Supporting Information

Approaches to Open Fullerenes: Synthesis and Thermal Stability of *cis-1* Bis(isobenzofuran) Diels-Alder Adducts of C₆₀

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General Methods. All reactions were performed under argon unless otherwise noted. Chemicals were used as purchased without further purification. Distilled solvents were dried as follows: THF and toluene from sodium/benzophenone; dichloromethane, acetonitrile, 1,2-dichloroethane, and 1,2-dichlorobenzene (ODCB) from calcium hydride. ^1H and ^{13}C NMR data were recorded using 400 or 500 MHz spectrometers. UV–Vis data were recorded using diode-array single beam spectrometers. High-resolution mass spectra of non- C_{60} products were ionized by EI. High- and low-resolution mass spectra of C_{60} derivatives were ionized using FAB^+ , FAB^- , and MALDI techniques. Thermogravimetric analysis (TGA) was performed using a TG/DTA instrument.

Synthesis of Methylene-Bridged Benzyne Adduct 2b. Bis(2-furyl)methane **1b** was prepared using the known procedure.¹ The two diastereoisomers of the double [4+2] addition of benzyne were obtained chromatographically (EtOAc/hexanes, 1:3) according to general procedure A using 5.48 g (40 mmol) of anthranilic acid, 11.2 mL (1.5 mol) of isoamyl nitrite, and 2.25 g (15.2 mmol) of the bisfuran **1b**.

(rac)-Bis[1-(11-oxatricyclo[6.2.1.0^{2,7}]undeca-2,4,6,9-tetraenyl)]methane. Yield: 1.35 g (30%); colorless crystals from hexanes/EtOAc (6:1); m.p. 109 °C; ^1H NMR (500 MHz, CDCl_3) δ (ppm) 3.24 (d, $J = 15.6$ Hz, 1H), 3.45 (d, $J = 15.6$ Hz, 1H), 5.67 (d, $J = 1.5$ Hz, 2H), 6.88–6.89 (m, 2H), 6.94–7.00 (m, 6H), 7.19–7.20 (m, 2H), 7.34–7.35 (m, 2H); ^{13}C NMR (125.7 Hz, CDCl_3) δ (ppm) 30.1, 81.7, 90.5, 119.8, 120.0, 124.7, 124.8, 143.5, 145.0, 150.2, 151.1; FT-IR (KBr) ν (cm^{-1}) 3069, 3015, 2950, 1452, 1287, 1039, 956; EI-

¹ Masau, R. M.; Whiting, A. J. *Chem. Soc., Perkin Trans.* **1994**, *1*, 2881–2888.

MS: m/z (rel. intensity) 300 (59), 157 (100), 145 (98), 129 (87), 115 (95); HRMS (m/z): calcd for $C_{21}H_{16}O_2$, 300.1150; found, 300.1153.

(*meso*)-Bis[1-(11-oxatricyclo[6.2.1.0^{2,7}]undeca-2,4,6,9-tetraenyl)]methane. Yield: 1.60 g (35%); colorless crystals from hexanes/EtOAc (5:1); m.p. 162 °C; 1H NMR (500 MHz, $CDCl_3$) δ (ppm) 3.31 (s, 2H), 5.69 (d, J = 1.6 Hz, 2H), 6.95–7.02 (m, 6H), 7.06–7.07 (m, 2H), 7.23–7.26 (m, 4H); ^{13}C NMR (125.7 Hz, $CDCl_3$) δ (ppm) 29.5, 81.6, 90.5, 119.1, 119.9, 124.9, 142.5, 144.8, 150.2, 151.5; FT-IR (KBr) ν (cm^{-1}) 3069, 3051, 3015, 1452, 1295, 1041, 958; EI-MS: m/z (rel. intensity) 300 (76), 144 (65), 141 (70), 128 (100), 115 (80); HRMS (m/z): calcd for $C_{21}H_{16}O_2$, 300.1150; found, 300.1145.

Synthesis of Methylene-Bridged Benzyne Adduct 2c. Methyl 2-furoate was reacted with *p*-formaldehyde in conc. H_2SO_4 to give the bisfuran **1c**.² Double [4+2] addition of benzyne following procedure A using 2.74 g (20 mmol) of anthranilic acid, 6.3 mL (48 mmol) of isoamyl nitrite, and 1.35 g (5.11 mmol) of the bisfuran **1c** gave adduct **2c**. Yield: 1.22 g (57%). The inseparable mixture of diastereomers could be differentiated in the 1H -NMR and ^{13}C -NMR spectra. Diastereomer with C_2 -symmetry: 1H NMR (500 MHz, $CDCl_3$) δ (ppm) 3.41 (s, 2H), 3.99 (s, 6H), 7.01–7.07 (m, 6H), 7.22–7.26 (m, 4H), 7.30–7.32 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 29.2, 52.8, 89.7, 91.2, 119.4, 125.3, 125.8, 141.8, 145.3, 148.7, 149.8, 168.3. Diastereomer with C_s -symmetry: 1H NMR (500 MHz, $CDCl_3$) δ (ppm) 3.36 (d, J = 16.0 Hz, 1H), 3.52 (d, J = 16.0 Hz, 1H), 3.97 (s, 6H), 6.95 (d, J = 5.3 Hz, 2H), 6.98–7.06 (m, 4H), 7.01 (d, J = 5.2 Hz, 2H), 7.32 (d, J = 7.0 Hz, 2H), 7.44 (d, J = 6.8 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$)

² Pennanen, S.; Nyman, G. *Acta Chem. Scand.* **1972**, 26, 1018–1022.

δ (ppm) 30.3, 52.7, 89.6, 91.0, 119.4, 121.0, 125.1, 125.6, 142.9, 145.6, 148.5, 149.2, 168.2; FT-IR (KBr) ν (cm⁻¹) 3068, 2955, 1751, 1452, 1349, 1328, 1237, 1194, 1152, 1105, 1059, 1024, 975, 958, 819, 803, 758, 733, 693, 644; HRMS–EI (m/z): calcd for C₂₅H₂₀O₆, 416.1260; found, 416.1249.

Synthesis of *gem*-Dimethylmethylene-Bridged Benzyne Adduct **2d.** Furan was reacted with acetone in conc. H₂SO₄ to give the bisfuran **1d**.³ The double [4+2] addition of benzyne according to general procedure A using 5.48 g (40 mmol) of anthranilic acid, 13.1 mL (0.1 mol) of isoamyl nitrite, and 2.64 g (15.0 mmol) of the bisfuran **1d** gave adduct **2d**. Yield: 3.39 g (69%). Spectral data for the major product: ¹H NMR (500 MHz, CDCl₃) δ (ppm) 1.74 (s, 3H), 1.75 (s, 3H), 5.73 (d, J = 1.4 Hz, 2H), 6.97–7.03 (m, 6H), 7.20–7.22 (m, 2H), 7.26–7.31 (m, 2H), 7.63–7.65 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ (ppm) 22.6, 38.2, 81.1, 99.5, 119.8, 123.1, 124.3, 124.4, 142.4, 144.2, 150.0, 151.7; FT-IR (KBr) ν (cm⁻¹) 3047, 2992, 2946, 1596, 1464, 1456, 1388, 1369, 1286, 1266, 1166, 1131, 1050, 764, 693; HRMS–EI (m/z): calcd for C₂₃H₂₀O₂, 328.1463; found, 328.1455.

2,3-Bis(11-oxatricyclo[6,2,1,0^{2,7}]undeca-2,4,6,9-tetraen-1-yl)quinoxaline (2e**).** Compound **2e** was synthesized starting from 2,3-bisfurylquinoxaline (**1e**) using 3.43 g (25 mmol) of anthranilic acid, 6.3 mL (48 mmol) of isoamyl nitrite, and 1.84 g (7.0 mmol) of the bisfuran **1e**.^{13c} Column chromatography (CH₂Cl₂/EtOAc, 15:1) provided the diastereomeric adducts in two fractions. The first fraction yielded the major isomer (1.69 g, 58%) as a yellow solid; m.p. 236 °C (dec.); ¹H

³ Ackman, R. G.; Brown, W. H. Wright, G. F. *J. Org. Chem.* **1955**, 20, 1147–1158.

NMR (500 MHz, CDCl₃) δ (ppm) 5.79 (d, J = 2.0 Hz, 2H), 6.90 (br dt, J = 7.3, 0.8 Hz, 2H), 6.96–7.00 (m, 4H), 7.05 (d, J = 7.3 Hz, 2H), 7.24 (d, J = 7.3 Hz, 2H), 7.40 (d, J = 5.4 Hz, 2H), 7.83 (dd, J = 6.4, 3.4 Hz, 2H), 8.28 (dd, J = 6.4, 3.4 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ (ppm) 82.0, 94.4, 120.0, 121.5, 124.7, 125.1, 129.3, 130.6, 140.7, 141.8, 145.9, 148.1, 148.6, 151.4; IR (KBr) ν (cm⁻¹) 3068, 3049, 3024, 2996, 1453, 1089, 1037, 994, 947, 922, 762, 691; MS-EI: m/z (rel. intensity) 415 (43, M⁺), 385 (100), 357 (46), 271 (80, [M – C₁₀H₇O]⁺); HRMS-EI (m/z): calcd for C₂₈H₁₈N₂O₂, 413.1290; found, 413.1275. The second fraction yielded the minor isomer (493 mg, 17%) as a yellow solid; m.p. 225 °C (dec.); ¹H NMR (500 MHz, CDCl₃) δ (ppm) 5.81 (d, J = 2.0 Hz, 2H), 6.79 (br dt, J = 7.3, 0.8, 2H), 6.95 (br dt, J = 7.3, 0.8, 2H), 7.08 (dd, J = 5.3, 2.0 Hz, 2H), 7.12 (d, J = 7.2 Hz, 2H), 7.24 (d, J = 7.2 Hz, 2H), 7.51 (d, J = 5.3 Hz, 2H), 7.83 (dd, J = 6.4, 3.4 Hz, 2H), 8.29 (dd, J = 6.4, 3.4 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ (ppm) 81.9, 94.0, 119.8, 121.8, 124.6, 124.9, 129.3, 130.6, 140.5, 141.8, 146.7, 148.3, 149.0, 151.1.

2,3-Bis(5-ethoxymethyl-2-furyl)quinoxaline (1i). Ethyl bromide (1.70 g, 15.0 mmol) was added via syringe to a solution of **6** (0.990 g, 3.10 mmol), tetrabutylammonium bromide (0.0452 g, 0.300 mmol), and sodium hydride (1.26, 52.0 mmol) in dry THF (250 mL) under Ar. The resulting solution was stirred vigorously for 47 h, by which time all of the starting material had disappeared (TLC). Saturated NH₄Cl solution was added and the mixture was extracted with CH₂Cl₂. After drying (Na₂SO₄) and concentrating the solution to ca. 3 mL, the mixture was passed through a short plug of silica gel (CH₂Cl₂/EtOAc, 9/1). The fractions containing the product were dried (Na₂SO₄) and the solvent evaporated to give **1i** (928 mg, 79%) as a yellow oil. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 1.23 (t, J = 7.0 Hz, 6H), 3.57 (q, J = 7.0 Hz, 4H), 4.52 (s,

4H), 6.48 (d, $J = 3.4$ Hz, 2H), 6.73 (d, $J = 3.4$ Hz, 2H), 7.74 (dd, $J = 6.4, 3.4$ Hz, 2H), 8.13 (dd, $J = 6.4, 3.5$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 15.1, 64.7, 66.0, 110.9, 113.9, 129.0, 130.5, 140.5, 142.5, 150.7, 154.3; HRMS–EI (m/z): calcd for $\text{C}_{22}\text{H}_{22}\text{N}_2\text{O}_4$, 378.1580; found, 378.1575.

