₁₈H₂₂O₂ (270.37): C 79.96, H 8.20; found: C 79.93, H 8.23.

4ea: IR (CHCl₃) 2255 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, 25 °C): δ 0.93 (t, J = 7.2 Hz, 3 H), 1.28-1.41 (m, 2 H), 1.53-1.64 (m, 2 H), 2.61 (t, J = 7.8 Hz, 2 H), 3.69 (s, 4 H), 7.10 (s, 1 H), 7.11 (d, J = 8.1 Hz, 1 H), 7.18 (d, J = 8.1 Hz, 1 H); ¹³C NMR (75 MHz, CDCl₃, 25 °C): δ 13.92, 22.29, 33.63, 33.74, 35.38, 44.40, 44.63, 116.30, 124.29, 124.49, 128.65, 133.25, 136.13, 143.52; MS (FAB): m/z (%): 223 (56) [M⁺-H], 198 (60) [M⁺-CN], 181 (100) [M⁺-CH₂CH₂CH₃]; EA calcd (%) for C₁₅H₁₆N₂ (224.30): C 80.32, H 7.19, N 12.49; found: C 80.06, H 7.28, N 12.21.

4fa: ¹H NMR (300 MHz, CDCl₃, 25 °C): δ 0.92 (t, J = 7.2 Hz, 3 H), 1.27-1.40 (m, 2 H), 1.51-1.62 (m, 2 H), 2.58 (t, J = 7.5 Hz, 2 H), 3.94 (s, 6 H), 6.99-7.45 (m, 8 H); ¹³C NMR (75 MHz, CDCl₃, 25 °C): δ 14.01, 22.31, 33.96, 35.56, 58.67, 58.89, 60.26, 121.85, 122.17, 126.72, 126.90, 128.18, 128.60, 138.92, 140.02, 141.30; MS (FAB): m/z (%): 264 (100) [M⁺-H], 91 (96) [CH₂Ph]; EA calcd (%) for C₁₉H₂₃N (265.39): C 85.98, H 8.74, N 5.28; found: C 85.89, H 8.71, N 5.20.

4ga: mp. 70-72 °C; IR (CHCl₃) 1346, 1162 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, 25 °C): δ 0.91 (t, J = 7.5 Hz, 3 H), 1.26-1.41 (m, 2 H), 1.49-1.60 (m, 2 H), 2.40 (s, 3 H), 2.57 (t, J = 7.5 Hz, 2 H), 4.59 (s, 4 H), 6.98-7.10 (m, 3 H), 7.31 (d, J = 7.8 Hz, 2 H), 7.78 (d, J = 7.8 Hz, 2 H); ¹³C NMR (75 MHz, CDCl₃, 25 °C): δ 13.94, 21.51, 22.29, 33.78, 35.42, 53.51, 53.64, 122.18, 122.27, 127.43, 127.82, 129.60, 133.14, 133.60, 135.98, 142.59, 143.38; MS (FAB): m/z (%): 330 (100) [MH⁺]; EA calcd (%) for C₁₉H₂₃NO₂S (329.46): C 69.27, H 7.04, N 4.25; found: C 69.28, H 7.05, N 4.02.

4ha: ¹H NMR (300 MHz, CDCl₃, 25 °C): δ 0.94 (t, J = 7.2 Hz, 3 H), 1.30-1.43 (2 H, m), 1.55-1.65 (m, 2 H), 2.63 (t, J = 7.5 Hz, 2 H), 5.09 (s, 4 H), 7.06 (s, 1 H), 7.08 (d, J = 7.8 Hz, 1 H), 7.14 (d, J = 7.8 Hz, 1 H); ¹³C NMR (75 MHz, CDCl₃, 25 °C): δ 14.04, 22.42, 33.98, 35.56, 73.43, 73.49, 120.54, 120.72, 127.41, 136.27, 139.18, 142.07; MS (FAB): m/z (%): 175 (100) [M⁺-H]; EA calcd

(%) for $C_{12}H_{16}O$ (176.25): This compound is unstable and decompose slowly even at $-15\text{ }^{\circ}\text{C}$. Thus, elemental analysis was omitted.

4ia: ^1H NMR (300 MHz, CDCl_3 , $25\text{ }^{\circ}\text{C}$): δ 0.93 (t, $J = 7.5\text{ Hz}$, 3 H), 1.29-1.42 (m, 2 H), 1.53-1.64 (m, 2 H), 2.60 (t, $J = 7.8\text{ Hz}$, 2 H), 4.24 (s, 4 H), 7.03 (d, $J = 7.5\text{ Hz}$, 1 H), 7.07 (s, 1 H), 7.15 (d, $J = 7.5\text{ Hz}$, 1 H); ^{13}C NMR (75 MHz, CDCl_3 , $25\text{ }^{\circ}\text{C}$): δ 14.03, 22.41, 33.87, 35.28, 37.80, 38.05, 124.23, 124.45, 126.91, 137.48, 140.35, 141.50; MS (FAB): m/z (%): 191 (100) $[\text{M}^+-\text{H}]$, 147 (25) $[\text{M}^+-\text{H}-\text{CH}_3\text{CH}_2\text{CH}_3]$; EA calcd (%) for $C_{12}H_{16}S$ (192.32): C 74.94, H 8.39; found: C 74.77, H 8.33.

8: IR (CHCl_3) 1731 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3 , $25\text{ }^{\circ}\text{C}$): δ 0.90 (t, $J = 7.5\text{ Hz}$, 3 H), 1.20 (t, $J = 7.2\text{ Hz}$, 12 H), 1.25-1.38 (m, 2 H), 1.49-1.60 (m, 2 H), 2.52 (t, $J = 7.8\text{ Hz}$, 2 H), 3.47 (s, 2 H), 3.49 (s, 2 H), 4.17 (q, $J = 7.2\text{ Hz}$, 4 H), 4.19 (q, $J = 7.2\text{ Hz}$, 4 H), 6.87 (s, 1 H), 6.91 (d, $J = 8.0\text{ Hz}$, 1 H), 6.97 (d, $J = 8.0\text{ Hz}$, 1 H); ^{13}C NMR (75 MHz, CDCl_3 , $25\text{ }^{\circ}\text{C}$): δ 13.82, 13.99, 22.38, 33.52, 34.42, 34.75, 35.21, 57.48, 57.54, 61.66, 126.25, 127.85, 129.59, 132.22, 140.37, 169.74; MS (FAB): m/z (%): 477 (10) $[\text{MH}^+]$, 431 (100) $[\text{M}^+-\text{OEt}]$, 357 (35) $[\text{M}^+-\text{CO}_2\text{Et}-\text{HOEt}]$, 329 (43) $[\text{M}^+-2\text{CO}_2\text{Et}-\text{H}]$, 283 (35) $[\text{M}^+-2\text{CO}_2\text{Et}-\text{H}-\text{HOEt}]$, 257 (81) $[\text{M}^+-3\text{CO}_2\text{Et}]$; EA calcd (%) for $\text{C}_{26}\text{H}_{36}\text{O}_8$ (476.56): C 65.53, H 7.61; found: C 65.62, H 7.52.

meta-10aa: IR (CHCl_3) 1738 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3 , $25\text{ }^{\circ}\text{C}$): δ 0.91 (t, $J = 7.5\text{ Hz}$, 3 H), 1.28-1.41 (m, 2 H), 1.50-1.61 (m, 2 H), 2.23 (s, 3 H), 2.53 (t, $J = 7.5\text{ Hz}$, 2 H), 3.50 (2 H, s), 3.58 (2 H, s), 3.75 (6 H, s), 6.81 (1 H, s), 6.85 (1 H, s); ^{13}C NMR (75 MHz, CDCl_3 , $25\text{ }^{\circ}\text{C}$): δ 14.06, 19.06, 22.55, 33.98, 35.53, 39.25, 40.79, 52.94, 59.95, 121.36, 128.02, 133.20, 135.83, 139.50, 142.02, 172.15; MS (FAB): m/z (%): 305 (100) $[\text{MH}^+]$, 245 (86) $[\text{M}^+-\text{CO}_2\text{Me}]$, 201 (32) $[\text{M}^+-\text{CO}_2\text{Me}-\text{CH}_3\text{CH}_2\text{CH}_3]$; EA calcd (%) for $\text{C}_{18}\text{H}_{24}\text{O}_4$ (304.38): C 71.03, H 7.95; found: C 70.99, H 7.99.

meta-10ab: IR (CHCl_3) 1738 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3 , $25\text{ }^{\circ}\text{C}$): δ 2.25 (s, 3 H), 3.37 (s, 3 H), 3.51 (s, 2 H), 3.60 (s, 2 H), 3.75 (s, 6 H), 4.37 (s, 2 H), 6.95 (s, 1 H), 7.00 (s, 1 H); ^{13}C NMR (75 MHz, CDCl_3 , $25\text{ }^{\circ}\text{C}$): δ 19.03, 39.29, 40.73, 52.99, 58.12, 59.97, 74.75, 120.93, 127.49, 133.57,

137.21, 138.16, 139.76, 171.99; MS (FAB): m/z (%): 291 (44) [$M^+ - H$], 261 (73) [$M^+ - OMe$], 232 (60) [$M^+ - H - CO_2Me$], 201 (100) [$M^+ - H - OMe - CO_2Me$]; EA calcd (%) for $C_{16}H_{20}O_5$ (292.33): C 65.74, H 6.90; found: C 65.75, H 6.88.

meta-10ag: IR ($CHCl_3$) 1738 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$, 25 °C): δ 2.33 (s, 3 H), 3.59 (s, 2 H), 3.68 (s, 2 H), 3.78 (s, 6 H), 7.23 (s, 1 H), 7.26 (s, 1 H), 7.28-7.60 (m, 5 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ 19.21, 39.31, 40.84, 53.01, 59.97, 120.26, 126.87, 126.97, 126.99, 128.50, 133.83, 137.81, 140.14, 140.57, 141.23, 172.00, 172.06; MS (FAB): m/z (%): 324 (100) [M^+], 265 (77) [$M^+ - CO_2Me$], 205 (65) [$M^+ - H - 2CO_2Me$]; EA calcd (%) for $C_{20}H_{20}O_4$ (324.37): C 74.06, H 6.21; found: C 73.89, H 6.28.

meta-10ai: IR ($CHCl_3$) 1738 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$, 25 °C): δ 2.22 (s, 3 H), 2.28 (s, 3 H), 3.49 (s, 2 H), 3.57 (s, 2 H), 3.75 (s, 6 H), 6.81 (s, 1 H), 6.85 (s, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ 18.97, 21.21, 39.16, 40.73, 52.93, 59.98, 122.02, 128.61, 133.25, 135.57, 136.77, 139.57, 172.09; MS (FAB): m/z (%): 263 (58) [MH^+], 202 (73) [$M^+ - H - CO_2Me$], 143 (100) [$M^+ - H - 2CO_2Me$]; EA calcd (%) for $C_{15}H_{18}O_4$ (262.30): C 68.68, H 6.92; found: C 68.84, H 7.06.