2,3-Bis(8-ethoxymethyl-11-oxatricyclo[6,2,1,0^{2,7}]undeca-2,4,6,9-tetraen-1-yl)quinoxaline (2i). Compound **2i** was prepared according to general procedure A using 885 mg (6.39 mmol) of anthranilic acid, 1.14 mL (8.50 mmol) of isoamyl nitrite, and 805 mg (2.13 mmol) of the bisfuran **1i**. A mixture of two diastereomers was obtained as a white solid (total yield: 790 mg, 70%). ^1H NMR (400 MHz, CDCl_3) δ (ppm) 1.04 (t, $J = 7.0$ Hz, 6H), 3.34 (m, 4H), 3.92 (d, $J = 11.2$, 2H), 4.17 (d, $J = 13.0$ Hz, 2H), 6.72 (td, $J = 7.5, 1.0$ Hz, 2H), 6.85 (td, $J = 7.4, 1.0$ Hz, 2H), 6.92 (d, $J = 5.3$ Hz, 2H), 7.07 (d, $J = 7.2$ Hz, 2H), 7.12 (d, $J = 7.0$ Hz, 2H), 7.49 (d, $J = 5.3$, 2H), 7.72 (dd, $J = 6.4, 3.4$ Hz, 2H), 8.19 (dd, $J = 6.4, 3.4$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 15.0, 67.1, 67.9, 91.4, 93.6, 118.8, 121.4, 124.4, 124.6, 129.2, 130.3, 140.2, 141.8, 147.4, 148.3, 149.1, 152.5; FTIR (KBr) ν (cm^{-1}) 694, 762, 879, 928, 951, 1054, 1112, 1303, 1380, 1454, 1479, 1561, 1673, 2855, 2926, 2974, 3067; HRMS–EI (m/z) calcd for $\text{C}_{34}\text{H}_{30}\text{N}_2\text{O}_4$, 530.2206; found, 530.2205.

1,2-Bis(5-methyl-2-furyl)-2-hydroxyethanone (8).⁴ Thiamine hydrochloride (Vitamin B1; 3.68 g, 10.9 mmol) was added to a solution of freshly distilled 5-methylfurfural **7** (24.0 g, 218 mmol) in dry ethanol (65 mL). While stirring under an Ar atmosphere, triethylamine (9.2 mL, 66 mmol) was added rapidly and then the reaction

mixture was heated under reflux for 24 h. After cooling to 20 °C, the resulting solution was poured into ice water (500 mL) and the aqueous layer was extracted with EtOAc. The combined organic extracts were then washed with brine, dried (Na₂SO₄), and filtered. The solvent was removed on a rotary evaporator and the residual yellow oil was taken up in *tert*-butyl methyl ether (50 mL). On cooling to 0 °C, a yellow solid separated, which was isolated on a Büchner funnel and dried under vacuum, giving **8** as a yellow oil (8.3 g, 34%). ¹H NMR (500 MHz, CDCl₃) δ (ppm) 2.24 (s, 3H), 2.38 (s, 3H), 5.65 (s, 1H), 5.92 (d, *J* = 3.1 Hz, 1H), 6.15 (d, *J* = 3.5 Hz, 1H), 6.25 (d, *J* = 3.1 Hz, 1H), 7.13 (d, *J* = 3.5 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃) δ (ppm) 13.5, 14.0, 68.8, 106.6, 109.4, 109.9, 122.2, 148.1, 149.7, 153.0, 159.2, 183.5.

2,3-Bis(5-methyl-2-furyl)quinoxaline (1j).⁵ The preparation of this dimethyl derivative was similar to the procedure described previously. ¹H NMR (500 MHz, CDCl₃) δ (ppm) 2.42 (s, 6H), 6.16 (d, *J* = 3.3 Hz, 2H), 6.61 (d, *J* = 3.3 Hz, 2H), 7.70 (dd, *J* = 6.4, 3.4 Hz, 2H), 8.09 (dd, *J* = 6.4, 3.4 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ (ppm) 13.9, 108.2, 114.3, 129.0, 129.9, 140.4, 142.8, 149.3, 154.5; IR (KBr) ν (cm⁻¹) 3123, 3063, 2978, 2949, 2917, 1533, 1516, 1208, 1091, 1022, 805, 761.

2,3-Bis(8-methyl-11-oxatricyclo[6,2,1,0^{2,7}]undeca-2,4,6,9-tetraen-1-yl)quinoxaline (2j). Compound **2j** was prepared according to general procedure A using 2.74 g (20 mmol) of anthranilic acid, 5.0 mL (38 mmol) of isoamyl nitrite, and 1.16 g (4.0 mmol) of the bisfuran **1j**. Column chromatography

⁴ Lee, C. K.; Kim, M. S.; Gong, J. S.; Lee, I.-S. H. *J. Heterocycl. Chem.* **1992**, 29, 149–153.

⁵ Behr, D.; Brandange, S.; Lindstrom, B. *Acta. Chim. Scand.* **1973**, 27, 2411–2414.

(hexanes/EtOAc, 2:1) provided the two different isomeric adducts in two separate fractions. The first fraction yielded the minor isomer of **2j** (203 mg, 11%) as a yellow oil. ¹H NMR (500 MHz, CDCl₃) δ (ppm) 1.87 (s, 6H), 6.79 (br dt, *J* = 7.3, 0.9 Hz, 2H), 6.83 (d, *J* = 5.2 Hz), 6.97 (br dt, *J* = 7.3, 0.9 Hz, 2H), 7.13 (d, *J* = 7.3 Hz, 2H), 7.16 (d, *J* = 7.3 Hz, 2H), 7.55 (d, *J* = 5.2 Hz, 2H), 7.81 (dd, *J* = 6.4, 3.4 Hz, 2H), 8.31 (dd, *J* = 6.4, 3.4 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ (ppm) 15.1, 88.7, 93.2, 117.9, 121.4, 124.1, 124.6, 129.2, 130.2, 140.3, 144.1, 147.7, 149.4, 150.5, 152.6. The second fraction yielded the major isomer of **2j** (1.24 g, 70%) as a yellow solid; m.p. 106 °C. ¹H NMR (500 MHz, CDCl₃) δ (ppm) 1.85 (s, 6H), 6.72 (d, *J* = 5.2 Hz), 6.87 (br dt, *J* = 7.3, 0.9 Hz, 2H), 6.98 (br dt, *J* = 7.3, 0.9 Hz, 2H), 7.04 (d, *J* = 7.3 Hz, 2H), 7.16 (d, *J* = 7.3 Hz, 2H), 7.32 (d, *J* = 5.2 Hz, 2H), 7.80 (dd, *J* = 6.4, 3.4 Hz, 2H), 8.28 (dd, *J* = 6.4, 3.4 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ (ppm) 15.2, 89.0, 93.6, 118.2, 121.2, 124.2, 124.9, 129.4, 130.3, 140.6, 144.1, 147.2, 149.0, 150.5, 152.9; IR (KBr) ν (cm⁻¹) 3076, 3044, 2978, 2930, 1453, 1387, 1116, 1076, 1053, 753, 729, 692, 649; HRMS–EI (*m/z*): calcd for C₃₀H₂₂N₂O₂, 442.1681; found, 442.1673.

Bis-5,5'-(acetoxymethyl)furfuryl Ether (1k). Triethylamine (8.31 mL, 60 mmol) and a catalytic amount of DMAP (244 mg, 2.0 mmol) were added to a CH₂Cl₂ (200 mL) solution of bis-5,5'-(hydroxymethyl)furfuryl ether **9**⁶ (2.38 g, 10.0 mmol) and acetic anhydride (3.77 mL, 40 mmol). After stirring for 10 h, the solution was washed

⁶ Timko, J. M.; Moore, S. S.; Walba, D. M.; Hilberly, P. C.; Cram, D. J. *J. Am. Chem. Soc.* **1977**, 99, 4207–4119.

sequentially with water, sat. NaHCO₃, and water. The organic layer was then dried (MgSO₄) and filtered through a plug of SiO₂. Evaporation of the solvent under reduced pressure gave a colorless oil (2.60 g, 81%). ¹H NMR (500 MHz, CDCl₃) δ (ppm) 2.06 (s, 6H), 4.47 (s, 4H), 5.02 (s, 4H), 6.31 (d, *J* = 3.1, 2H), 6.36 (d, *J* = 3.1 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ (ppm) 25.5, 57.7, 63.5, 110.3, 111.1, 149.6, 151.8, 170.2; IR (neat) ν (cm⁻¹) 3125, 2936, 2850, 1743, 1440, 1376, 1238, 1067, 1023, 803; MS-EI *m/z* (rel. intensity) 322 (14, M⁺), 293 (29), 262 (92, [M – AcO]⁺), 221 (65), 202 (42, [M – 2AcO]⁺), 153 (100), 94.0 (100, [C₆H₆O]⁺); HRMS–EI (*m/z*): calcd for C₁₆H₁₈O₇, 322.1052; found, 322.1057.

***anti/syn*-1,3-Bis-8,8'-(1-acetoxymethyl-11-oxatricyclo[6,2,1,0^{2,7}]undeca-2,4,6,9-tetraenyl)-2-oxapropane (2k).** This was prepared through the reaction of the bisacetate **1k** (2.60 g, 7.07 mmol), anthranilic acid (3.87 g, 28.2 mmol), and isoamyl nitrite (4.73 g, 40.4 mmol) according to the general procedure A. Column chromatography (toluene/EtOAc, 8:2) provided a 1:1 mixture of the two isomers of **2k** (3.05 g, 80%) as a yellow oil. ¹H NMR (500 MHz, CDCl₃) δ (ppm) 2.132 (s, 6H), 2.136 (s, 6H), 4.43 (d, *J* = 11.87 Hz, 4H), 4.49 (d, *J* = 11.90 Hz, 4H), 4.54 (d, *J* = 11.90 Hz, 4H), 4.59 (d, *J* = 11.87 Hz, 4H), 4.86 (d, *J* = 12.6 Hz, 4H), 4.99 (d, *J* = 12.6 Hz, 4H), 6.87 (s, 2H), 6.88 (s, 4H), 6.95–7.00 (m, 8H), 7.20–7.26 (m, 8H); ¹³C NMR (125 MHz, CDCl₃) δ (ppm) 20.8, 61.3, 68.8, 90.7, 92.4, 119.1, 119.2, 119.9, 120.0, 125.0, 125.1, 125.2, 125.3, 128.4, 128.4, 129.0, 130.0, 137.8, 143.1, 143.2, 144.6, 144.6, 148.9, 149.0, 149.4, 149.5, 170.9; IR (neat) ν (cm⁻¹) 2925, 1743, 1454, 1236; MS-EI *m/z* (rel. intensity) 474 (38, M⁺), 415 (5, [M – OAc]⁺), 355 (16, [M – 2OAc]⁺), 337 (29), 325 (25), 229 (56), 216 (58), 199 (43),

169 (52), 157 (75, $[\text{C}_{11}\text{H}_9\text{O}]^+$), 128 (100); HRMS (m/z): calcd for $\text{C}_{28}\text{H}_{26}\text{O}_7$, 474.1679; found, 474.1678.