meta-10ba: IR ($CHCl_3$) 1738 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$, 25 °C): δ 0.91 (t, $J = 7.2\text{ Hz}$, 3 H), 1.25-1.42 (m, 2 H), 1.51-1.62 (m, 2 H), 2.56 (t, $J = 7.2\text{ Hz}$, 2 H), 3.38 (s, 3 H), 3.56 (s, 3 H), 3.57 (s, 2 H), 3.74 (s, 6 H), 4.40 (s, 2 H), 6.96 (s, 1 H), 6.97 (s, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ 14.05, 22.52, 33.89, 35.54, 38.77, 40.51, 52.96, 58.17, 60.29, 72.88, 123.47, 126.72, 133.29, 135.68, 140.16, 142.08, 172.02; MS (FAB): m/z (%): 335 (35) [MH^+], 303 (100) [$M^+ - OMe$], 243 (79) [$M^+ - H - OMe - CO_2Me$]; EA calcd (%) for $C_{19}H_{26}O_5$ (334.41): C 68.24, H 7.84; found: C 68.20, H 7.88.

meta-10ca: IR ($CHCl_3$) 1738 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$, 25 °C): δ 0.94 (t, $J = 7.5\text{ Hz}$, 3 H), 1.32-1.45 (m, 2 H), 1.57-1.68 (m, 2 H), 2.63 (t, $J = 7.5\text{ Hz}$, 2 H), 3.64 (s, 4 H), 3.73 (s, 6 H), 7.04 (s, 2 H), 7.25-7.45 (m, 5 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ 14.06, 22.54, 33.86, 35.56,

40.12, 40.67, 52.93, 60.36, 123.12, 126.87, 127.70, 128.21, 128.34, 134.62, 137.85, 140.48, 140.70, 142.34, 171.91; MS (FAB): m/z (%): 367 (99) $[MH^+]$, 307 (100) $[M^+ - CO_2Me]$; EA calcd (%) for $C_{23}H_{26}O_4$ (336.45): C 75.38, H 7.15; found: C 75.28, H 7.25.

meta-10da: IR ($CHCl_3$) 1739, 1250, 893 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$, 25 $^{\circ}C$): δ 0.30 (s, 9 H), 0.93 (t, $J = 7.5$ Hz, 3 H), 1.30-1.43 (m, 2 H), 1.51-1.62 (m, 2 H), 2.56 (t, $J = 7.5$ Hz, 2 H), 3.55 (s, 2 H), 3.59 (s, 2 H), 3.74 (s, 6 H), 7.02 (s, 1 H), 7.10 (s, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 $^{\circ}C$): δ -0.67, 14.08, 22.64, 34.00, 35.70, 40.12, 41.27, 52.93, 60.67, 124.93, 132.66, 134.94, 139.03, 140.86, 142.17, 172.00; MS (FAB): m/z (%): 363 (99) $[MH^+]$, 303 (100) $[M^+ - CO_2Me]$, 259 (54) $[MH^+ - CO_2Me - 3CH_3]$, 231 (65) $[MH^+ - CO_2Me - SiMe_3]$; EA calcd (%) for $C_{20}H_{30}O_4Si$ (362.54): C 66.26, H 8.34; found: C 65.98, H 8.48.

meta-10ea: mp. 59-60 $^{\circ}C$; IR ($CHCl_3$) 1348, 1165 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$, 25 $^{\circ}C$): δ 0.90 (t, $J = 7.5$ Hz, 3 H), 1.23-1.38 (m, 2 H), 1.47-1.58 (m, 2 H), 2.18 (s, 3 H), 2.41 (s, 3 H), 2.53 (t, $J = 7.5$ Hz, 2 H), 4.52 (s, 2 H), 4.60 (s, 2 H), 6.81 (s, 1 H), 6.84 (s, 1 H), 7.31 (d, $J = 8.2$ Hz, 2 H), 7.78 (d, $J = 8.2$ Hz, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 $^{\circ}C$): δ 14.00, 18.70, 21.57, 22.40, 33.92, 35.44, 52.93, 54.01, 119.58, 127.46, 128.66, 129.65, 132.23, 132.34, 133.69, 135.78, 143.03, 143.40; MS (FAB): m/z (%): 342 (100) $[M^+ - H]$, 188 (49) $[MH^+ - SO_2C_6H_4Me]$; EA calcd (%) for $C_{20}H_{25}NO_2S$ (343.48): C 69.93, H 7.34, N 4.08; found: C 69.63, H 7.25, N 3.94.

meta-10fa: 1H NMR (300 MHz, $CDCl_3$, 25 $^{\circ}C$): δ 0.94 (t, $J = 7.2$ Hz, 3 H), 1.30-1.43 (m, 2 H), 1.54-1.64 (m, 2 H), 2.22 (s, 3 H), 2.59 (t, $J = 7.2$ Hz, 2 H), 5.06 (s, 2 H), 5.10 (s, 2 H), 6.88 (s, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 $^{\circ}C$): δ 14.06, 18.86, 22.49, 34.07, 35.51, 72.95, 73.97, 117.94, 128.29, 130.86, 135.32, 138.85, 142.53; MS (FAB): m/z (%): 189 (100) $[M^+ - H]$; EA calcd (%) for $C_{13}H_{18}O$ (190.28): This compound is unstable and decomposes slowly even at -15 $^{\circ}C$. Thus, elemental analysis was omitted.

12: IR ($CHCl_3$) 1738 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$, 25 $^{\circ}C$): δ 0.94 (t, $J = 7.2$ Hz, 3 H), 1.32-

1.56 (m, 4 H), 2.16 (s, 3 H), 2.20 (s, 3 H), 2.54 (t, $J = 7.8$ Hz, 2 H), 3.53 (2 H, s), 3.56 (2 H, s), 3.76 (6 H, s), 6.80 (1 H, s); ^{13}C NMR (75 MHz, CDCl_3 , 25 °C): δ 14.10, 15.18, 18.69, 22.89, 32.93, 33.15, 39.65, 40.32, 52.96, 59.55, 128.50, 128.97, 130.25, 135.64, 138.76, 139.84, 172.28; MS (FAB): m/z (%): 318 (100) $[\text{M}^+]$, 259 (100) $[\text{M}^+-\text{CO}_2\text{Me}]$, 215 (83) $[\text{M}^+-\text{CO}_2\text{Me}-\text{CH}_3\text{CH}_2\text{CH}_3]$; EA calcd (%) for $\text{C}_{19}\text{H}_{26}\text{O}_4$ (318.41): C 71.67, H 8.23; found: C 71.45, H 8.44.

15: IR (CHCl_3) 1732 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3 , 25 °C): δ 1.11 (t, $J = 7.2$ Hz, 6 H), 2.19 (s, 6 H), 2.64 (t, $J = 7.2$ Hz, 4 H), 3.56 (s, 4 H), 3.75 (s, 6 H); ^{13}C NMR (75 MHz, CDCl_3 , 25 °C): δ 14.91, 15.84, 22.44, 40.58, 52.94, 59.06, 128.81, 136.18, 138.99, 172.38; MS (FAB): m/z (%): 317 (51) $[\text{M}^+-\text{H}]$, 259 (100) $[\text{M}^+-\text{CO}_2\text{Me}]$, 199 (75) $[\text{M}^+-\text{H}-2\text{CO}_2\text{Me}]$; EA calcd (%) for $\text{C}_{19}\text{H}_{26}\text{O}_4$ (318.41): C 71.67, H 8.23; found: C 71.70, H 8.20.

18b: IR (CHCl_3) 1733 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3 , 25 °C): δ 3.49 (s, 2 H), 3.61 (s, 2 H), 3.76 (s, 6 H), 5.04 (2 H, s), 5.08 (2 H, s), 7.05 (d, $J = 7.8$ Hz, 1 H), 7.11 (d, $J = 7.8$ Hz, 1 H); ^{13}C NMR (75 MHz, CDCl_3 , 25 °C): δ 38.61, 39.94, 52.72, 60.22, 72.01, 73.27, 119.12, 122.71, 132.49, 134.48, 137.73, 138.86, 171.38; MS (FAB): m/z (%): 275 (100) $[\text{M}^+-\text{H}]$, 215 (31) $[\text{M}^+-2\text{H}-\text{CO}_2\text{Me}]$; EA calcd (%) for $\text{C}_{15}\text{H}_{16}\text{O}_5$ (276.28): C 65.21, H 5.84; found: C 65.34, H 5.71.

18f: mp. 60.5-61.2 °C; ^1H NMR (300 MHz, CDCl_3 , 25 °C): δ 1.80-1.88 (m, 2 H), 2.83-2.87 (m, 2 H), 4.03-4.07 (m, 2 H), 4.67 (s, 2 H), 5.13 (s, 4 H), 6.99 (d, $J = 7.5$ Hz, 1 H), 7.09 (d, $J = 7.5$ Hz, 1 H); ^{13}C NMR (75 MHz, CDCl_3 , 25 °C): δ 29.68, 31.25, 72.92, 74.08, 74.30, 75.38, 118.07, 128.00, 135.62, 137.82, 138.44, 139.30; MS (FAB): m/z (%): 189 (100) $[\text{M}^+-\text{H}]$; EA calcd (%) for $\text{C}_{12}\text{H}_{14}\text{O}_2$ (190.24): C 75.76, H 7.42; found: C 75.64, H 7.54.

18g: ^1H NMR (300 MHz, CDCl_3 , 25 °C): δ 2.25 (s, 3 H), 5.00 (s, 2 H), 5.05 (s, 2 H), 5.09 (s, 4 H), 6.94 (s, 1 H); ^{13}C NMR (75 MHz, CDCl_3 , 25 °C): δ 18.76, 72.00, 72.65, 72.93, 73.17, 120.38, 129.31, 130.22, 131.50, 137.31, 139.08; MS (FAB): m/z (%): 175 (100) $[\text{M}^+-\text{H}]$, 147 (64) $[\text{M}^+-\text{H}-\text{CO}]$, 119 (62) $[\text{M}^+-\text{H}-2\text{CO}]$; EA calcd (%) for $\text{C}_{11}\text{H}_{12}\text{O}_2$ (176.21): C 74.98, H 6.86; found: C 74.92,

H 6.92.

18h: mp. 207-208 °C; ¹H NMR (300 MHz, CDCl₃, 25 °C): δ 2.15 (s, 6 H), 5.03 (s, 4 H), 5.09 (s, 4 H); ¹³C NMR (75 MHz, CDCl₃, 25 °C): δ 15.45, 72.80, 73.24, 128.35, 128.61, 137.95; MS (FAB): *m/z* (%): 189 (100) [M⁺-H]; EA calcd (%) for C₁₂H₁₄O₂ (190.24): C 75.76, H 7.42; found: C 75.77, H 7.40.

The analytical data for **18a,c-e** were consistent with those reported in the literatures.^{1,2}

(1) Peters, J.-U.; Blechert, S. *Chem. Commun.* **1997**, 1983-1984.

(2) Ojima, I.; Vu, A. T.; McCullagh, J. V.; Kinoshita, A. *J. Am. Chem. Soc.* **1999**, *121*, 3230-3231.

Summary of DFT Calculation Data

Compound	Energy (a.u.)	ZPE (kcal/mol)	Imadinary frequency (cm ⁻¹)
acetylene	-77.35659878	16.722	
Ia	-903.52847612	89.699	
TS_{Ia-IIa}	-903.50750530	90.465	432.43i
IIa	-903.58897609	93.886	
IIIa	-980.94987524	112.789	
TS_{IIIa-IVa}	-980.92596174	112.528	360.87i
IVa	-981.09656553	117.741	
TS_{IIIa-Va}	-980.94946945	112.710	162.41i
Va	-980.98384130	114.978	
TS_{Va-VIa}	-980.97664226	114.266	172.53i
VIa	-981.01111085	114.952	
TS_{VIa-IVa}	-981.00178251	114.944	182.88i

VIb	-1177.64710373	203.499	
TS_{VIb-IVb}	-1177.64334767	202.601	220.14i
IVb	-1177.74006824	205.586	
Ic	-1056.21320513	117.213	
TS_{Ic-IIc}	-1056.19360137	117.068	349.26i
IIc	-1056.25171543	118.984	
propyne	-116.69275399	34.974	
IIe	-942.92009432	111.269	
IIIe			
<i>trans-anti</i>	-1059.60950097	148.708	
<i>trans-syn</i>	-1059.60950097	148.708	
<i>cis-anti</i>	-1059.61000678	148.562	
<i>cis-syn</i>	-1059.60960037	148.827	
TS_{IIIe-Ve}			
<i>trans-anti</i>	-1059.60785891	148.448	236.57i
<i>trans-syn</i>	-1059.60770042	148.859	217.90i
<i>cis-anti</i>	-1059.60655697	148.588	148.588i
<i>cis-syn</i>	-1059.60681195	148.873	148.873i
Ve			
<i>trans-anti</i>	-1059.64470150	149.737	
<i>trans-syn</i>	-1059.64329711	150.163	
<i>cis-anti</i>	-1059.63574903	150.481	
<i>cis-syn</i>	-1059.63634132	150.315	
norbornene	-272.79958688	96.407	
VII	-1176.38449297	192.270	
TS_{VII-VIII}	-1176.38064770	192.672	205.920i
VIII	-1176.40097791	193.843	
TS_{VII-IX}	-1176.37906713	192.788	185.320i
IX	-1176.40187096	193.167	

TS_{IX-X}	-1176.38412047	193.433	255.950i
X	-1176.46299153	195.153	
TS_{VIII-XI}	-1176.37394659	193.017	201.170i
XI	-1176.40154220	193.517	

Standard orientations

Ia

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.046157	0.156313	-0.000414
2	17	-1.950116	-1.422577	-0.000677
3	6	2.074487	0.508194	0.713396
4	1	2.324494	1.344441	1.353095
5	6	2.075372	0.511988	-0.707602
6	1	2.328547	1.351352	-1.342903
7	6	1.681468	-0.795322	-1.155691
8	1	1.592954	-1.119027	-2.183968
9	6	1.459181	-1.602090	-0.003377
10	1	1.109247	-2.625069	-0.007199
11	6	1.678539	-0.801704	1.153307
12	1	1.586790	-1.130114	2.180029
13	6	-1.060776	0.588552	1.929791
14	1	-1.433406	-0.173808	2.583262
15	6	-0.847858	1.690487	1.393796
16	1	-0.893554	2.757634	1.291955
17	6	-0.850553	1.692659	-1.390203
18	1	-0.898914	2.759345	-1.285042
19	6	-1.060035	0.592221	-1.929210
20	1	-1.432220	-0.168638	-2.584739

TS_{Ia-IIa}

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.046322	-0.110560	-0.000388

2	17	-1.435717	1.923005	0.000288
3	6	1.948099	-0.880791	-0.742336
4	1	2.014103	-1.742893	-1.392698
5	6	1.952731	-0.910577	0.697617
6	1	2.022317	-1.800451	1.311213
7	6	1.883342	0.431219	1.168722
8	1	1.861449	0.753585	2.200231
9	6	1.796976	1.278083	0.025065
10	1	1.661398	2.351230	0.047779
11	6	1.870768	0.479898	-1.155200
12	1	1.842460	0.845901	-2.172624
13	6	-1.340631	-0.503858	-1.592509
14	1	-1.659204	0.129623	-2.401408
15	6	-1.429423	-1.625659	-0.990211
16	1	-1.574516	-2.683768	-1.136795
17	6	-1.427157	-1.623283	0.994794
18	1	-1.573500	-2.681471	1.144211
19	6	-1.337153	-0.500621	1.595499
20	1	-1.654469	0.135315	2.403605

IIa

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.003076	0.102892	-0.000055
2	17	-0.748604	2.343945	-0.000027
3	6	1.396247	-1.650963	0.003932
4	1	0.989756	-2.652510	0.007912
5	6	1.774599	-0.883672	1.154949
6	1	1.634484	-1.182042	2.185943
7	6	2.397729	0.313082	0.704975
8	1	2.750382	1.118817	1.335992
9	6	2.396636	0.308773	-0.711025
10	1	2.749382	1.109430	-1.347008
11	6	1.773171	-0.891110	-1.152051
12	1	1.631416	-1.195946	-2.181057

13	6	-1.328014	-0.625598	-1.235082
14	1	-1.117538	-0.714095	-2.304081
15	6	-2.533843	-1.081784	-0.702102
16	1	-3.376989	-1.412460	-1.306117
17	6	-2.532881	-1.081595	0.701897
18	1	-3.376807	-1.413480	1.304882
19	6	-1.327831	-0.626616	1.234918
20	1	-1.117378	-0.715148	2.303919

IIIa

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.053954	0.040187	0.109773
2	17	-0.999641	2.239165	-0.590583
3	6	-0.463390	-1.950051	-0.775574
4	1	0.359608	-2.467222	-1.247558
5	6	-1.353458	-1.028794	-1.393727
6	1	-1.334629	-0.705018	-2.424050
7	6	-2.306241	-0.613719	-0.400080
8	1	-3.070970	0.134849	-0.551071
9	6	-2.019864	-1.276308	0.812963
10	1	-2.543241	-1.142895	1.749272
11	6	-0.856261	-2.066181	0.609223
12	1	-0.371360	-2.690415	1.347568
13	6	1.721615	-0.873925	0.800992
14	1	1.712879	-1.363667	1.770931
15	6	2.781240	-0.823475	-0.032467
16	1	3.732523	-1.306640	0.192765
17	6	2.574900	-0.021078	-1.216721
18	1	3.362690	0.143176	-1.952429
19	6	1.346212	0.533671	-1.313996
20	1	1.035940	1.197067	-2.116528
21	6	-0.019649	1.119261	2.042678
22	1	-0.886147	1.349951	2.629088
23	6	1.137044	1.231877	1.597462
24	1	2.117694	1.629107	1.427383

TSIIIa-IVa

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.075273	-0.007582	0.080884
2	17	-0.888678	2.372733	-0.186127
3	6	-1.094411	-1.571247	-1.151780
4	1	-0.555736	-1.995758	-1.987735
5	6	-1.894981	-0.406618	-1.157459
6	1	-2.090568	0.238304	-2.001688
7	6	-2.468205	-0.246008	0.174889
8	1	-3.091407	0.582351	0.479166
9	6	-2.000777	-1.278270	0.988634
10	1	-2.205852	-1.411155	2.043103
11	6	-1.088978	-2.057259	0.202717
12	1	-0.562990	-2.937367	0.543989
13	6	1.547910	-1.292726	0.507917
14	1	1.458981	-2.091967	1.239314
15	6	2.627816	-1.185936	-0.322218
16	1	3.494945	-1.839627	-0.232786
17	6	2.583587	-0.079710	-1.215745
18	1	3.423282	0.192451	-1.853846
19	6	1.422913	0.637424	-1.159190
20	1	1.233587	1.507746	-1.784387
21	6	1.457195	1.409685	1.211071
22	1	1.522975	2.452377	0.989572
23	6	1.319523	0.322197	1.823308
24	1	1.322768	-0.209380	2.757688

IVa

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.662976	0.084504	-0.005043
2	17	-1.616058	2.265804	-0.000300
3	6	-0.119717	-2.051170	0.020869
4	1	0.902836	-2.401720	0.031039

5	6	-0.890066	-1.739055	-1.142323
6	1	-0.562232	-1.846719	-2.168883
7	6	-2.186759	-1.263641	-0.715829
8	1	-2.991613	-0.943034	-1.363776
9	6	-2.197297	-1.248128	0.711275
10	1	-3.011315	-0.913631	1.339793
11	6	-0.906057	-1.712542	1.166429
12	1	-0.593880	-1.800081	2.198900
13	6	3.241856	-0.532998	0.705507
14	1	3.913026	-1.193654	1.248036
15	6	3.238960	-0.542839	-0.700353
16	1	3.908647	-1.210495	-1.236126
17	6	2.393988	0.305802	-1.402881
18	1	2.402758	0.313382	-2.489511
19	6	1.540159	1.186484	-0.709143
20	1	0.958099	1.929569	-1.249237
21	6	1.543012	1.196532	0.698705
22	1	0.963544	1.946200	1.230947
23	6	2.398974	0.324458	1.400883
24	1	2.411748	0.345939	2.486979

TSIIIa-Va

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	44	-0.062530	0.041056	0.099498
2	17	-0.954540	2.268875	-0.561788
3	6	-0.524289	-1.913009	-0.849214
4	1	0.271826	-2.404419	-1.389591
5	6	-1.438802	-0.955972	-1.369518
6	1	-1.477755	-0.582621	-2.383085
7	6	-2.327931	-0.580433	-0.301116
8	1	-3.091127	0.181944	-0.369720
9	6	-1.980601	-1.307186	0.857156
10	1	-2.442193	-1.215244	1.831264
11	6	-0.837406	-2.094704	0.546323
12	1	-0.316831	-2.755401	1.224354
13	6	1.721242	-0.853441	0.816516
14	1	1.710001	-1.365115	1.774657
15	6	2.764920	-0.846830	-0.045897

16	1	3.701922	-1.363199	0.162214
17	6	2.558292	-0.054346	-1.230863
18	1	3.344229	0.102205	-1.970020
19	6	1.331180	0.511295	-1.327724
20	1	1.031850	1.183134	-2.127473
21	6	0.014898	1.102123	2.014250
22	1	-0.830366	1.448900	2.575522
23	6	1.200815	1.133360	1.615591
24	1	2.183031	1.547322	1.491339