***cis-1* Bis(isobenzofuran)- C_{60} Adduct 4f.** Compound **4f** was prepared according to general procedure B described above using 288 mg (0.4 mmol) of C_{60} , 223 mg (0.4 mmol) of quinoxaline **2f**, and 0.5 mL (1.5 mmol) of a 3 M solution of the parent tetrazine **3b** in CH_2Cl_2 . After column chromatography and eluting with toluene/ethyl acetate 9:1 ($R_f = 0.22$), the cycloadduct was obtained as a brown solid to give 42 mg (8.6%; 32% based on recovered C_{60}). ^1H NMR (500 MHz, $\text{CS}_2/\text{CDCl}_3$, 9:1) δ (ppm) 2.08 (s, 6H), 5.41 (d, $J = 12.6$ Hz, 2H), 5.68 (d, $J = 12.6$ Hz, 2H), 7.30–7.40 (m, 6H), 7.89–7.93 (m, 4H), 8.29 (dd, $J = 6.4, 3.4$ Hz, 2H); ^{13}C NMR (125 MHz, $\text{CS}_2/\text{CDCl}_3$, 9:1) δ (ppm) 34.2, 61.7, 74.3, 79.0, 93.3, 93.4, 119.5, 126.4, 127.1, 129.1, 129.7, 131.2, 135.3, 136.1, 138.3, 140.0, 140.7, 140.8, 140.9, 141.8, 142.0, 142.2, 142.3, 142.4, 142.7, 142.9, 143.2, 143.4, 143.6, 143.7, 143.8, 144.2, 144.3, 144.6, 144.9, 145.5, 145.6, 146.1, 146.4, 146.5, 147.1, 147.5, 147.6, 148.5, 149.2, 149.7, 169.0; IR (KBr) ν (cm^{-1}) 1749, 1223, 1050, 752; MS-FAB m/z (rel. intensity) 1227 (21, MH^+), 720 (100, C_{60}^+); HRMS–FAB (m/z): MH^+ calcd for $\text{C}_{90}\text{H}_{23}\text{N}_2\text{O}_6$, 1227.1556; found, 1227.1540.

***cis-1* Bis(isobenzofuran)- C_{60} Adduct 4g.** Compound **4g** was prepared according to general procedure B described above using 144 mg (0.2 mmol) of C_{60} , 95 mg (0.2 mmol) of quinoxaline **2g**, and 1.0 mL (3.0 mmol) of a 3 M solution of the parent tetrazine **3b** in CH_2Cl_2 . After column chromatography and eluting with toluene/THF 1:1 ($R_f = 0.5$), the cycloadduct was obtained as

a brown solid (112 mg, 49%; 77% based on recovered C₆₀). ¹H NMR (500 MHz, CDCl₃) δ (ppm) 5.22 (d, *J* = 12.9 Hz, 2H), 5.27 (d, *J* = 12.9 Hz, 2H), 7.36–7.41 (m, 4H), 7.46 (t, *J* = 6.2 Hz, 2H), 7.96 (dd, *J* = 6.4, 3.4 Hz, 2H), 8.00 (d, *J* = 7.5 Hz, 2H), 8.37 (dd, *J* = 6.4, 3.4 Hz, 2H); ¹³C NMR (125 MHz, THF-*d*₈) δ (ppm) 62.3, 76.2, 80.8, 94.8, 97.2, 121.6, 126.9, 127.9, 128.9, 129.7, 130.2, 130.7, 132.6, 136.4, 137.1, 139.9, 140.8, 142.2, 142.6, 142.8, 142.9, 143.0, 143.3, 143.6, 143.7, 143.8, 144.4, 144.5, 144.6, 144.9, 145.2, 145.3, 145.5, 145.9, 146.1, 146.8, 147.2, 147.6, 147.9, 148.4, 148.7, 148.7, 149.6, 150.4, 151.8, 152.6; IR (KBr) ν (cm⁻¹) 3436, 1630, 1461, 1050, 752; MS-FAB *m/z* (rel. intensity) 1144 (46, MH⁺), 720 (100, C₆₀⁺); HRMS-FAB (*m/z*): MH⁺ calcd for C₈₆H₁₉N₂O₄, 1143.1345; found, 1143.1344.

***cis-I* Bis(isobenzofuran)-C₆₀ Adduct 4h.** 3,6-Dihydro-1,2,4,5-tetrazine **3b** (0.37 M, 1.3 mL, 0.480 mmol) was added to a solution of C₆₀ (0.130 g, 0.180 mmol) and compound **2h** (0.0661 g, 0.120 mmol) in dry *o*-dichlorobenzene (7 mL). The resulting solution was stirred at room temperature for 2.5 h. Hexanes (5 mL) was added to the mixture, which was then placed onto a silica gel column; C₆₀ was eluted using hexanes and then the desired product was eluted using toluene/EtOAc (9/1). The fractions containing the product were concentrated and added to hexanes. The precipitate that formed was filtered and dried to give **4h** as a brown solid [8 mg, 4% (25% based on consumed C₆₀)]. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 4.31 (d, *J* = 5.7 Hz, 4H), 5.22 (ddd, *J* = 11.8, 2.8, 1.2 Hz, 2H), 5.35 (ddd, *J* = 11.8, 2.8, 1.2 Hz, 2H), 5.98 (m, 2H), 7.38 (dt, *J* = 7.4, 1.2 Hz, 2H), 7.44 (dt, *J* = 7.5, 1.2 Hz, 2H), 7.58 (d, *J* = 7.4 Hz, 2H), 7.93 (d, *J* = 6.5, 3.4 Hz, 2H), 7.98 (d, *J* = 7.3 Hz, 2H), 8.35 (dd, *J* = 6.5, 3.4 Hz, 2H); FTIR (KBr) ν (cm⁻¹) 525, 739,

752, 762, 923, 966, 989, 1049, 1104, 1147, 1263, 1349, 1462, 1491, 1531, 1608, 1645, 2584, 2923, 3074; HRMS–FAB⁺ (*m/z*): [M + Na]⁺ calcd for C₉₂H₂₆N₂O₄Na, 1245.1785; found, 1245.1864.

***cis-I* Bis(isobenzofuran)-C₆₀ Adduct 4i.** Compound **4i** was prepared according to general procedure B described above using 183 mg (0.250 mmol) of C₆₀, 135 mg (0.250 mmol) of quinoxaline **2i**, and 2.7 mL (1.02 mmol) of a 0.37 M solution of the parent tetrazine **3b** in CH₂Cl₂ in dry toluene (190 mL). The resulting solution was stirred at room temperature for 4 h. Hexanes (100 mL) was added to the mixture, which was then placed onto a silica gel column; C₆₀ (60% recovery) was eluted using hexanes. The desired product was then eluted using toluene/EtOAc (9/1) to give **4i** as a brown solid (40 mg, 13%; 33% based on consumed C₆₀). ¹H NMR (400 MHz, CDCl₃) δ (ppm) 1.22 (m, 6H), 3.76 (m, 4H), 4.83 (d, *J* = 10.6 Hz, 2H), 4.97 (d, *J* = 10.5 Hz, 2H), 7.31 (m, 4H), 7.51 (m, 2H), 7.87 (m, 4H), 8.27 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ (ppm) 15.3, 67.7, 69.6, 74.5, 79.5, 93.6, 93.8, 120.5, 126.3, 127.2, 129.0, 129.8, 131.2, 135.1, 136.1, 138.6, 139.7, 141.0, 141.1, 141.5, 141.7, 141.9, 142.4, 142.5, 142.6, 143.0, 143.4, 143.6, 143.7, 143.9, 144.05, 144.09, 144.3, 144.4, 144.8, 144.9, 145.7, 146.3, 146.6, 146.9, 147.4, 147.7, 147.8, 148.6, 149.0, 150.0, 150.8; FTIR (KBr) ν (cm⁻¹) 525, 661, 693, 740, 751, 761, 875, 923, 961, 1016, 1048, 1065, 1118, 1148, 1176, 1194, 1348, 1376, 1462, 1514, 2869, 2925, 2971, 3045, 3070; HRMS–FAB⁺ (*m/z*): [M + H]⁺ calcd for C₉₀H₂₇N₂O₄, 1199.1965; found, 1199.2020.

***cis-I* Bis(isobenzofuran)-C₆₀ Adduct 4j.** Compound **4j** is prepared according to general procedure B described above using 455 mg (0.2 mmol) of C₆₀, 280

mg (0.2 mmol) of quinoxaline **2j**, and 2.0 mL (6.0 mmol) of a 3 M solution of the parent tetrazine **3b** in CH₂Cl₂. After column chromatography and eluting with toluene/ethyl acetate 9:1 (*R_f* = 0.7), the cycloadduct was obtained as a brown solid to give 389 mg (56%, 92% based on recovered C₆₀). ¹H NMR (500 MHz, CS₂/CDCl₃, 9:1) δ (ppm) 2.60 (s, 6H), 7.29–7.35 (m, 6H), 7.87–7.90 (m, 4H), 8.26 (dd, *J* = 6.4, 3.4 Hz, 2H); ¹³C NMR (125 MHz, CS₂/CDCl₃, 9:1) δ (ppm) 16.4, 74.5, 80.2, 92.9, 93.0, 118.3, 125.1, 126.0, 126.9, 127.9, 128.7, 128.9, 129.6, 130.9, 134.9, 136.0, 138.4, 140.1, 140.9, 141.0, 141.4, 141.7, 142.0, 142.1, 142.3, 142.8, 143.2, 143.3, 143.6, 143.6, 143.7, 144.2, 144.2, 144.3, 144.66, 144.67, 145.5, 145.6, 146.0, 146.5, 146.9, 147.1, 147.6, 148.5, 150.5, 150.55, 150.57; IR (KBr) ν (cm⁻¹) 1384, 1125, 1042, 751; MS-FAB *m/z* (rel. intensity) 1111 (37, MH⁺), 720 (100, C₆₀⁺); HRMS-FAB (*m/z*): MH⁺ calcd for C₈₆H₁₉N₂O₂, 1111.1447; found, 1111.1431.

Mono(isobenzofuran)-C₆₀ Adducts: *syn*- and *anti*-9,10-(1-Acetoxymethyl-8-(2'-oxa-3'-(8''-(1''-acetoxymethyl-11''-oxatricyclo[6,2,1,0^{2,7}]undeca-2'',4'',6'',9''-tetraenyl))propyl)-11-oxatricyclo[6,2,1,0^{2,7}]undeca-2,4,6-trieno)-1''',2'''-

buckminsterfullerene (4k'). Compound **4k'** was prepared according to general procedure B described above using 180 mg (0.25 mmol) of C₆₀, 119 mg (0.25 mmol) of bisacetate **2k**, and tetrazine **3a** (148 mg, 1.12 mmol) in 100 mL toluene. After column chromatography and eluting with toluene/ethyl acetate 9:1 (*R_f* = 0.7), the cycloadduct was obtained as a brown solid to give 213 mg (73%, 81% based on recovered C₆₀). ¹H NMR (500 MHz, CDCl₃/CS₂, 3:1) δ (ppm) 2.11 (s, 3H), 2.12 (s, 3H), 2.13 (s, 3H), 2.14 (s, 3H), 4.51 (d, *J* = 11.7 Hz, 1H), 4.63 (d, *J* = 11.6

Hz, 2H), 4.69 (d, $J = 11.6$ Hz, 2H), 4.76 (d, $J = 11.7$ Hz, 1H), 4.82 (d, $J = 12.7$ Hz, 1H), 4.83 (d, $J = 12.7$ Hz, 1H), 4.94 (d, $J = 13.1$ Hz, 1H), 4.97 (d, $J = 13.1$ Hz, 1H), 5.07 (d, $J = 11.5$ Hz, 1H), 5.09 (d, $J = 11.5$ Hz, 1H), 5.32 (d, $J = 11.3$ Hz, 1H), 5.38 (d, $J = 11.3$ Hz, 1H), 5.46 (d, $J = 12.6$ Hz, 1H), 5.47 (d, $J = 12.6$ Hz, 1H), 5.79 (d, $J = 12.6$ Hz, 2H), 6.83–7.00 (m, 4H), 7.46–7.50 (m, 4H), 7.60–7.64 (m, 2H), 7.75–7.84 (m, 2H); ^{13}C NMR (125 MHz, $\text{CDCl}_3/\text{CS}_2$ 3:1) δ (ppm) 20.67, 20.69, 61.2, 62.9, 63.0, 69.5, 71.5, 79.66, 79.68, 78.0, 90.7, 90.7, 91.0, 92.0, 94.3, 95.2, 95.3, 119.15, 119.19, 119.6, 119.9, 121.5, 121.6, 123.0, 125.0, 125.1, 125.17, 125.21, 125.3, 128.97, 128.01, 128.10, 128.14, 128.2, 129.0, 137.5, 137.6, 137.68, 137.70, 137.8, 137.9, 138.0, 139.3, 139.4, 139.5, 139.75, 139.78, 139.9, 141.7, 141.77, 141.80, 141.9, 142.00, 142.06, 142.11, 142.59, 142.61, 142.64, 142.7, 143.0, 143.05, 143.10, 143.3, 143.48, 143.53, 144.0, 144.1, 144.2, 144.36, 144.44, 144.48, 144.52, 144.7, 145.1, 145.20, 145.23, 145.31, 145.34, 145.39, 145.42, 145.9, 146.0, 146.09, 146.13, 146.3, 146.45, 146.49, 147.0, 148.8, 148.9, 149.3, 149.5, 151.2, 151.8, 151.87, 151.89, 151.9, 152.2, 152.3, 170.3, 170.6; IR (KBr) ν (cm^{-1}) 2913, 2862, 1747, 1225, 1045, 751, 527.

Ortep drawing of Compound 4b

* For detailed bond lengths, bond angles, and torsional angles, see the supplied CIF file.

Table 1. Crystal data and structure refinement for Compound **4b**

Empirical formula	$C_{77}H_{12}O_2 \cdot 1.2(CHCl_3)$	
Formula weight	1112.11	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C m	
Unit cell dimensions	$a = 20.310(4)$ Å	$\alpha = 90^\circ$.
	$b = 20.105(3)$ Å	$\beta = 99.637(3)^\circ$.
	$c = 27.042(5)$ Å	$\gamma = 90^\circ$.
Volume	$10887(3)$ Å ³	
Z	2	
Density (calculated)	1.696 Mg/m ³	
Absorption coefficient	0.314 mm ⁻¹	
F(000)	5596	
Crystal size	$0.20 \times 0.10 \times 0.10$ mm ³	
Theta range for data collection	1.44 to 28.29° .	
Index ranges	$-20 \leq h \leq 27$; $-22 \leq k \leq 26$; $-36 \leq l \leq 34$	
Reflections collected	35,674	
Independent reflections	19,360 [R(int) = 0.0563]	
Completeness to $\theta = 28.29^\circ$	96.7%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.9299	
Refinement method	Full-matrix-block least-squares on F ²	
Data / restraints / parameters	19,360 / 38 / 1917	
Goodness-of-fit on F ²	0.883	
Final R indices [I > 2sigma(I)]	R1 = 0.0569, wR2 = 0.1129	
R indices (all data)	R1 = 0.1476, wR2 = 0.1396	
Absolute structure parameter	0.00(19)	
Largest diff. peak and hole	0.984 and -0.754 e.Å ⁻³	

¹H NMR Spectrum of Compound **4b'**

¹³C NMR Spectrum of Compound **4b'**

¹H NMR Spectrum of Compound **4b**

¹³C NMR Spectrum of Compound **4b**

¹H NMR Spectrum of Compound **4e**

¹³C NMR Spectrum of Compound **4e**

¹H NMR Spectrum of Compound **4f**

¹³C NMR Spectrum of Compound **4f**

Chemical structure of the compound is shown above the spectrum. The compound is a C₆₀ fullerene derivative with a pyrazine ring fused to the cage, and two hydroxymethyl groups (HOCH₂) attached to the cage. The spectrum shows peaks corresponding to the protons in the molecule, with chemical shifts (ppm) and integrations provided.

Chemical structure: OCC1C2C(C1)C3C(C2)C4C(C3)C5C(C4)C6C(C5)C7C(C6)C8C(C7)C9C(C8)C10C(C9)C11C(C10)C12C(C11)C13C(C12)C14C(C13)C15C(C14)C16C(C15)C17C(C16)C18C(C17)C19C(C18)C20C(C19)C21C(C20)C22C(C21)C23C(C22)C24C(C23)C25C(C24)C26C(C25)C27C(C26)C28C(C27)C29C(C28)C30C(C29)C31C(C30)C32C(C31)C33C(C32)C34C(C33)C35C(C34)C36C(C35)C37C(C36)C38C(C37)C39C(C38)C40C(C39)C41C(C40)C42C(C41)C43C(C42)C44C(C43)C45C(C44)C46C(C45)C47C(C46)C48C(C47)C49C(C48)C50C(C49)C51C(C50)C52C(C51)C53C(C52)C54C(C53)C55C(C54)C56C(C55)C57C(C56)C58C(C57)C59C(C58)C60C(C59)C61C(C60)C62C(C61)C63C(C62)C64C(C63)C65C(C64)C66C(C65)C67C(C66)C68C(C67)C69C(C68)C70C(C69)C71C(C70)C72C(C71)C73C(C72)C74C(C73)C75C(C74)C76C(C75)C77C(C76)C78C(C77)C79C(C78)C80C(C79)C81C(C80)C82C(C81)C83C(C82)C84C(C83)C85C(C84)C86C(C85)C87C(C86)C88C(C87)C89C(C88)C90C(C89)C91C(C90)C92C(C91)C93C(C92)C94C(C93)C95C(C94)C96C(C95)C97C(C96)C98C(C97)C99C(C98)C100C(C99)C101C(C100)C102C(C101)C103C(C102)C104C(C103)C105C(C104)C106C(C105)C107C(C106)C108C(C107)C109C(C108)C110C(C109)C111C(C110)C112C(C111)C113C(C112)C114C(C113)C115C(C114)C116C(C115)C117C(C116)C118C(C117)C119C(C118)C120C(C119)C121C(C120)C122C(C121)C123C(C122)C124C(C123)C125C(C124)C126C(C125)C127C(C126)C128C(C127)C129C(C128)C130C(C129)C131C(C130)C132C(C131)C133C(C132)C134C(C133)C135C(C134)C136C(C135)C137C(C136)C138C(C137)C139C(C138)C140C(C139)C141C(C140)C142C(C141)C143C(C142)C144C(C143)C145C(C144)C146C(C145)C147C(C146)C148C(C147)C149C(C148)C150C(C149)C151C(C150)C152C(C151)C153C(C152)C154C(C153)C155C(C154)C156C(C155)C157C(C156)C158C(C157)C159C(C158)C160C(C159)C161C(C160)C162C(C161)C163C(C162)C164C(C163)C165C(C164)C166C(C165)C167C(C166)C168C(C167)C169C(C168)C170C(C169)C171C(C170)C172C(C171)C173C(C172)C174C(C173)C175C(C174)C176C(C175)C177C(C176)C178C(C177)C179C(C178)C180C(C179)C181C(C180)C182C(C181)C183C(C182)C184C(C183)C185C(C184)C186C(C185)C187C(C186)C188C(C187)C189C(C188)C190C(C189)C191C(C190)C192C(C191)C193C(C192)C194C(C193)C195C(C194)C196C(C195)C197C(C196)C198C(C197)C199C(C198)C200C(C199)C201C(C200)C202C(C201)C203C(C202)C204C(C203)C205C(C204)C206C(C205)C207C(C206)C208C(C207)C209C(C208)C210C(C209)C211C(C210)C212C(C211)C213C(C212)C214C(C213)C215C(C214)C216C(C215)C217C(C216)C218C(C217)C219C(C218)C220C(C219)C221C(C220)C222C(C221)C223C(C222)C224C(C223)C225C(C224)C226C(C225)C227C(C226)C228C(C227)C229C(C228)C230C(C229)C231C(C230)C232C(C231)C233C(C232)C234C(C233)C235C(C234)C236C(C235)C237C(C236)C238C(C237)C239C(C238)C240C(C239)C241C(C240)C242C(C241)C243C(C242)C244C(C243)C245C(C244)C246C(C245)C247C(C246)C248C(C247)C249C(C248)C250C(C249)C251C(C250)C252C(C251)C253C(C252)C254C(C253)C255C(C254)C256C(C255)C257C(C256)C258C(C257)C259C(C258)C260C(C259)C261C(C260)C262C(C261)C263C(C262)C264C(C263)C265C(C264)C266C(C265)C267C(C266)C268C(C267)C269C(C268)C270C(C269)C271C(C270)C272C(C271)C273C(C272)C274C(C273)C275C(C274)C276C(C275)C277C(C276)C278C(C277)C279C(C278)C280C(C279)C281C(C280)C282C(C281)C283C(C282)C284C(C283)C285C(C284)C286C(C285)C287C(C286)C288C(C287)C289C(C288)C290C(C289)C291C(C290)C292C(C291)C293C(C292)C294C(C293)C295C(C294)C296C(C295)C297C(C296)C298C(C297)C299C(C298)C300C(C299)C301C(C300)C302C(C301)C303C(C302)C304C(C303)C305C(C304)C306C(C305)C307C(C306)C308C(C307)C309C(C308)C310C(C309)C311C(C310)C312C(C311)C313C(C312)C314C(C313)C315C(C314)C316C(C315)C317C(C316)C318C(C317)C319C(C318)C320C(C319)C321C(C320)C322C(C321)C323C(C322)C324C(C323)C325C(C324)C326C(C325)C327C(C326)C328C(C327)C329C(C328)C330C(C329)C331C(C330)C332C(C331)C333C(C332)C334C(C333)C335C(C334)C336C(C335)C337C(C336)C338C(C337)C339C(C338)C340C(C339)C341C(C340)C342C(C341)C343C(C342)C344C(C343)C345C(C344)C346C(C345)C347C(C346)C348C(C347)C349C(C348)C350C(C349)C351C(C350)C352C(C351)C353C(C352)C354C(C353)C355C(C354)C356C(C355)C357C(C356)C358C(C357)C359C(C358)C360C(C359)C361C(C360)C362C(C361)C363C(C362)C364C(C363)C365C(C364)C366C(C365)C367C(C366)C368C(C367)C369C(C368)C370C(C369)C371C(C370)C372C(C371)C373C(C372)C374C(C373)C375C(C374)C376C(C375)C377C(C376)C378C(C377)C379C(C378)C380C(C379)C381C(C380)C382C(C381)C383C(C382)C384C(C383)C385C(C384)C386C(C385)C387C(C386)C388C(C387)C389C(C388)C390C(C389)C391C(C390)C392C(C391)C393C(C392)C394C(C393)C395C(C394)C396C(C395)C397C(C396)C398C(C397)C399C(C398)C400C(C399)C401C(C400)C402C(C401)C403C(C402)C404C(C403)C405C(C404)C406C(C405)C407C(C406)C408C(C407)C409C(C408)C410C(C409)C411C(C410)C412C(C411)C413C(C412)C414C(C413)C415C(C414)C416C(C415)C417C(C416)C418C(C417)C419C(C418)C420C(C419)C421C(C420)C422C(C421