Va

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.114011	0.077718	0.010550
2	17	-0.930767	2.403346	0.016405
3	6	-1.675662	-1.076552	-1.369074
4	1	-1.709918	-0.892332	-2.433801
5	6	-2.433397	-0.399855	-0.378662
6	1	-3.117185	0.417333	-0.561416
7	6	-2.115812	-0.937795	0.909924
8	1	-2.536911	-0.610810	1.850569
9	6	-1.102241	-1.895342	0.729073
10	1	-0.628476	-2.480050	1.506790
11	6	-0.795492	-1.963090	-0.689967
12	1	-0.094837	-2.644935	-1.153084
13	6	1.760078	-0.993391	0.506774
14	1	1.654172	-2.057999	0.739610
15	6	2.745684	-0.717920	-0.546758
16	1	3.688919	-1.266333	-0.582157
17	6	2.429570	0.248663	-1.459423
18	1	3.130662	0.608778	-2.211371
19	6	1.128014	0.786622	-1.300493
20	1	0.841750	1.647034	-1.908472
21	6	0.854850	0.676803	1.726307
22	1	0.543655	1.479836	2.386434
23	6	1.920201	-0.114293	1.739428
24	1	2.772931	-0.160094	2.421051

TS_{Va-VIa}

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.143124	0.094086	0.023835
2	17	-1.104138	2.343225	-0.096051
3	6	-0.938920	-1.749708	-1.189320
4	1	-0.479784	-2.047713	-2.123220
5	6	-1.927786	-0.744897	-1.017250
6	1	-2.388811	-0.146066	-1.792154
7	6	-2.252392	-0.685172	0.394605
8	1	-2.963314	-0.003835	0.840976
9	6	-1.464060	-1.643072	1.067589
10	1	-1.448688	-1.822068	2.134077
11	6	-0.630195	-2.278760	0.099914
12	1	0.099769	-3.051264	0.304105
13	6	2.140647	-0.803159	0.727432
14	1	2.323936	-1.763416	1.218948
15	6	2.668985	-0.685304	-0.548861
16	1	3.346946	-1.474352	-0.885751
17	6	2.286569	0.314100	-1.495540
18	1	2.980793	0.608739	-2.282942
19	6	1.014631	0.813911	-1.421789
20	1	0.657765	1.566806	-2.121946
21	6	0.610850	0.816279	1.750425
22	1	0.208958	1.588981	2.395888
23	6	1.835573	0.303453	1.722363
24	1	2.666799	0.623554	2.358721

VIa

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.022685	0.149335	-0.000898
2	17	-0.492021	2.412355	-0.018780
3	6	-1.417730	-1.436673	0.013805

4	1	-0.839741	-2.363464	0.023999
5	6	-2.237542	-1.081764	-1.164458
6	1	-1.953444	-1.271737	-2.192796
7	6	-3.369325	-0.458030	-0.727055
8	1	-4.148923	-0.031809	-1.348916
9	6	-3.370552	-0.442272	0.730862
10	1	-4.151327	-0.004264	1.341945
11	6	-2.238900	-1.057221	1.182416
12	1	-1.957110	-1.226167	2.214973
13	6	3.435003	-0.550421	0.703721
14	1	4.416918	-0.725067	1.140399
15	6	3.434191	-0.562701	-0.697225
16	1	4.416223	-0.744974	-1.131514
17	6	2.418604	-0.416903	-1.645674
18	1	2.756980	-0.539318	-2.677597
19	6	1.051700	-0.154372	-1.510152
20	1	0.493774	-0.067606	-2.452022
21	6	1.053315	-0.129877	1.512750
22	1	0.496168	-0.029610	2.453833
23	6	2.420183	-0.390008	1.651216
24	1	2.759293	-0.495319	2.685224

TS_{VIa-IVa}

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	0.494393	-0.151908	0.094597
2	17	1.940204	-2.017938	0.303631
3	6	0.900667	1.217013	-1.538842
4	1	0.821719	0.859551	-2.557152
5	6	2.109505	1.272569	-0.746966
6	1	3.071465	0.875888	-1.040654
7	6	1.806604	1.887088	0.487257
8	1	2.489890	2.030130	1.314255
9	6	0.409171	2.161206	0.498188
10	1	-0.145398	2.568433	1.332043
11	6	-0.156559	1.792263	-0.762708
12	1	-1.183397	1.921324	-1.069590
13	6	-3.187416	0.456660	0.327696

14	1	-4.074100	1.069587	0.482730
15	6	-3.083685	-0.221601	-0.867579
16	1	-3.905925	-0.111245	-1.573096
17	6	-2.134863	-1.245310	-1.140163
18	1	-2.480147	-2.018269	-1.833855
19	6	-0.899574	-1.448040	-0.576729
20	1	-0.495086	-2.458657	-0.652718
21	6	-1.026264	-0.140218	1.442414
22	1	-0.533636	-0.253240	2.416157
23	6	-2.326236	0.272634	1.449335
24	1	-2.770230	0.479827	2.426440

Iib

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.415354	-0.363011	-0.000889
2	17	-0.385154	-2.743116	-0.004563
3	6	0.434571	1.703903	0.007913
4	6	-0.395492	2.956305	0.013823
5	1	-1.041979	3.010145	-0.866110
6	1	0.240853	3.852201	0.018813
7	1	-1.042448	3.000345	0.894868
8	6	1.002989	1.068375	-1.160054
9	6	0.785049	1.508007	-2.576677
10	1	0.933376	0.689042	-3.286299
11	1	1.485318	2.311488	-2.844976
12	1	-0.227707	1.897998	-2.721579
13	6	1.911156	0.054163	-0.715181
14	6	2.713407	-0.878060	-1.574066
15	1	2.562621	-1.920674	-1.269452
16	1	3.787228	-0.660774	-1.493196
17	1	2.437532	-0.796003	-2.627850
18	6	1.912272	0.047072	0.710804
19	6	2.716553	-0.893435	1.558901

20	1	2.446668	-0.817995	2.615107
21	1	3.790496	-0.678772	1.472762
22	1	2.559830	-1.933298	1.248520
23	6	1.005879	1.057803	1.166925
24	6	0.791706	1.484927	2.588276
25	1	-0.218989	1.877510	2.738385
26	1	1.494188	2.283877	2.862966
27	1	0.938278	0.659778	3.290641
28	6	-1.900060	-0.039503	1.232927
29	1	-1.724363	0.083842	2.305359
30	6	-3.182498	0.086048	0.702127
31	1	-4.086008	0.173533	1.304271
32	6	-3.181318	0.090300	-0.704866
33	1	-4.084352	0.182630	-1.307713
34	6	-1.898426	-0.030868	-1.236057
35	1	-1.722104	0.100349	-2.306612

VIIb

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	0.018325	-0.545901	-0.245856
2	17	-0.891159	-2.533901	-1.206463
3	6	1.489240	-1.572302	0.494025
4	6	2.787156	-1.278424	0.870838
5	6	3.630174	-0.230960	0.437951
6	6	3.519544	0.615746	-0.655204
7	6	2.478642	0.767529	-1.599827
8	6	1.152038	0.386210	-1.548761
9	1	0.546807	0.742821	-2.390277
10	1	2.776441	1.305188	-2.504413
11	1	4.408009	1.210405	-0.866350
12	1	4.591949	-0.182201	0.948942
13	1	3.279615	-2.000552	1.529701
14	1	1.183583	-2.600718	0.725205
15	6	-0.600540	0.561464	1.570522
16	6	-0.183809	1.634601	0.725609
17	6	-1.207542	1.828249	-0.291717
18	6	-2.186451	0.836920	-0.137984
19	6	-1.813251	0.018004	0.989386
20	6	0.940393	2.587759	1.001114

21	1	0.575503	3.472492	1.543736
22	1	1.413485	2.937472	0.077910
23	1	1.718405	2.117360	1.607079
24	6	-0.042787	0.228763	2.925556
25	1	-0.503417	0.872587	3.689034
26	1	1.039486	0.377259	2.962494
27	1	-0.244009	-0.809676	3.201018
28	6	-2.659046	-1.079142	1.570279
29	1	-3.478421	-0.651910	2.167107
30	1	-2.078201	-1.733426	2.226691
31	1	-3.095097	-1.704675	0.787963
32	6	-3.397916	0.588876	-0.987781
33	1	-3.400175	-0.438519	-1.369955
34	1	-3.439353	1.264998	-1.845762
35	1	-4.321044	0.727630	-0.409332
36	6	-1.129485	2.885706	-1.345058
37	1	-1.101798	3.887675	-0.898263
38	1	-1.978168	2.848631	-2.032457
39	1	-0.208350	2.779144	-1.936224

TS_{Vib-IVb}

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.128773	-0.527779	-0.148406
2	17	-1.290115	-2.511714	-0.864412
3	6	-0.675691	0.752460	1.549551
4	6	-0.343790	0.417325	2.973472
5	1	-0.827209	1.129799	3.656111
6	1	0.732997	0.457365	3.149940
7	1	-0.689495	-0.585669	3.242065
8	6	-1.922207	0.427849	0.870613
9	6	-3.045433	-0.391717	1.437075
10	1	-3.811801	0.262950	1.875726
11	1	-2.697610	-1.065564	2.224767
12	1	-3.518135	-1.004108	0.665299
13	6	-1.926650	1.072339	-0.398913
14	6	-3.035228	0.983267	-1.404478
15	1	-3.402686	-0.044485	-1.488032

16	1	-2.709106	1.302127	-2.397412
17	1	-3.882203	1.618842	-1.110820
18	6	-0.685492	1.765153	-0.535508
19	6	-0.268055	2.624927	-1.687074
20	1	-0.372361	3.686187	-1.427161
21	1	-0.874374	2.438782	-2.578438
22	1	0.781351	2.450050	-1.945778
23	6	0.085867	1.594915	0.677681
24	6	1.300711	2.389244	1.051179
25	1	1.002749	3.351070	1.492801
26	1	1.928031	2.601518	0.182128
27	1	1.919673	1.861710	1.779349
28	6	3.529997	0.396014	-0.488013
29	1	4.387166	1.052968	-0.636437
30	6	3.535560	-0.400255	0.641370
31	1	4.402627	-0.324977	1.296463
32	6	2.655064	-1.481404	0.863225
33	1	3.050652	-2.283942	1.494368
34	6	1.417975	-1.711007	0.300729
35	1	1.115206	-2.760006	0.235087
36	6	1.324421	-0.197912	-1.536914
37	1	0.817700	-0.226693	-2.507575
38	6	2.600420	0.311708	-1.557062
39	1	2.959966	0.686084	-2.519161

IVb

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.310671	0.431834	-0.000718
2	17	-0.956411	2.752627	-0.005280
3	6	-0.166965	-1.785057	0.020458
4	6	1.020327	-2.700618	0.038842
5	1	0.696662	-3.751722	0.040716
6	1	1.640273	-2.545146	0.926279
7	1	1.658284	-2.551639	-0.835709
8	6	-0.857108	-1.320599	-1.152267
9	6	-0.491998	-1.640721	-2.572094
10	1	-0.983701	-2.570073	-2.894672