¹³C NMR Spectrum of Compound **4g**

¹H NMR Spectrum of Compound 4b

¹H NMR Spectrum of Compound **4i**

¹³C NMR Spectrum of Compound **4i**

¹H NMR Spectrum of Compound **4j**

¹³C NMR Spectrum of Compound **4j**

¹H NMR Spectrum of Compound **4k'**

¹³C NMR Spectrum of Compound **4k'**

Linker -CH₂- A

X = CH₂

AM1 optimized geometry; Nimag=0

E = 0.088648858126

0 1

6 0	2.204223	-1.458563	0.179494
1 0	1.443886	-2.082823	0.672715
6 0	3.247867	-1.992891	-0.517219
1 0	3.366184	-3.083603	-0.600143
6 0	4.221365	-1.163413	-1.166164
1 0	5.037655	-1.661186	-1.710819
6 0	4.146818	0.197629	-1.119269
1 0	4.887945	0.838090	-1.617517
6 0	3.076750	0.803623	-0.404172
6 0	2.086008	-0.043385	0.262304
6 0	1.178645	0.815312	0.873680
6 0	2.701382	2.116270	-0.153443
1 0	3.091261	3.094890	-0.414701
8 0	1.549506	2.137967	0.619307
6 0	-0.014167	0.634880	1.720120
1 0	0.293815	0.088644	2.656978
1 0	-0.419607	1.642679	2.018486
6 0	-1.086963	-0.116082	1.046601
6 0	-2.174327	0.244865	0.258151
6 0	-2.879511	-0.995511	-0.070363
6 0	-2.171669	-2.021679	0.540365
1 0	-2.275319	-3.100334	0.603343
8 0	-1.080790	-1.502284	1.221352
6 0	-2.672892	1.483615	-0.232138
1 0	-2.136716	2.410727	0.016117
6 0	-3.799922	1.483313	-1.000405
1 0	-4.208501	2.425533	-1.395502
6 0	-4.050824	-0.943125	-0.875763
1 0	-4.574586	-1.877935	-1.120005
6 0	-4.489996	0.268223	-1.322802
1 0	-5.392458	0.341381	-1.948073

X = CH₂

PM3 optimized geometry; Nimag=0

E = 0.061802573795

SPE (B3LYP/3-21G*//PM3) =

-800.985187453 hartrees

SPE (B3LYP/6-31G*//PM3) =

-805.423552613 hartrees

0 1

6 0	3.039206	-1.219514	0.687263
1 0	2.533472	-1.952302	1.323956
6 0	4.291831	-1.418872	0.199630
1 0	4.839287	-2.337088	0.436957
6 0	4.941593	-0.448898	-0.635606
1 0	5.951144	-0.677411	-0.992987
6 0	4.337472	0.718489	-0.980206
1 0	4.824614	1.463599	-1.615887
6 0	3.022373	0.970386	-0.490892
6 0	2.365723	-0.009274	0.349936
6 0	1.119432	0.516407	0.659483
6 0	2.130658	2.019905	-0.632233
1 0	2.153737	2.969121	-1.158297
8 0	0.982237	1.752738	0.058993
6 0	-0.000022	0.000143	1.482306
1 0	0.394139	-0.798833	2.143105
1 0	-0.394224	0.799221	2.142953
6 0	-1.119434	-0.516269	0.659516
6 0	-2.365754	0.009312	0.349920
6 0	-3.022320	-0.970435	-0.490862
6 0	-2.130525	-2.019891	-0.632142
1 0	-2.153563	-2.969117	-1.158193
8 0	-0.982126	-1.752601	0.059069
6 0	-3.039298	1.219544	0.687150
1 0	-2.533560	1.952418	1.323740
6 0	-4.291953	1.418770	0.199550
1 0	-4.839473	2.336964	0.436816
6 0	-4.337443	-0.718656	-0.980173
1 0	-4.824540	-1.463830	-1.615814
6 0	-4.941655	0.448693	-0.635613
1 0	-5.951226	0.677113	-0.992998

Linker -CH₂- A and C₆₀ B

X = CH₂

AM1 optimized geometry; Nimag=0

E = 1.596572473317

0 1

6 0	-0.390267	-1.227905	-2.329641
6 0	0.852344	-1.733761	-2.907136
6 0	-0.665797	0.114036	-2.322704
6 0	-0.701243	-2.049575	-1.144801
6 0	1.774710	-0.857282	-3.456706
6 0	0.316060	1.033230	-2.873455
6 0	-1.268113	-1.472385	-0.038713
6 0	0.354299	-3.050227	-1.009971
6 0	-1.509090	0.824225	-1.273231
6 0	-7.390698	-1.065399	2.049033
6 0	1.314677	-2.859183	-2.095996
6 0	1.496449	0.572753	-3.438040
6 0	0.326072	2.229574	-2.040786
6 0	-5.535692	-1.167413	0.776465
6 0	-0.651332	2.044075	-0.980947
6 0	0.802186	-3.428517	0.245771
6 0	-1.852641	-0.066516	0.009955
6 0	-0.773608	-1.848272	1.275795
6 0	3.205924	-1.046732	-3.213693
6 0	-2.944225	1.156083	-1.811522
8 0	-6.004483	-1.086489	2.092105
6 0	-7.823606	-1.126789	0.731620
6 0	2.667923	-3.043840	-1.868552
6 0	3.812781	0.275527	-3.048311
6 0	-0.765276	-0.653016	2.110030
6 0	-3.434170	-0.076239	-0.029776
6 0	0.218727	-2.805433	1.426399
6 0	2.232757	-3.619891	0.490782
6 0	3.140427	-3.430595	-0.537430
6 0	3.640172	-2.109340	-2.439581
6 0	-1.256005	0.455540	1.307316
6 0	-0.356782	2.508005	0.274635
6 0	1.516788	2.904001	-1.813689

8 0	-3.648713	-0.080399	-1.486590
6 0	-6.618186	-1.190902	-0.096415
6 0	-3.576791	2.122710	-0.830512
6 0	-9.101917	-1.140918	0.107432
6 0	2.755720	1.278069	-3.190959
6 0	-0.668807	1.685072	1.458833
6 0	1.283421	-2.614547	2.413289
6 0	4.398727	-2.728515	-0.282836
6 0	4.707531	-1.912018	-1.458305
6 0	2.530509	-3.114814	1.832517
6 0	0.238245	-0.475275	3.051129
6 0	2.765611	2.413015	-2.399996
6 0	4.821666	0.462963	-2.117881
6 0	0.895939	3.210293	0.539148
6 0	1.812189	3.412708	-0.480836
6 0	-4.078605	-1.272737	0.622071
6 0	-3.889108	1.331341	0.320123
6 0	-6.741290	-1.252846	-1.512493
6 0	-9.170196	-1.211083	-1.252937
1 0	-10.003834	-1.095313	0.733600
6 0	-3.879936	3.464289	-0.872702
6 0	3.720612	-2.448189	2.073129
6 0	5.281510	-0.661309	-1.301361
6 0	4.680528	-2.250264	0.986131
6 0	3.833253	2.613712	-1.418811
6 0	0.839189	0.840770	3.221802
6 0	4.832176	1.664084	-1.280784
6 0	0.397352	1.892697	2.435178
6 0	3.243488	3.233619	-0.230624
6 0	-7.988560	-1.264123	-2.064148
1 0	-5.824386	-1.274060	-2.121581
1 0	-10.144334	-1.225720	-1.764558
6 0	-4.501940	1.892084	1.418070
6 0	-4.504135	4.032809	0.253852
1 0	-3.649891	4.081914	-1.751971
6 0	1.364505	2.833868	1.872054
6 0	1.292991	-1.479609	3.204105
6 0	3.730980	-1.247030	2.910209
6 0	5.577231	-0.155267	0.040077
6 0	2.550766	-0.776542	3.462041
6 0	3.683723	2.869991	1.030715
6 0	2.270039	0.660409	3.473999
6 0	5.298476	1.281793	0.052849
6 0	2.717896	2.669036	2.113067
1 0	-8.117447	-1.311358	-3.155853
6 0	-4.807062	3.265500	1.371646

1 0	-4.763486	1.287255	2.299240
1 0	-4.757922	5.103600	0.239112
6 0	5.285182	-0.927414	1.151705
6 0	4.740592	1.868607	1.176589
6 0	4.697462	-0.307168	2.340364
6 0	3.183944	1.548667	2.932951
1 0	-5.300527	3.730877	2.238375
6 0	4.431752	1.052105	2.352069
1 0	-7.874560	-1.010864	3.019164
1 0	-3.026512	1.357487	-2.895336
1 0	-3.852782	-2.179992	-0.007833
1 0	-3.601290	-1.418981	1.631548

X = CH₂

PM3 optimized geometry; Nimag=0

E = 1.312574865910

SPE (B3LYP/3-21G*//PM3) =

-3074.54999994 hartrees

SPE (B3LYP/6-31G*//PM3) =

-3091.61521055 hartrees

0 1

6 0	-0.660172	-1.570210	-1.849995
6 0	0.490544	-2.323291	-2.319140
6 0	-0.815721	-0.251074	-2.182750
6 0	-0.968900	-2.029851	-0.486059
6 0	1.451113	-1.713066	-3.109694
6 0	0.203824	0.393087	-2.980112
6 0	-1.417474	-1.143932	0.457623
6 0	-0.002975	-3.059085	-0.140236
6 0	-1.534320	0.777651	-1.321158
6 0	-7.775504	0.097923	1.249538
6 0	0.898472	-3.244680	-1.268297

6 0	1.303029	-0.311388	-3.447507
6 0	0.369260	1.747827	-2.484618
6 0	-5.660369	-0.533112	0.955748
6 0	-0.550085	1.934628	-1.384619
6 0	0.484642	-3.155424	1.152952
6 0	-1.880764	0.278236	0.162789
6 0	-0.878890	-1.223557	1.797611
6 0	2.866007	-1.977865	-2.878571
6 0	-2.968943	1.103957	-1.873472
8 0	-6.479396	0.404374	1.557590
6 0	-7.817137	-1.033546	0.453597
6 0	2.240223	-3.502947	-1.051170
6 0	3.593413	-0.730689	-3.079177
6 0	-0.716053	0.130507	2.295532
6 0	-3.463400	0.430278	0.170845
6 0	0.033844	-2.205674	2.150497
6 0	1.899104	-3.421357	1.384929
6 0	2.754870	-3.588657	0.310473
6 0	3.250467	-2.848957	-1.874464
6 0	-1.155564	1.041080	1.261522
6 0	-0.141476	2.662380	-0.298315
6 0	1.626521	2.332945	-2.478901
8 0	-3.760974	0.082050	-1.221250
6 0	-6.441975	-1.446603	0.262619
6 0	-3.452196	2.351131	-1.159405
6 0	-8.873329	-1.782338	-0.143524
6 0	2.626822	0.300310	-3.434616
6 0	-0.452006	2.200617	1.065187
6 0	1.164682	-1.882213	3.012309
6 0	4.077559	-2.978776	0.330322
6 0	4.383748	-2.521672	-1.019764
6 0	2.319907	-2.631855	2.535774
6 0	0.356077	0.437355	3.119927
6 0	2.784628	1.590006	-2.962166
6 0	4.668842	-0.418096	-2.265156
6 0	1.175684	3.274373	-0.267483
6 0	2.042795	3.123333	-1.337644
6 0	-4.200695	-0.440900	1.174134
6 0	-3.757138	1.926262	0.156372
6 0	-6.151439	-2.603638	-0.518176
6 0	-8.550927	-2.877036	-0.881040
1 0	-9.908321	-1.460772	0.004380
6 0	-3.626048	3.659035	-1.549460
6 0	3.575910	-2.049659	2.553615
6 0	5.074311	-1.337010	-1.209486
6 0	4.477285	-2.228260	1.422719

6 0	3.917803	1.921011	-2.107783
6 0	1.075686	1.680113	2.925415
6 0	4.835188	0.941651	-1.767006
6 0	0.681199	2.536538	1.910339
6 0	3.459246	2.871268	-1.102060
6 0	-7.188342	-3.288400	-1.068147
1 0	-5.108213	-2.904079	-0.658233
1 0	-9.334954	-3.476586	-1.355365
6 0	-4.223851	2.815180	1.098123
6 0	-4.109776	4.561069	-0.590767
1 0	-3.396606	3.986542	-2.567920
6 0	1.686871	3.200641	1.093522
6 0	1.322046	-0.592580	3.484720
6 0	3.742091	-0.689853	3.051747
6 0	5.492516	-0.545691	-0.059142
6 0	2.644077	0.020007	3.507257
6 0	3.940676	2.794182	0.192999
6 0	2.492075	1.427847	3.161694
6 0	5.343319	0.862663	-0.403622
6 0	3.031785	2.968424	1.319835
1 0	-7.002971	-4.180634	-1.675370
6 0	-4.398265	4.149287	0.702526
1 0	-4.459324	2.492160	2.117596
1 0	-4.261384	5.608558	-0.872857
6 0	5.201871	-0.979597	1.222409
6 0	4.908161	1.765778	0.551028
6 0	4.746278	-0.028588	2.228612
6 0	3.445088	2.054365	2.378055
1 0	-4.773225	4.875705	1.431617
6 0	4.601938	1.308663	1.901131
1 0	-8.527341	0.764462	1.660073
1 0	-3.095298	1.044450	-2.967576
1 0	-3.791336	-1.472718	1.134359
1 0	-3.984650	-0.051356	2.190514

Linker -CH₂- and C₆₀ C

X = CH₂

AM1 optimized geometry; Nimag=0

E=1.570171596446

0 1

6 0	1.150016	0.683259	-2.256224
6 0	0.009628	1.393790	-2.827402
6 0	1.150012	-0.683279	-2.256224
6 0	1.834293	1.581732	-1.240736
6 0	-1.060380	0.726524	-3.399664
6 0	0.009645	-1.393816	-2.827384
6 0	2.355839	0.794874	0.023387
6 0	0.748042	2.609842	-0.966823
6 0	1.834299	-1.581719	-1.240725
6 0	3.145211	2.284062	-1.751278
6 0	-0.238226	2.585667	-2.027951
6 0	-1.060371	-0.726560	-3.399651
6 0	-0.238202	-2.585676	-2.027925
6 0	3.905835	1.172991	0.004871
6 0	0.748063	-2.609830	-0.966811
6 0	0.369401	3.031046	0.279202
6 0	2.355804	-0.794865	0.023375
6 0	1.631042	1.173261	1.289335
6 0	-2.433153	1.183717	-3.173412
6 0	3.145220	-2.284045	-1.751263
8 0	4.138024	1.268443	-1.450383
6 0	3.526516	3.348197	-0.730486
6 0	-1.535555	3.029903	-1.813938
6 0	-3.281376	-0.000023	-3.024731
6 0	1.359102	0.000004	2.089220
6 0	3.905919	-1.172979	0.004851
6 0	0.831249	2.277288	1.457370
6 0	-0.994111	3.481961	0.536497
6 0	-1.928157	3.490369	-0.488037
6 0	-2.665591	2.304275	-2.396189
6 0	1.631034	-1.173236	1.289323
6 0	0.369421	-3.031028	0.279215
6 0	-1.535530	-3.029909	-1.813904

8 0	4.138039	-1.268424	-1.450353
6 0	4.039386	2.622586	0.398224
6 0	3.526489	-3.348188	-0.730468
6 0	3.503924	4.723205	-0.733259
6 0	-2.433148	-1.183763	-3.173412
6 0	0.831261	-2.277265	1.457379
6 0	-0.252271	2.290001	2.435423
6 0	-3.298211	3.039849	-0.236256
6 0	-3.754867	2.306511	-1.418892
6 0	-1.381896	3.029307	1.871567
6 0	0.352511	0.000006	3.050270
6 0	-2.665576	-2.304312	-2.396173
6 0	-4.312100	-0.000023	-2.098398
6 0	-0.994085	-3.481952	0.536522
6 0	-1.928132	-3.490382	-0.488007
6 0	4.696899	0.000024	0.537710
6 0	4.039445	-2.622575	0.398204
6 0	4.516137	3.284025	1.505931
6 0	3.995704	5.393862	0.403650
1 0	3.118788	5.293213	-1.590410
6 0	3.503976	-4.723201	-0.733268
6 0	-2.678250	2.607385	2.113474
6 0	-4.553586	1.184211	-1.272483
6 0	-3.662175	2.609321	1.028487
6 0	-3.754845	-2.306543	-1.418870
6 0	-0.484295	-1.178851	3.227446
6 0	-4.553566	-1.184246	-1.272468
6 0	-0.252257	-2.289977	2.435431
6 0	-3.298185	-3.039869	-0.236232
6 0	4.489002	4.692156	1.495420
1 0	4.910754	2.742738	2.377098
1 0	3.988206	6.494364	0.417519
6 0	4.516114	-3.284013	1.505951
6 0	3.995895	-5.393853	0.403577
1 0	3.119142	-5.293217	-1.590548
6 0	-1.381873	-3.029303	1.871594
6 0	-0.484302	1.178870	3.227434
6 0	-2.921079	1.424495	2.942400
6 0	-4.940499	0.731847	0.064759
6 0	-1.853960	0.732108	3.489788
6 0	-3.662151	-2.609331	1.028507
6 0	-1.853953	-0.732085	3.489795
6 0	-4.940491	-0.731876	0.064766
6 0	-2.678226	-2.607381	2.113496
1 0	4.869974	5.238489	2.371560
6 0	4.488843	-4.692139	1.495503

1 0	4.910501	-2.742707	2.377207
1 0	3.987984	-6.494351	0.417638
6 0	-4.506936	1.424409	1.183174
6 0	-4.506921	-1.424423	1.183186
6 0	-4.049131	0.692738	2.365663
6 0	-2.921069	-1.424484	2.942419
1 0	4.870200	-5.238484	2.371469
6 0	-4.049125	-0.692737	2.365670
1 0	3.175236	2.539468	-2.825984
1 0	3.175281	-2.539403	-2.825977
1 0	4.725964	0.000010	1.653923
1 0	5.739318	0.000082	0.129255

X = CH₂

PM3 optimized geometry; Nimag=0

E = 1.279349634894

SPE (B3LYP/3-21G*//PM3) =

-3074.58545861 hartrees

SPE (B3LYP/6-31G*//PM3) =

-3091.61521055 hartrees

0 1

6 0	-1.128507	-0.684039	-2.276530
6 0	0.014621	-1.389365	-2.830054
6 0	-1.128504	0.684043	-2.276528
6 0	-1.821353	-1.583289	-1.262645
6 0	1.089786	-0.722531	-3.392355
6 0	0.014625	1.389369	-2.830052
6 0	-2.359031	-0.793878	-0.004099
6 0	-0.727925	-2.599933	-0.982892
6 0	-1.821345	1.583294	-1.262642
6 0	-3.126322	-2.318749	-1.758208
6 0	0.258829	-2.575645	-2.031588