11	1	0.587046	-1.779811	-2.689576
12	1	-0.804248	-0.848344	-3.258023
13	6	-2.044341	-0.594422	-0.731949
14	6	-3.094521	-0.015068	-1.631098
15	1	-3.908291	-0.735924	-1.791446
16	1	-2.682600	0.246454	-2.610067
17	1	-3.522813	0.894382	-1.202452
18	6	-2.061352	-0.581121	0.707012
19	6	-3.133545	0.008735	1.572836
20	1	-3.949316	-0.711975	1.723490
21	1	-3.553830	0.911950	1.123500
22	1	-2.744637	0.283493	2.557832
23	6	-0.883126	-1.297048	1.168662
24	6	-0.547040	-1.587658	2.601746
25	1	-1.048749	-2.506591	2.936134
26	1	-0.869302	-0.778317	3.262764
27	1	0.529004	-1.728802	2.741274
28	6	3.758575	-0.351279	0.703199
29	1	4.430783	-1.013072	1.244648
30	6	3.758584	-0.356457	-0.700791
31	1	4.430798	-1.021226	-1.237339
32	6	2.912316	0.494690	-1.402940
33	1	2.922318	0.504688	-2.488983
34	6	2.062033	1.372995	-0.706179
35	1	1.473799	2.112837	-1.241914
36	6	2.061025	1.376179	0.699819
37	1	1.472785	2.119953	1.230077
38	6	2.912300	0.503030	1.401048
39	1	2.923289	0.520039	2.486994

Ic

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.374383	0.054556	0.000101
2	17	-1.215533	2.379619	0.000308
3	6	-0.716268	-2.062216	0.710014
4	1	0.001303	-2.564356	1.345748
5	6	-0.716087	-2.062464	-0.710986

6	1	0.002451	-2.563753	-1.346252
7	6	-1.829714	-1.268541	-1.154565
8	1	-2.106902	-1.075716	-2.181464
9	6	-2.520778	-0.802811	-0.000317
10	1	-3.377443	-0.141211	-0.000967
11	6	-1.830866	-1.268946	1.153435
12	1	-2.108426	-1.075219	2.180538
13	6	0.365518	0.824937	1.943490
14	1	-0.220665	1.398610	2.631792
15	6	1.352149	0.319194	1.374218
16	6	1.352118	0.320610	-1.373781
17	6	0.365672	0.825958	-1.942510
18	1	-0.221311	1.399164	-2.632209
19	6	2.768434	-0.071080	1.176002
20	1	3.094605	-0.706813	2.005671
21	1	3.396285	0.836957	1.173463
22	8	3.003430	-0.826029	-0.000390
23	6	2.769389	-0.069672	-1.175998
24	1	3.096129	-0.702392	-2.006327
25	1	3.396062	0.839146	-1.170536

TS_{IC-IIc}

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.483238	0.031007	-0.000078
2	17	-1.055516	2.427141	-0.000169
3	6	-1.205429	-1.982692	0.720924
4	1	-0.604638	-2.618978	1.357976
5	6	-1.203211	-1.984588	-0.717076
6	1	-0.601145	-2.623829	-1.351024
7	6	-2.165161	-1.028701	-1.161157
8	1	-2.404030	-0.783131	-2.187178
9	6	-2.735787	-0.425426	-0.002206
10	1	-3.446751	0.388917	-0.004269
11	6	-2.167566	-1.024789	1.159843
12	1	-2.409755	-0.776379	2.183822
13	6	0.633938	0.723195	1.627974
14	1	0.319504	1.287482	2.488942

15	6	1.613407	0.180371	1.020047
16	6	1.613532	0.180323	-1.019953
17	6	0.634137	0.723119	-1.627025
18	1	0.319810	1.287366	-2.488058
19	6	2.949269	-0.476891	1.146144
20	1	2.811310	-1.560517	1.313161
21	1	3.483323	-0.056267	2.004168
22	8	3.742986	-0.250416	0.000187
23	6	2.949343	-0.475946	-1.146856
24	1	2.812403	-1.559513	-1.313839
25	1	3.483502	-0.055362	-2.002833

IIc

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	0.000000	0.721729	0.000000
2	17	-2.321126	1.177397	0.000000
3	6	2.215737	1.077836	0.000000
4	1	2.891706	0.233338	0.000000
5	6	1.739095	1.784137	1.153000
6	1	1.931865	1.512458	2.182999
7	6	1.001468	2.914236	0.708000
8	1	0.475908	3.617067	1.342001
9	6	1.001468	2.914236	-0.708000
10	1	0.475908	3.617067	-1.342001
11	6	1.739095	1.784137	-1.153000
12	1	1.931865	1.512458	-2.182999
13	6	-0.030940	-0.780450	-1.258000
14	1	0.150896	-0.645896	-2.327000
15	6	-0.241593	-2.037662	-0.700000
16	6	-0.241593	-2.037662	0.700000
17	6	-0.030940	-0.780450	1.258000
18	1	0.150896	-0.645896	2.327000
19	6	-0.469995	-3.441766	-1.186000
20	1	0.306952	-3.803239	-1.874001
21	1	-1.440812	-3.542533	-1.696000
22	8	-0.444128	-4.251230	0.000000
23	6	-0.469995	-3.441766	1.186000
24	1	0.306952	-3.803239	1.874001
25	1	-1.440812	-3.542533	1.696000

IId

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	44	-0.005186	-0.473135	0.082647
2	17	0.016579	-1.039441	2.393360
3	6	0.224377	-0.782262	-2.145980
4	1	0.440924	0.062781	-2.784779
5	6	-1.078368	-1.292063	-1.835264
6	1	-2.018597	-0.847295	-2.131520
7	6	-0.918765	-2.483978	-1.081432
8	1	-1.719453	-3.078476	-0.661264
9	6	0.473358	-2.715410	-0.911686
10	1	0.913782	-3.522073	-0.340410
11	6	1.183833	-1.684694	-1.578461
12	1	2.258784	-1.592192	-1.644170
13	6	1.277312	1.020962	0.174705
14	6	0.706885	2.310116	0.282752
15	1	1.301602	3.212140	0.418937
16	6	-0.680116	2.316526	0.289209
17	1	-1.265400	3.225050	0.430802
18	6	-1.264692	1.034931	0.183582
19	6	2.730354	0.844823	0.093339
20	6	3.353894	-0.252820	0.723637
21	1	2.740276	-0.941853	1.296175
22	6	4.734937	-0.422241	0.657405
23	1	5.199358	-1.264803	1.164056
24	6	5.521444	0.488198	-0.051438
25	1	6.598479	0.350514	-0.108054
26	6	4.921905	1.581885	-0.683810
27	1	5.530519	2.292590	-1.236976
28	6	3.544860	1.763101	-0.605376
29	1	3.081440	2.609562	-1.105961
30	6	-2.719651	0.863701	0.107029
31	6	-3.532144	1.766733	-0.610539
32	1	-3.069565	2.604774	-1.126502
33	6	-4.909099	1.580600	-0.691366
34	1	-5.517483	2.279134	-1.259435

35	6	-5.509559	0.496202	-0.041532
36	1	-6.585523	0.354813	-0.100671
37	6	-4.723066	-0.398026	0.687193
38	1	-5.187645	-1.232154	1.208223
39	6	-3.342110	-0.223704	0.756816
40	1	-2.728729	-0.899579	1.345272

Ile

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	0.110942	0.089777	-0.224638
2	17	-0.596923	2.341395	-0.413758
3	6	1.392984	-1.506259	0.723248
4	1	0.923406	-2.392262	1.129957
5	6	1.744081	-0.318847	1.448109
6	1	1.532362	-0.121828	2.489263
7	6	2.440356	0.543431	0.558989
8	1	2.787357	1.541442	0.792547
9	6	2.557917	-0.102105	-0.696947
10	1	3.014912	0.313158	-1.586098
11	6	1.898693	-1.358935	-0.608494
12	1	1.819613	-2.095121	-1.397047
13	6	-0.936994	-0.840654	-1.557383
14	1	-0.508451	-1.125812	-2.521676
15	6	-2.243773	-1.214477	-1.217191
16	1	-2.952247	-1.642378	-1.925687
17	6	-2.549656	-0.975584	0.124430
18	1	-3.512907	-1.208857	0.575684
19	6	-1.499131	-0.372877	0.830700
20	6	-1.622643	-0.048679	2.286426
21	1	-2.576801	-0.391745	2.708388
22	1	-1.544208	1.037601	2.430598
23	1	-0.807786	-0.498210	2.870703

IIIe *trans-anti*

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	0.255272	-0.008408	-0.176606
2	17	0.037174	2.353069	0.640897
3	6	1.638165	-1.529889	0.652546
4	1	1.201899	-2.379349	1.158375
5	6	1.992035	-0.278872	1.232714
6	1	1.875557	0.010038	2.267017
7	6	2.574903	0.535628	0.199087
8	1	2.884074	1.564592	0.322860
9	6	2.580506	-0.196252	-1.003679
10	1	2.923786	0.160486	-1.965719
11	6	1.959046	-1.452265	-0.749164
12	1	1.803477	-2.241494	-1.471744
13	6	-0.808596	-1.609200	-1.008699
14	1	-0.607558	-1.892716	-2.040482
15	6	-1.725341	-2.201784	-0.223178
16	1	-2.316130	-3.060608	-0.545781
17	6	-1.905207	-1.585176	1.070313
18	1	-2.615133	-1.979966	1.800732
19	6	-1.158222	-0.481884	1.319104
20	6	-1.237458	0.241350	2.633415
21	1	-0.272402	0.269682	3.155239
22	1	-1.537325	1.285090	2.506055
23	1	-1.959081	-0.262803	3.292414
24	6	-0.297961	1.010656	-2.081899
25	1	0.449289	1.453632	-2.708810
26	6	-1.431244	0.810012	-1.622918
27	6	-2.853905	0.866420	-1.294708
28	1	-3.007190	1.558842	-0.460180
29	1	-3.415940	1.228039	-2.163549
30	1	-3.231577	-0.118164	-1.008588

IIIe *trans-syn*

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	0.055398	0.101379	0.065897

2	17	0.822924	-1.703462	-1.507507
3	6	-0.444121	2.198618	-0.448441
4	1	-1.458229	2.521909	-0.262794
5	6	0.051301	1.588525	-1.633470
6	1	-0.511816	1.362316	-2.526605
7	6	1.457327	1.350007	-1.443511
8	1	2.097394	0.832945	-2.143765
9	6	1.833070	1.821886	-0.169161
10	1	2.819237	1.756753	0.269738
11	6	0.659261	2.297395	0.476528
12	1	0.603357	2.707844	1.474017
13	6	-0.993712	0.495643	1.845053
14	1	-0.440441	0.844024	2.713753
15	6	-2.324660	0.293602	1.810555
16	1	-2.975981	0.503697	2.660101
17	6	-2.817618	-0.280556	0.585254
18	1	-3.876259	-0.505919	0.443432
19	6	-1.896403	-0.539244	-0.377742
20	6	-2.284504	-1.131159	-1.702972
21	1	-1.965882	-0.508385	-2.548139
22	1	-1.819203	-2.107803	-1.860368
23	1	-3.377135	-1.242201	-1.756990
24	6	1.358076	-1.217442	1.422742
25	6	2.824441	-1.286769	1.397695
26	1	3.162503	-2.116067	2.031479
27	1	3.163935	-1.476353	0.373652
28	1	3.294588	-0.366736	1.762050
29	6	0.167615	-1.523479	1.605854
30	1	-0.683733	-2.110020	1.888309

IIIe *cis-anti*

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	0.255437	0.041194	-0.023224
2	17	0.832318	2.478449	0.200053
3	6	1.360843	-1.650491	0.869012
4	1	0.839535	-2.260273	1.592693
5	6	2.110243	-0.469487	1.135700

6	1	2.256909	-0.004202	2.099766
7	6	2.674447	-0.019314	-0.107011
8	1	3.246926	0.889212	-0.236818
9	6	2.283210	-0.906030	-1.129807
10	1	2.522718	-0.810737	-2.180867
11	6	1.442513	-1.893937	-0.549815
12	1	0.994574	-2.725395	-1.073735
13	6	-1.399251	-1.315250	-0.039095
14	6	-1.719704	-2.209345	-1.205298
15	1	-2.732402	-2.623419	-1.099581
16	1	-1.674971	-1.670346	-2.158283
17	1	-1.034046	-3.064570	-1.289781
18	6	-2.138920	-1.294634	1.092765
19	1	-3.001504	-1.951596	1.225048
20	6	-1.757886	-0.321918	2.091582
21	1	-2.295160	-0.217130	3.034176
22	6	-0.718611	0.460778	1.740948
23	1	-0.312879	1.258781	2.356303
24	6	-0.531504	0.736518	-1.990502
25	1	0.080675	0.718458	-2.868657
26	6	-1.488020	1.063272	-1.274992
27	6	-2.675266	1.661377	-0.670901
28	1	-2.371509	2.464698	0.007754
29	1	-3.314472	2.079807	-1.458295
30	1	-3.245604	0.921298	-0.104280

IIIe *cis-syn*

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.079051	-0.109468	-0.098882
2	17	-1.967835	0.409480	-1.690452
3	6	0.372032	-2.157197	0.636614
4	1	1.310696	-2.600227	0.333567
5	6	-0.857998	-2.215269	-0.069213
6	1	-1.038005	-2.699722	-1.017998
7	6	-1.844748	-1.520500	0.718789
8	1	-2.864951	-1.340933	0.413135
9	6	-1.237988	-1.059638	1.903663

10	1	-1.714994	-0.475443	2.680113
11	6	0.138293	-1.400939	1.842526
12	1	0.874388	-1.190798	2.603555
13	6	1.961660	0.353956	0.397173
14	6	2.371461	0.928605	1.723186
15	1	3.385518	1.346458	1.661491
16	1	1.698952	1.733483	2.039956
17	1	2.382749	0.184245	2.531410
18	6	2.830883	0.103103	-0.610316
19	1	3.903301	0.275798	-0.494387
20	6	2.258359	-0.328277	-1.862097
21	1	2.874015	-0.527461	-2.739663
22	6	0.911237	-0.423600	-1.866395
23	1	0.317771	-0.706457	-2.731277
24	6	-0.526937	2.073349	0.435113
25	6	-1.667365	2.516087	1.247840
26	1	-1.708882	3.613173	1.257844
27	1	-2.594429	2.138773	0.805014
28	1	-1.602530	2.163968	2.282721
29	6	0.395229	2.057630	-0.394614
30	1	1.083128	2.376706	-1.150602

TS_{Me-Ve} *trans-anti*

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	44	0.261530	-0.047868	-0.153569
2	17	0.328692	2.445975	-0.201020
3	6	1.535828	-1.474041	0.974370
4	1	1.061088	-2.094222	1.721129
5	6	2.073285	-0.168410	1.166440
6	1	2.093949	0.391470	2.089263
7	6	2.623836	0.263484	-0.090621
8	1	3.043352	1.240718	-0.279600
9	6	2.444228	-0.761970	-1.042227
10	1	2.718373	-0.715981	-2.088163
11	6	1.731231	-1.818849	-0.410074
12	1	1.420346	-2.743641	-0.875011
13	6	-1.111696	-1.635092	-0.411041

14	1	-1.005205	-2.304154	-1.259708
15	6	-1.941269	-1.850727	0.639163
16	1	-2.600603	-2.717431	0.698007
17	6	-1.907824	-0.839974	1.655984
18	1	-2.581453	-0.871287	2.514614
19	6	-1.014563	0.173023	1.484645
20	6	-0.909143	1.299361	2.472340
21	1	0.107770	1.414786	2.869102
22	1	-1.159045	2.260295	2.012623
23	1	-1.585594	1.123823	3.321124
24	6	-0.422324	0.400383	-2.151654
25	1	0.153157	0.913893	-2.899710
26	6	-1.540507	0.109398	-1.653578
27	6	-3.000752	0.255949	-1.508277
28	1	-3.248611	0.508727	-0.472725
29	1	-3.344545	1.067583	-2.158953
30	1	-3.530038	-0.665169	-1.770427

TS_{Me-Ve} *trans-syn*

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	44	0.067700	0.107059	0.048478
2	17	0.818940	-1.695274	-1.511738
3	6	-0.460817	2.210502	-0.453695
4	1	-1.491211	2.510352	-0.324805
5	6	0.114270	1.620187	-1.612983
6	1	-0.385865	1.396547	-2.543336
7	6	1.509724	1.395883	-1.338051
8	1	2.200761	0.900261	-2.006481
9	6	1.798878	1.860283	-0.037628
10	1	2.755796	1.801106	0.462213
11	6	0.579575	2.317116	0.535137
12	1	0.455571	2.718865	1.530115
13	6	-0.964439	0.354890	1.879465
14	1	-0.428033	0.735534	2.742650
15	6	-2.310319	0.219744	1.802148
16	1	-2.971723	0.452039	2.635934
17	6	-2.795100	-0.303443	0.558849

18	1	-3.852289	-0.528418	0.408587
19	6	-1.872331	-0.524841	-0.419210
20	6	-2.268115	-1.080971	-1.756977
21	1	-1.796662	-2.049387	-1.945733
22	1	-1.960723	-0.431354	-2.586794
23	1	-3.359220	-1.199635	-1.805552
24	6	1.315855	-1.172859	1.383755
25	6	2.765713	-1.410352	1.317401
26	1	3.031114	-2.291422	1.914438
27	1	3.052061	-1.595500	0.277155
28	1	3.344502	-0.557455	1.694123
29	6	0.113582	-1.425011	1.667481
30	1	-0.653709	-2.119267	1.959848

TS_{Me-Ve cis-anti}

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	44	0.318758	0.068618	-0.005416
2	17	1.020245	2.460322	0.037048
3	6	1.353525	-1.669632	0.937219
4	1	0.862738	-2.161143	1.765188
5	6	2.212399	-0.537199	1.008680
6	1	2.511768	-0.007025	1.901255
7	6	2.642472	-0.234062	-0.332025
8	1	3.253773	0.612650	-0.610327
9	6	2.074967	-1.177696	-1.214516
10	1	2.184414	-1.188879	-2.290515
11	6	1.246826	-2.041046	-0.449384
12	1	0.669071	-2.867663	-0.836499
13	6	-1.526055	-1.056928	0.000181
14	6	-1.882218	-2.068505	-1.061919
15	1	-2.971135	-2.124228	-1.199116
16	1	-1.441187	-1.821299	-2.030903
17	1	-1.547453	-3.078534	-0.784644
18	6	-2.164174	-0.990930	1.204440
19	1	-3.029594	-1.619599	1.423769
20	6	-1.654198	-0.041775	2.149913
21	1	-2.156130	0.151860	3.098484

22	6	-0.539653	0.620744	1.754381
23	1	-0.072458	1.417416	2.328894
24	6	-0.546581	0.788128	-1.826207
25	1	-0.023534	1.206928	-2.666603
26	6	-1.606631	0.765963	-1.138241
27	6	-2.919639	1.336124	-0.774964
28	1	-2.932752	1.593730	0.287832
29	1	-3.087227	2.250034	-1.357553
30	1	-3.736045	0.631994	-0.966119

TS_{Me-Ve} *cis-syn*

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	44	-0.113476	-0.114518	-0.121131
2	17	-1.970300	0.836948	-1.498691
3	6	0.347680	-2.272663	0.217449
4	1	1.270882	-2.663155	-0.185200
5	6	-0.902845	-2.186713	-0.454451
6	1	-1.118288	-2.496547	-1.466424
7	6	-1.849603	-1.614637	0.467812
8	1	-2.871919	-1.357876	0.226577
9	6	-1.201290	-1.381722	1.700878
10	1	-1.645434	-0.930154	2.578255
11	6	0.160677	-1.743473	1.544905
12	1	0.922755	-1.678583	2.306236
13	6	1.925324	0.366890	0.388465
14	6	2.392686	0.504284	1.815498
15	1	3.242736	1.197935	1.880272
16	1	1.604709	0.884394	2.470395
17	1	2.735776	-0.457761	2.220536
18	6	2.778303	0.220597	-0.667097
19	1	3.859225	0.294506	-0.538819
20	6	2.171276	0.029605	-1.948825
21	1	2.757549	0.015539	-2.868752
22	6	0.818272	-0.078899	-1.936590
23	1	0.207968	-0.155835	-2.831515
24	6	-0.394572	1.848716	0.855100
25	6	-1.561931	2.361411	1.592594

26	1	-1.510018	3.455181	1.671888
27	1	-2.473445	2.095255	1.047590
28	1	-1.631024	1.949749	2.607202
29	6	0.635690	1.962916	0.130620
30	1	1.218578	2.560183	-0.548865

Ve *trans-anti*

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	44	-0.292783	-0.081829	0.056661
2	17	-1.261561	1.285569	1.875545
3	6	-0.948088	-1.466149	-1.626979
4	1	-0.357089	-1.563248	-2.527457
5	6	-2.077708	-0.613416	-1.461297
6	1	-2.434532	0.121118	-2.170610
7	6	-2.567818	-0.819339	-0.154279
8	1	-3.353527	-0.252408	0.323897
9	6	-1.828971	-1.892053	0.462958
10	1	-1.978960	-2.259030	1.468661
11	6	-0.839314	-2.301585	-0.443114
12	1	-0.104614	-3.077603	-0.283278
13	6	1.713753	-0.639086	-0.674480
14	1	1.780993	-1.615587	-1.168506
15	6	2.222069	0.466665	-1.496528
16	1	3.138141	0.354325	-2.080141
17	6	1.509957	1.625166	-1.499719
18	1	1.856824	2.525117	-2.009766
19	6	0.282111	1.607132	-0.766486
20	6	-0.486607	2.893003	-0.705500
21	1	-1.566438	2.733577	-0.661038
22	1	-0.229571	3.402701	0.234192
23	1	-0.237226	3.560684	-1.541771
24	6	1.187396	-0.342585	1.469637
25	1	1.051956	-0.215746	2.540109
26	6	2.257807	-0.658948	0.749448
27	6	3.676318	-0.984534	1.120602
28	1	4.381068	-0.238925	0.729228
29	1	3.794566	-1.016074	2.209302