6 0	1.089788	0.722533	-3.392359	6 0	3.759569	2.300607	-1.396296
6 0	0.258835	2.575654	-2.031587	6 0	0.462878	1.172765	3.213986
6 0	-3.906011	-1.177507	-0.046854	6 0	4.556606	1.178864	-1.243338
6 0	-0.727917	2.599938	-0.982887	6 0	0.237125	2.281450	2.417922
6 0	-0.362699	-3.019119	0.266573	6 0	3.295198	3.030378	-0.222424
6 0	-2.359027	0.793884	-0.004097	6 0	-4.508308	-4.654304	1.516072
6 0	-1.638705	-1.167780	1.271172	1 0	-4.951986	-2.683282	2.336651
6 0	2.455374	-1.178023	-3.155794	1 0	-3.979413	-6.471669	0.494884
6 0	-3.126310	2.318758	-1.758206	6 0	-4.542915	3.251381	1.495489
8 0	-4.131860	-1.324588	-1.495097	6 0	-3.991832	5.377214	0.451331
6 0	-3.515313	-3.360713	-0.712414	1 0	-3.080943	5.311473	-1.527069
6 0	1.553491	-3.020308	-1.806387	6 0	1.366323	3.017552	1.865178
6 0	3.298843	-0.000002	-3.001125	6 0	0.462876	-1.172773	3.213984
6 0	-1.372905	-0.000002	2.068273	6 0	2.895852	-1.420363	2.945104
6 0	-3.906006	1.177516	-0.046855	6 0	4.930923	-0.728666	0.091186
6 0	-0.834798	-2.267858	1.437717	6 0	1.825181	-0.728664	3.484732
6 0	0.991312	-3.467718	0.532828	6 0	3.648510	2.600149	1.044608
6 0	1.932993	-3.478725	-0.484285	6 0	1.825182	0.728656	3.484738
6 0	2.682964	-2.297919	-2.377715	6 0	4.930925	0.728656	0.091188
6 0	-1.638703	1.167779	1.271176	6 0	2.660143	2.597472	2.117128
6 0	-0.362692	3.019121	0.266579	1 0	-4.900420	-5.183336	2.391376
6 0	1.553498	3.020321	-1.806390	6 0	-4.508283	4.654315	1.516076
8 0	-4.131844	1.324590	-1.495099	1 0	-4.951950	2.683294	2.336660
6 0	-4.045697	-2.620957	0.379848	1 0	-3.979394	6.471679	0.494883
6 0	-3.515297	3.360723	-0.712412	6 0	4.488412	-1.420723	1.205508
6 0	-3.484079	-4.734987	-0.688909	6 0	4.488415	1.420712	1.205511
6 0	2.455374	1.178019	-3.155788	6 0	4.023350	-0.692373	2.379454
6 0	-0.834788	2.267852	1.437720	6 0	2.895853	1.420352	2.945107
6 0	0.237124	-2.281450	2.417910	1 0	-4.900394	5.183346	2.391380
6 0	3.295189	-3.030383	-0.222430	6 0	4.023351	0.692360	2.379456
6 0	3.759563	-2.300611	-1.396301	1 0	-3.140074	-2.618386	-2.819059
6 0	1.366319	-3.017561	1.865173	1 0	-3.140061	2.618395	-2.819057
6 0	-0.368792	-0.000004	3.032329	1 0	-4.731510	0.000009	1.593598
6 0	2.682966	2.297913	-2.377706	1 0	-5.749460	0.000009	0.134482
6 0	4.322286	-0.000003	-2.067500				
6 0	0.991318	3.467709	0.532834				
6 0	1.933000	3.478716	-0.484279				
6 0	-4.702053	0.000007	0.488548				
6 0	-4.045685	2.620968	0.379846				
6 0	-4.542936	-3.251369	1.495487				
6 0	-3.991846	-5.377203	0.451333				
1 0	-3.080942	-5.311464	-1.527060				
6 0	-3.484066	4.734996	-0.688911				
6 0	2.660139	-2.597483	2.117123				
6 0	4.556602	-1.178871	-1.243339				
6 0	3.648504	-2.600159	1.044603				

Linker quinoxaline-2,3-diyl and C₆₀ A

X = quinoxaline-2,3-diyl

AM1 optimized geometry; Nimag=0

E=0.228249956152

0 1

6 0	-3.852910	-0.338703	-0.590331
1 0	-3.736785	0.689078	-0.964006
6 0	-5.022370	-1.030589	-0.723482
1 0	-5.889560	-0.570454	-1.220772
6 0	-5.168120	-2.366356	-0.225792
1 0	-6.138675	-2.864962	-0.367808
6 0	-4.143313	-3.008493	0.406379
1 0	-4.247798	-4.032483	0.791334
6 0	-2.905472	-2.329028	0.569881
6 0	-2.756095	-0.966261	0.060386
6 0	-1.449806	-0.576619	0.357924
6 0	-1.688117	-2.665288	1.150602
1 0	-1.292764	-3.535962	1.665933
8 0	-0.796195	-1.614078	1.029315
6 0	1.449816	-0.576639	-0.357927
6 0	2.756087	-0.966336	-0.060396
6 0	2.905381	-2.329142	-0.569811
6 0	1.687980	-2.665386	-1.150436
1 0	1.292556	-3.536107	-1.665637
8 0	0.796123	-1.614118	-1.029211
6 0	3.852969	-0.338734	0.590172
1 0	3.736869	0.689075	0.963775
6 0	5.022411	-1.030645	0.723305
1 0	5.889652	-0.570515	1.220509
6 0	4.143235	-3.008602	-0.406372
1 0	4.247669	-4.032638	-0.791224
6 0	5.168091	-2.366449	0.225693
1 0	6.138650	-2.865063	0.367663
6 0	-0.697829	5.409865	0.117656
6 0	-1.393161	4.233817	0.236533
6 0	-0.708729	2.982869	0.124118
6 0	0.708790	2.982858	-0.124096
6 0	1.393237	4.233798	-0.236521
6 0	0.697923	5.409855	-0.117641
1 0	-1.221610	6.374367	0.205220
1 0	-2.478963	4.233065	0.422719

1 0	2.479046	4.233035	-0.422662
1 0	1.221710	6.374350	-0.205241
6 0	0.716211	0.659436	-0.154722
6 0	-0.716173	0.659448	0.154745
7 0	1.399882	1.799186	-0.271465
7 0	-1.399833	1.799203	0.271487

X = quinoxaline-2,3-diyl

PM3 optimized geometry; Nimag=0

E = 0.172298115054

SPE (B3LYP/3-21G**//PM3) =

-1176.34803704 hartrees

SPE (B3LYP/6-31G**//PM3) =

-1182.88352469 hartrees

0 1

6 0	-3.715084	-0.451929	-0.774318
1 0	-3.558974	0.524877	-1.242244
6 0	-4.851437	-1.173601	-0.965467
1 0	-5.649610	-0.787915	-1.608521
6 0	-5.052555	-2.450016	-0.342114
1 0	-5.992944	-2.974424	-0.541577
6 0	-4.115610	-3.002466	0.472756
1 0	-4.258377	-3.974405	0.953908
6 0	-2.908371	-2.280577	0.701416
6 0	-2.703883	-0.991930	0.072660
6 0	-1.447966	-0.557983	0.481527
6 0	-1.772120	-2.532750	1.452567
1 0	-1.454060	-3.346571	2.097102
8 0	-0.888539	-1.501394	1.326382
6 0	1.447199	-0.559401	-0.480938
6 0	2.703116	-0.994056	-0.072793
6 0	2.906168	-2.283205	-0.700981
6 0	1.769178	-2.534930	-1.451167
1 0	1.450034	-3.348862	-2.095025
8 0	0.886468	-1.502848	-1.324894
6 0	3.715326	-0.454380	0.773182

1 0	3.560285	0.522785	1.240715
6 0	4.851309	-1.176770	0.963828
1 0	5.650240	-0.791340	1.606093
6 0	4.113031	-3.005877	-0.472828
1 0	4.254711	-3.978183	-0.953557
6 0	5.051000	-2.453683	0.341040
1 0	5.991159	-2.978672	0.540060
6 0	-0.678887	5.419455	0.187258
6 0	-1.361422	4.244353	0.376160
6 0	-0.679396	3.013771	0.189648
6 0	0.681961	3.013104	-0.189600
6 0	1.365129	4.243020	-0.376326
6 0	0.683685	5.418789	-0.187632
1 0	-1.188257	6.379201	0.327229
1 0	-2.417939	4.241553	0.669207
1 0	2.421641	4.239189	-0.669380
1 0	1.193947	6.378037	-0.327771
6 0	0.691852	0.660311	-0.214724
6 0	-0.691464	0.661001	0.215189
7 0	1.343096	1.806998	-0.393589
7 0	-1.341646	1.808312	0.393847

Linker quinoxaline-2,3-di-yl and C₆₀ B

X = quinoxaline-2,3-diyl

AM1 optimized geometry; Nimag=0
E=1.742187457231

0 1			
6 0	0.395839	-2.075930	-1.036087
6 0	-0.646273	-2.593930	-1.918785
6 0	0.339286	-2.289237	0.315713
6 0	0.813055	-0.760336	-1.556533
6 0	-1.711707	-3.310365	-1.396545
6 0	-0.793310	-3.015988	0.864100
6 0	1.147505	0.246668	-0.689226
6 0	0.021020	-0.487061	-2.753294
6 0	0.912895	-1.352568	1.369510
6 0	6.131038	-2.769560	0.612622
6 0	-0.880030	-1.616175	-2.980639
6 0	-1.786670	-3.527543	0.042179
6 0	-1.147398	-2.399685	2.136645
6 0	5.358071	-0.905365	-0.368132
6 0	-0.230090	-1.296538	2.369210
6 0	-0.409241	0.801428	-3.027702
6 0	1.376011	0.073329	0.807126
6 0	0.665070	1.590349	-0.963346
6 0	-3.069025	-3.079137	-1.894065
6 0	2.255235	-1.905506	1.956795
8 0	5.730322	-1.466677	0.854647
6 0	6.025089	-3.058414	-0.743040
6 0	-2.161953	-1.399080	-3.456859
6 0	-3.985241	-3.158342	-0.754650
6 0	0.312548	2.208165	0.308602
6 0	2.913449	0.069030	1.190390
6 0	-0.075386	1.874660	-2.101043
6 0	-1.765633	1.034979	-3.526621
6 0	-2.618938	-0.035546	-3.733345
6 0	-3.288080	-2.147972	-2.894995
6 0	0.580583	1.244337	1.363543
6 0	-0.712607	-0.147050	2.938378
6 0	-2.477774	-2.324727	2.522186
8 0	3.216538	-1.353202	1.003505
6 0	5.530900	-1.840592	-1.386123
6 0	2.573839	-1.096936	3.197099
6 0	6.290891	-4.209912	-1.533135
6 0	-3.192284	-3.439679	0.443189
6 0	-0.293822	1.168129	2.417129
6 0	-1.220302	2.784192	-2.026447
6 0	-4.023356	0.060334	-3.334087
6 0	-4.436886	-1.245123	-2.815989
6 0	-2.267858	2.262248	-2.905542
6 0	-0.765410	3.078437	0.378396
6 0	-3.528724	-2.853982	1.650532