30	1	3.981967	-1.958726	0.714261
----	---	----------	-----------	----------

Ve *trans-syn*

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	0.182107	-0.066828	-0.018449
2	17	0.671084	2.106756	1.068565
3	6	1.198443	-2.066680	-0.342095
4	1	0.622295	-2.979369	-0.402052
5	6	1.857809	-1.576212	0.821104
6	1	1.790150	-1.988104	1.819201
7	6	2.520552	-0.387150	0.453331
8	1	3.029998	0.289816	1.125872
9	6	2.384117	-0.188922	-0.967113
10	1	2.789726	0.643384	-1.526061
11	6	1.580670	-1.225972	-1.464497
12	1	1.275154	-1.367866	-2.491956
13	6	-1.403867	-1.094922	-1.157472
14	1	-1.068463	-1.910436	-1.807875
15	6	-2.461431	-1.499740	-0.223497
16	1	-3.285352	-2.133576	-0.556988
17	6	-2.368519	-1.057822	1.059700
18	1	-3.145024	-1.239877	1.802876
19	6	-1.192200	-0.311847	1.377026
20	6	-1.087064	0.206199	2.779773
21	1	-0.059654	0.194023	3.148739
22	1	-1.381694	1.265459	2.784846
23	1	-1.742304	-0.342112	3.471164
24	6	-0.877348	1.095068	-1.404259
25	6	-0.723863	2.533528	-1.775264
26	1	-1.376129	2.774769	-2.628091
27	1	-0.977667	3.186008	-0.934548
28	1	0.310502	2.773214	-2.048546
29	6	-1.713530	0.185894	-1.897376
30	1	-2.485275	0.291699	-2.666616

Ve *cis-anti*

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.447378	-0.115580	0.029215
2	17	-1.576310	-2.289483	-0.274090
3	6	-0.996990	2.040680	0.529887
4	1	-0.371118	2.642594	1.173653
5	6	-2.129185	1.286798	0.939781
6	1	-2.469999	1.134398	1.953703
7	6	-2.672059	0.682516	-0.223166
8	1	-3.480608	-0.035191	-0.240899
9	6	-1.958545	1.153052	-1.375761
10	1	-2.149594	0.856254	-2.398262
11	6	-0.923072	1.984589	-0.919947
12	1	-0.203231	2.503118	-1.534700
13	6	1.737313	0.580705	0.159869
14	6	2.194934	1.975092	-0.266379
15	1	3.289181	2.051175	-0.168168
16	1	1.956376	2.168412	-1.316232
17	1	1.764974	2.776277	0.344940
18	6	2.161596	0.218471	1.511085
19	1	3.092300	0.630200	1.911582
20	6	1.373887	-0.613106	2.265184
21	1	1.704163	-1.017392	3.221410
22	6	0.133491	-0.945229	1.683204
23	1	-0.492896	-1.697059	2.166605
24	6	0.873968	-0.967399	-1.286863
25	1	0.630621	-1.729545	-2.019865
26	6	2.049458	-0.482969	-0.903273
27	6	3.448726	-0.829925	-1.339653
28	1	4.025371	-1.284508	-0.522911
29	1	3.419838	-1.547205	-2.165665
30	1	4.005385	0.055575	-1.674914

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.272261	0.052224	0.128062
2	17	-2.068302	-1.575466	0.646075
3	6	-0.064848	2.319850	0.112230
4	1	0.820288	2.795222	0.510295
5	6	-1.273530	2.089030	0.820433
6	1	-1.452841	2.277625	1.870214
7	6	-2.175414	1.467630	-0.082362
8	1	-3.148838	1.074627	0.173612
9	6	-1.579554	1.417493	-1.385451
10	1	-2.036720	0.998402	-2.271154
11	6	-0.278187	1.932103	-1.272959
12	1	0.435435	2.043766	-2.074916
13	6	2.001513	0.054080	-0.188565
14	6	2.767439	1.111374	-0.979887
15	1	3.825616	0.810739	-1.048808
16	1	2.397102	1.190848	-2.005108
17	1	2.748525	2.104609	-0.516017
18	6	2.570066	-0.193365	1.135772
19	1	3.644786	-0.057922	1.289615
20	6	1.746927	-0.566280	2.166557
21	1	2.131033	-0.880143	3.136701
22	6	0.374647	-0.568321	1.853143
23	1	-0.333807	-0.951750	2.588530
24	6	0.479264	-1.451807	-1.097322
25	6	-0.228108	-2.520901	-1.862795
26	1	-0.779269	-3.186503	-1.192008
27	1	-0.966701	-2.093844	-2.551489
28	1	0.490215	-3.110999	-2.449139
29	6	1.784070	-1.214798	-0.995965
30	1	2.620108	-1.786131	-1.415300

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-0.778732	-0.030004	0.039064
2	17	-0.874666	-0.808207	2.423836
3	6	-2.263943	-0.229438	-1.562427
4	1	-2.700750	0.676729	-1.957499
5	6	-2.752291	-0.997236	-0.460960
6	1	-3.617143	-0.770315	0.146261
7	6	-1.913199	-2.153122	-0.328391
8	1	-1.994922	-2.891370	0.456396
9	6	-0.912760	-2.102207	-1.318943
10	1	-0.111445	-2.817840	-1.448147
11	6	-1.090319	-0.898501	-2.061554
12	1	-0.494843	-0.571271	-2.902438
13	6	-0.209381	1.691162	-1.019156
14	1	0.473195	1.616808	-1.861138
15	6	-0.774453	2.863982	-0.667444
16	1	-0.570075	3.800559	-1.187105
17	6	-1.669190	2.770820	0.460906
18	1	-2.200631	3.629334	0.871427
19	6	-1.790764	1.519825	0.951222
20	1	-2.430012	1.254262	1.788608
21	6	1.533147	-0.801114	0.551228
22	1	1.193652	-1.485029	1.318507
23	6	1.537107	0.575794	0.681832
24	1	1.200237	1.114591	1.560507
25	6	2.608562	-1.163247	-0.460784
26	1	2.539654	-2.155382	-0.913452
27	6	3.943520	-0.898419	0.318603
28	1	4.796266	-1.256448	-0.270064
29	1	3.969367	-1.412577	1.284166
30	6	3.957598	0.658809	0.457172
31	1	4.813636	1.098358	-0.065499
32	1	3.999686	0.992571	1.498056
33	6	2.623926	1.088854	-0.251567
34	1	2.571017	2.144587	-0.519643
35	6	2.592717	0.054055	-1.399582
36	1	1.697478	0.102152	-2.020421
37	1	3.477495	0.109879	-2.043489

TS_{VII-VIII}

Center	Atomic	Coordinates (Angstroms)		
--------	--------	-------------------------	--	--

Number	Number	X	Y	Z
1	44	-0.766240	-0.028816	0.046603
2	17	-1.174518	-1.058706	2.310756
3	6	-2.291024	0.109090	-1.560961
4	1	-2.674162	1.089763	-1.807623
5	6	-2.779428	-0.762451	-0.547762
6	1	-3.617497	-0.585064	0.111328
7	6	-1.983409	-1.966806	-0.589700
8	1	-2.082175	-2.795948	0.096194
9	6	-1.023203	-1.841063	-1.610416
10	1	-0.256648	-2.563655	-1.856321
11	6	-1.162822	-0.541140	-2.175399
12	1	-0.565949	-0.128777	-2.976644
13	6	0.146110	1.705054	-0.848213
14	1	0.753218	1.612425	-1.742037
15	6	-0.353353	2.899509	-0.442428
16	1	-0.115638	3.833286	-0.952155
17	6	-1.237819	2.829003	0.684530
18	1	-1.638397	3.715728	1.176143
19	6	-1.532957	1.567392	1.080675
20	1	-2.196813	1.348163	1.912748
21	6	1.340826	-0.651554	0.628515
22	1	1.094378	-1.119387	1.573844
23	6	1.548288	0.747550	0.526614
24	1	1.367694	1.424089	1.356170
25	6	2.378622	-1.310151	-0.277480
26	1	2.166102	-2.335696	-0.590966
27	6	3.718430	-1.146543	0.510727
28	1	4.523581	-1.696723	0.009961
29	1	3.644679	-1.524183	1.534536
30	6	3.960223	0.396349	0.449415
31	1	4.898055	0.636847	-0.063392
32	1	3.999706	0.861707	1.439985
33	6	2.751144	0.918506	-0.396455
34	1	2.893042	1.916365	-0.815657
35	6	2.573171	-0.257768	-1.382805
36	1	1.705452	-0.159549	-2.038235
37	1	3.465972	-0.433356	-1.994404

VIII

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z

1	44	0.828078	-0.012274	-0.103497
2	17	1.255309	-1.396417	-2.129388
3	6	2.618631	0.310777	1.383519
4	1	3.214376	1.211556	1.327242
5	6	2.796554	-0.869010	0.618229
6	1	3.571953	-1.056498	-0.110010
7	6	1.779072	-1.823306	1.022204
8	1	1.653902	-2.809308	0.598132
9	6	0.969036	-1.215875	1.990537
10	1	0.104980	-1.652179	2.470742
11	6	1.443706	0.128387	2.169511
12	1	1.028368	0.858201	2.851534
13	6	-0.547245	1.675172	0.542935
14	1	-0.831012	1.703770	1.594614
15	6	0.100583	2.867439	0.087515
16	1	-0.022880	3.807274	0.629992
17	6	0.930877	2.764707	-1.017519
18	1	1.290684	3.631460	-1.570010
19	6	1.282414	1.445290	-1.333613
20	1	1.888685	1.241226	-2.217398
21	6	-1.209485	-0.428682	-0.593577
22	1	-1.182072	-0.717912	-1.641509
23	6	-1.691412	0.987969	-0.308754
24	1	-1.864585	1.582183	-1.211959
25	6	-2.127810	-1.330351	0.249394
26	1	-1.727693	-2.317452	0.495733
27	6	-3.471088	-1.380856	-0.531278
28	1	-3.330439	-1.675829	-1.576125
29	1	-4.153350	-2.106374	-0.072130
30	6	-4.015309	0.079457	-0.379775
31	1	-4.113352	0.593953	-1.341131
32	1	-5.002355	0.089833	0.094867
33	6	-2.966140	0.760365	0.539060
34	1	-3.330431	1.656265	1.054315
35	6	-2.538057	-0.426798	1.434386
36	1	-1.724137	-0.190007	2.124520
37	1	-3.372274	-0.839131	2.015392

TS^{VIII-IX}

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	1.021961	-0.060771	-0.182328

2	17	1.419070	-1.280215	-2.229244
3	1	2.980576	1.208549	1.514139
4	6	2.355442	0.328010	1.566596
5	6	2.626197	-0.953143	0.937415
6	1	0.608909	0.997562	2.770615
7	1	3.516931	-1.224586	0.383706
8	6	1.596511	-1.878300	1.359126
9	1	1.518936	-2.909691	1.046163
10	6	0.675099	-1.158477	2.108759
11	1	-0.251389	-1.544663	2.511578
12	6	1.119528	0.213255	2.231062
13	6	-1.108442	2.120185	0.532336
14	1	-1.649367	2.345541	1.453352
15	6	-0.106825	2.962342	0.196927
16	1	0.017003	3.858825	0.807691
17	6	0.835529	2.791487	-0.897953
18	1	1.080570	3.680510	-1.486451
19	6	1.414773	1.599883	-1.209442
20	1	2.056047	1.534416	-2.089294
21	6	-1.061857	-0.379721	-0.420305
22	1	-0.946692	-0.697461	-1.457765
23	6	-1.751446	1.016210	-0.321082
24	1	-1.858937	1.425795	-1.333122
25	6	-1.996154	-1.334880	0.338123
26	1	-1.522116	-2.241374	0.716921
27	6	-3.173066	-1.627585	-0.636291
28	1	-2.823893	-1.980064	-1.611609
29	1	-3.822514	-2.405651	-0.217586
30	6	-3.912460	-0.252236	-0.709000
31	1	-4.959140	-0.346455	-0.401245
32	1	-3.907928	0.179545	-1.716331
33	6	-3.127711	0.623380	0.296356
34	1	-3.686598	1.492018	0.661703
35	6	-2.696598	-0.411597	1.358358
36	1	-2.028548	0.005332	2.119469
37	1	-3.543429	-0.893443	1.861765

IX

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	1.009373	-0.151827	-0.179632
2	17	2.174331	-0.913095	-2.105180
3	6	1.342213	0.779089	1.805301

4	1	0.957252	1.774392	1.973646
5	6	2.585183	0.434862	1.174948
6	1	3.324255	1.131788	0.803474
7	6	2.722207	-1.004633	1.231275
8	1	3.540790	-1.568149	0.803142
9	6	1.590366	-1.537178	1.866083
10	1	1.378260	-2.586149	2.020311
11	6	0.715468	-0.445599	2.168571
12	1	-0.254200	-0.531694	2.639932
13	6	-1.784378	2.104601	0.466752
14	1	-2.489656	2.320682	1.269742
15	6	-0.776108	2.962646	0.235936
16	1	-0.747500	3.887049	0.817547
17	6	0.254095	2.795423	-0.786940
18	1	0.530466	3.711213	-1.319278
19	6	0.897933	1.658601	-1.124944
20	1	1.596906	1.719707	-1.960443
21	6	-1.051301	-0.262714	-0.274652
22	1	-0.679804	-0.588708	-1.285062
23	6	-2.085276	0.888698	-0.384644
24	1	-2.137006	1.219288	-1.431124
25	6	-1.817019	-1.403057	0.418365
26	1	-1.194343	-2.142162	0.927457
27	6	-2.725750	-2.031161	-0.682124
28	1	-2.162107	-2.319695	-1.575464
29	1	-3.203250	-2.937020	-0.291966
30	6	-3.775830	-0.905763	-0.950637
31	1	-3.735521	-0.531260	-1.979616
32	1	-4.795596	-1.265772	-0.776073
33	6	-3.391634	0.185676	0.074738
34	1	-4.197569	0.891262	0.299803
35	6	-2.871978	-0.655045	1.262116
36	1	-2.449980	-0.042740	2.066724
37	1	-3.626575	-1.325704	1.688243

TSIX-X

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	0.927715	-0.247985	0.016622
2	17	1.173998	-2.104777	-1.544289
3	6	1.793101	1.584946	0.933713
4	1	1.370076	2.564189	0.774870
5	6	2.749895	0.918990	0.075025

6	1	3.201552	1.330070	-0.817655
7	6	3.088394	-0.338245	0.686012
8	1	3.746659	-1.086020	0.264490
9	6	2.290722	-0.489958	1.837257
10	1	2.266365	-1.361938	2.478789
11	6	1.474947	0.698092	1.987975
12	1	0.783425	0.890135	2.798411
13	6	-1.827635	2.311726	-0.032914
14	1	-2.400965	2.850165	0.722410
15	6	-0.831667	2.920208	-0.692498
16	1	-0.615766	3.973402	-0.507332
17	6	-0.082412	2.216363	-1.739397
18	1	0.096047	2.754322	-2.673037
19	6	0.310096	0.931352	-1.660616
20	1	0.655742	0.404601	-2.547534
21	6	-1.167671	-0.133812	-0.635796
22	1	-1.286273	-0.656714	-1.582050
23	6	-2.289381	0.912172	-0.389239
24	1	-2.891767	0.998821	-1.306344
25	6	-1.356561	-1.154187	0.551267
26	1	-0.498276	-1.778690	0.856935
27	6	-2.541188	-2.056110	0.091847
28	1	-2.380375	-2.477797	-0.903847
29	1	-2.657277	-2.893149	0.790179
30	6	-3.752915	-1.072023	0.175520
31	1	-4.237864	-0.916689	-0.794510
32	1	-4.516533	-1.450040	0.863931
33	6	-3.128597	0.236104	0.727317
34	1	-3.857685	0.913676	1.184248
35	6	-2.024853	-0.306339	1.650145
36	1	-1.374558	0.475485	2.048872
37	1	-2.405617	-0.916937	2.477023

X

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	1.335598	-0.148557	-0.134133
2	17	1.129643	-2.475753	-0.687611
3	6	1.752269	1.127899	1.601250
4	1	0.986453	1.584389	2.213913
5	6	2.388649	1.722241	0.474494
6	1	2.179892	2.704109	0.071975
7	6	3.308250	0.767668	-0.070954

8	1	3.926467	0.907204	-0.947765
9	6	3.303799	-0.394203	0.780753
10	1	3.869324	-1.300989	0.619196
11	6	2.333546	-0.180506	1.798225
12	1	2.046534	-0.891173	2.562097
13	6	-1.776913	2.354671	-0.393193
14	1	-2.209855	3.250754	0.051051
15	6	-0.543782	2.404097	-0.917421
16	1	0.018642	3.334944	-0.904315
17	6	0.071123	1.233109	-1.558965
18	1	0.881450	1.414645	-2.262267
19	6	-0.582704	0.015589	-1.576213
20	1	-0.262035	-0.746107	-2.280925
21	6	-1.993651	-0.165157	-1.025858
22	1	-2.577873	-0.485926	-1.899887
23	6	-2.650472	1.129724	-0.404715
24	1	-3.558436	1.394583	-0.966176
25	6	-2.177353	-1.219487	0.106416
26	1	-1.525269	-2.085512	-0.007056
27	6	-3.684214	-1.561505	0.213218
28	1	-4.125438	-1.791952	-0.762887
29	1	-3.832421	-2.441530	0.848078
30	6	-4.301972	-0.281640	0.868194
31	1	-5.093665	0.169582	0.259575
32	1	-4.737041	-0.508394	1.849407
33	6	-3.078786	0.650709	1.019975
34	1	-3.229888	1.475555	1.724468
35	6	-1.967633	-0.359618	1.368800
36	1	-0.967592	0.086098	1.419547
37	1	-2.160455	-0.907532	2.299150

TS_{VIII-XI}

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-1.064099	0.018175	-0.100027
2	17	-1.177245	1.137188	2.085222
3	6	-2.435483	-1.226215	-1.311496
4	1	-2.847880	-0.799178	-2.216416
5	6	-2.984897	-1.121102	0.003899
6	1	-3.898185	-0.614366	0.284512
7	6	-2.180893	-1.943329	0.878274
8	1	-2.332488	-2.045276	1.945252
9	6	-1.133863	-2.487558	0.138646

10	1	-0.353524	-3.125944	0.528972
11	6	-1.227181	-1.984214	-1.213693
12	1	-0.594109	-2.275066	-2.042489
13	6	0.981310	1.390449	-0.704476
14	1	0.844168	0.928048	-1.676354
15	6	0.344985	2.688784	-0.575181
16	1	0.966339	3.539868	-0.294924
17	6	-0.981282	2.821531	-0.877258
18	1	-1.432612	3.797936	-1.047954
19	6	-1.712009	1.610110	-0.952650
20	1	-2.712905	1.650419	-1.396936
21	6	1.350343	-0.014954	0.561839
22	1	1.008505	0.086035	1.584905
23	6	2.242290	1.086536	0.014354
24	1	2.543041	1.858309	0.725100
25	6	2.066387	-1.294287	0.105344
26	1	1.479883	-2.209552	0.118618
27	6	3.340929	-1.366285	1.007127
28	1	3.105304	-1.218146	2.066534
29	1	3.801453	-2.355828	0.910582
30	6	4.265455	-0.244504	0.427116
31	1	4.541753	0.502141	1.179136
32	1	5.193188	-0.662439	0.022182
33	6	3.394403	0.361704	-0.700095
34	1	3.939948	0.971772	-1.425130
35	6	2.700679	-0.905948	-1.246676
36	1	1.974386	-0.731975	-2.044673
37	1	3.420233	-1.652967	-1.598962

XI

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	44	-1.618421	0.120573	0.066422
2	17	-1.093440	0.361752	2.371060
3	6	-2.024375	-1.199167	-1.690993
4	1	-1.445373	-1.190644	-2.605280
5	6	-3.150843	-0.373549	-1.396403
6	1	-3.559674	0.405433	-2.025692
7	6	-3.611545	-0.731162	-0.083128
8	1	-4.456141	-0.297489	0.436287
9	6	-2.880238	-1.917460	0.330822
10	1	-2.982496	-2.405251	1.290579
11	6	-1.911259	-2.186072	-0.626983

12	1	-1.142400	-2.944127	-0.560268
13	6	1.490455	0.996906	-0.339646
14	1	0.727026	0.251040	-0.111746
15	6	0.994287	2.330116	-0.663531
16	1	1.762596	3.078589	-0.860072
17	6	-0.306455	2.731129	-0.756529
18	1	-0.473078	3.771877	-1.040354
19	6	-1.473542	1.927434	-0.513933
20	1	-2.401896	2.465440	-0.746593
21	6	2.833060	0.917577	0.388575
22	1	3.282930	1.853503	0.710687
23	6	2.760623	0.524233	-1.064117
24	1	3.154579	1.158979	-1.853995
25	6	3.235779	-0.369377	1.116921
26	1	3.022641	-0.383454	2.188192
27	6	4.729872	-0.590838	0.737332
28	1	5.335127	0.306321	0.903371
29	1	5.162743	-1.394474	1.343660
30	6	4.655325	-0.998493	-0.776152
31	1	5.214995	-0.315587	-1.423594
32	1	5.056738	-2.004813	-0.937517
33	6	3.127848	-0.964847	-1.074404
34	1	2.828573	-1.516427	-1.969785
35	6	2.574454	-1.479925	0.272481
36	1	1.486214	-1.520843	0.345629
37	1	2.965225	-2.472103	0.524047

Figure S1. Calculated ground and transition state structures of **Ia-VIa** with natural electron populations.