6 0	-5.071488	-2.302183	-0.678588
6 0	-2.112483	-0.041663	3.340680
6 0	-2.977765	-1.106690	3.145693
6 0	2.991163	0.181892	2.709574
6 0	5.327093	-1.825172	-2.793001
6 0	6.078623	-4.148677	-2.879620
1 0	6.660032	-5.122037	-1.043784
6 0	2.546289	-1.368805	4.545691
6 0	-3.596884	2.352397	-2.525645
6 0	-5.303555	-1.319555	-1.738145
6 0	-4.498663	1.220956	-2.746302
6 0	-4.678469	-1.951698	1.732678
6 0	-1.674608	3.005391	1.514027
6 0	-5.427578	-1.682342	0.599088
6 0	-1.444083	2.063913	2.504617
6 0	-4.338163	-0.870197	2.659182
6 0	5.597523	-2.954744	-3.509754
1 0	4.962872	-0.904731	-3.271110
1 0	6.274458	-5.023231	-3.517958
6 0	3.369172	1.180245	3.578750
6 0	2.938808	-0.346378	5.430195
1 0	2.230140	-2.347846	4.931730
6 0	-2.567761	1.322083	3.075045
6 0	-1.556434	3.369708	-0.818951
6 0	-3.952819	2.972169	-1.247937
6 0	-5.804028	-0.092708	-1.115826
6 0	-2.960841	3.468732	-0.418301
6 0	-4.764266	0.421743	2.401749
6 0	-3.034377	3.243985	1.026695
6 0	-5.879576	-0.316783	0.328835
6 0	-3.855644	1.549323	2.620233
1 0	5.451101	-2.972934	-4.600247
6 0	3.338231	0.897305	4.957874
1 0	3.685629	2.170892	3.221807
1 0	2.927820	-0.544152	6.512786
6 0	-5.412869	1.141882	-1.605716
6 0	-5.557719	0.705987	1.205629
6 0	-5.074683	2.223746	-0.679322
6 0	-4.095135	2.534315	1.563514
1 0	3.641063	1.681613	5.668256
6 0	-5.144139	2.011490	0.687615
1 0	6.449166	-3.315916	1.495397
1 0	2.361429	-3.005654	1.987427
6 0	5.782629	4.926738	-1.864500
6 0	6.114419	3.596112	-1.878685
6 0	5.355998	2.662442	-1.104675

6 0	4.244835	3.140836	-0.326644
6 0	3.937530	4.537468	-0.338647
6 0	4.693819	5.398288	-1.092362
1 0	6.364291	5.648905	-2.458595
1 0	6.962644	3.227693	-2.477801
7 0	5.697425	1.326924	-1.095360
7 0	3.478196	2.265095	0.412836
1 0	3.088400	4.903738	0.260081
1 0	4.459616	6.474258	-1.105919
6 0	3.802276	0.973919	0.395552
6 0	4.957480	0.494575	-0.362346

X = quinoxaline-2,3-diyl
 PM3 optimized geometry; Nimag=0
 E = 1.429560474411

SPE (B3LYP/3-21G*//PM3) =
 -3449.89866985 hartrees
 SPE (B3LYP/6-31G*//PM3) =
 -3469.05664461 hartrees

0 1

6 0	-0.339071	2.324846	-0.208399
6 0	0.720276	3.083101	-0.851870
6 0	-0.284321	2.046484	1.130902
6 0	-0.795481	1.297112	-1.158400
6 0	1.804803	3.533474	-0.116218
6 0	0.863061	2.488773	1.890905
6 0	-1.173810	0.059027	-0.709897
6 0	-0.007372	1.441544	-2.371130
6 0	-0.902217	0.817844	1.783349
6 0	-6.417606	2.764058	0.974055
6 0	0.927475	2.542555	-2.187589

6 0	1.878064	3.224208	1.297881	6 0	1.539036	-3.379326	0.346844
6 0	1.187301	1.452430	2.854653	6 0	5.440541	1.186480	1.139053
6 0	-5.349228	1.202102	-0.190163	6 0	1.332729	-2.842416	1.607324
6 0	0.237473	0.375666	2.686893	6 0	4.312899	-0.262877	2.778267
6 0	0.380956	0.323698	-3.091523	6 0	-4.297204	4.090841	-2.332116
6 0	-1.415980	-0.300934	0.751769	1 0	-3.811942	2.006804	-2.554212
6 0	-0.731790	-1.106934	-1.442576	1 0	-4.907550	6.135114	-1.915430
6 0	3.150884	3.449816	-0.669782	6 0	-3.462875	-2.234579	2.996752
6 0	-2.231029	1.171529	2.537383	6 0	-2.979330	-1.463072	5.252684
8 0	-6.163980	1.424158	0.904328	1 0	-2.196565	0.559656	5.462267
6 0	-5.783046	3.422672	-0.065894	6 0	2.471547	-2.392240	2.394882
6 0	2.203127	2.468410	-2.718144	6 0	1.426285	-2.887894	-1.951872
6 0	4.058553	3.089872	0.412555	6 0	3.830341	-2.441893	-2.225183
6 0	-0.408662	-2.144203	-0.479852	6 0	5.773372	0.303885	-1.022217
6 0	-2.961703	-0.373960	1.136112	6 0	2.817637	-3.168111	-1.621783
6 0	0.008083	-0.990850	-2.609340	6 0	4.696946	-1.391249	2.075338
6 0	1.726448	0.239635	-3.646443	6 0	2.888011	-3.473224	-0.198168
6 0	2.615066	1.284267	-3.462599	6 0	5.846627	-0.002372	0.400871
6 0	3.344951	2.929367	-1.937173	6 0	3.753557	-2.486416	1.883244
6 0	-0.654015	-1.616010	0.843865	1 0	-3.729985	4.412347	-3.211986
6 0	0.675755	-0.916879	2.801564	6 0	-3.422700	-2.448290	4.382447
6 0	2.511768	1.199670	3.178468	1 0	-3.810174	-3.021737	2.319317
8 0	-3.202738	1.029574	1.474316	1 0	-2.963154	-1.657440	6.330505
6 0	-5.088293	2.405693	-0.829672	6 0	5.345170	-0.661118	-1.916947
6 0	-2.587344	-0.008885	3.416856	6 0	5.485118	-1.258208	0.857565
6 0	-5.711513	4.787968	-0.468915	6 0	4.967167	-1.984370	-1.436864
6 0	3.271673	2.953414	1.631442	6 0	3.967060	-3.036511	0.549981
6 0	0.217296	-1.943156	1.850247	1 0	-3.751152	-3.414579	4.780471
6 0	1.117506	-1.900664	-2.869077	6 0	5.034046	-2.274818	-0.084998
6 0	4.006898	1.007895	-3.133613	1 0	-7.046979	3.080084	1.800014
6 0	4.457901	2.024438	-2.190982	1 0	-2.291522	2.184433	2.970403
6 0	2.182409	-1.137911	-3.507463	6 0	-6.130100	-4.007294	-3.110782
6 0	0.640554	-3.015548	-0.730057	6 0	-6.376929	-2.701500	-2.769981
6 0	3.580725	1.965996	2.548529	6 0	-5.554793	-2.079054	-1.794618
6 0	5.114724	2.227520	0.172223	6 0	-4.501843	-2.802675	-1.193743
6 0	2.061935	-1.203602	3.128385	6 0	-4.268229	-4.153206	-1.562993
6 0	2.963797	-0.169686	3.322843	6 0	-5.077149	-4.732518	-2.507510
6 0	-3.047833	-1.008877	2.526218	1 0	-6.752713	-4.506139	-3.861754
6 0	-4.336958	2.777997	-1.982752	1 0	-7.192743	-2.135533	-3.235293
6 0	-4.984891	5.097327	-1.574724	7 0	-5.780249	-0.761437	-1.417205
1 0	-6.238892	5.547456	0.115516	7 0	-3.696478	-2.184134	-0.245642
6 0	-2.549119	-0.216509	4.776362	1 0	-3.449152	-4.712122	-1.095230
6 0	3.504665	-1.400889	-3.192102	1 0	-4.912633	-5.773370	-2.807543
6 0	5.319644	1.681769	-1.163203	6 0	-3.908076	-0.915972	0.098439
6 0	4.440147	-0.300205	-3.000932	6 0	-5.001132	-0.185417	-0.506057
6 0	4.693966	1.059629	2.298128				

Linker quinoxaline-2,3-diyl and C₆₀ C

X = quinoxaline-2,3-diyl

AM1 optimized geometry; Nimag=0

E=1.710101172044

0 1

6 0	-0.005867	0.679215	-2.515972
6 0	-1.222681	1.394473	-2.883912
6 0	-0.005871	-0.679283	-2.515948
6 0	0.859042	1.551625	-1.640295
6 0	-2.375309	0.727018	-3.262509
6 0	-1.222676	-1.394555	-2.883879
6 0	1.643787	0.802284	-0.460456
6 0	-0.160911	2.589697	-1.173375
6 0	0.859038	-1.551674	-1.640260
6 0	2.022750	2.245670	-2.443126
6 0	-1.319333	2.580203	-2.046787
6 0	-2.375305	-0.727118	-3.262494
6 0	-1.319324	-2.580269	-2.046734
6 0	3.084973	1.426774	-0.684072
6 0	-0.160911	-2.589737	-1.173320
6 0	-0.320385	3.016116	0.117291
6 0	1.643816	-0.802289	-0.460451
6 0	1.102324	1.168598	0.901823
6 0	-3.686003	1.184068	-2.797166
6 0	2.022733	-2.245749	-2.443089
8 0	3.149380	1.373282	-2.156331
6 0	2.385546	3.469382	-1.626820
6 0	-2.559291	3.026671	-1.611461
6 0	-4.494879	-0.000047	-2.502000
6 0	0.970355	0.000010	1.738037
6 0	3.085001	-1.426721	-0.684114
6 0	0.338457	2.269635	1.201135
6 0	-1.616608	3.473960	0.607127
6 0	-2.715185	3.486659	-0.237750
6 0	-3.775258	2.303767	-1.989226

6 0	1.102344	-1.168592	0.901839
6 0	-0.320372	-3.016133	0.117354
6 0	-2.559277	-3.026737	-1.611398
8 0	3.149340	-1.373316	-2.156389
6 0	3.011195	2.938288	-0.455122
6 0	2.385583	-3.469407	-1.626716
6 0	2.227804	4.823907	-1.807197
6 0	-3.685997	-1.184165	-2.797143
6 0	0.338471	-2.269619	1.201174
6 0	-0.558816	2.286609	2.352078
6 0	-4.021345	3.038773	0.248461
6 0	-4.677401	2.306161	-0.836760
6 0	-1.768016	3.025961	1.990632
6 0	0.143852	0.000022	2.858106
6 0	-3.775248	-2.303849	-1.989180
6 0	-5.346462	-0.000038	-1.408911
6 0	-1.616591	-3.473975	0.607199
6 0	-2.715168	-3.486698	-0.237679
6 0	3.011307	-2.938237	-0.455104
6 0	3.439013	3.780572	0.547927
6 0	2.686843	5.678379	-0.787196
1 0	1.759141	5.236052	-2.711428
6 0	2.227905	-4.823956	-1.807014
6 0	-3.003190	2.606541	2.454951
6 0	-5.439140	1.184271	-0.553472
6 0	-4.160508	2.608796	1.557355
6 0	-4.677389	-2.306221	-0.836713
6 0	-0.650263	-1.178299	3.175882
6 0	-5.439133	-1.184329	-0.553448
6 0	-0.558802	-2.286576	2.352118
6 0	-4.021330	-3.038807	0.248523
6 0	3.269194	5.166790	0.364827
1 0	3.906363	3.404707	1.469066
1 0	2.577654	6.766248	-0.911496
6 0	3.439217	-3.780437	0.547979
6 0	2.687062	-5.678346	-0.787002
1 0	1.759298	-5.236178	-2.711238
6 0	-1.767999	-3.025943	1.990692
6 0	-0.650271	1.178343	3.175859
6 0	-3.099546	1.424534	3.314866
6 0	-5.587476	0.731860	0.830658
6 0	-1.954289	0.732151	3.670994
6 0	-4.160494	-2.608803	1.557407
6 0	-1.954285	-0.732104	3.671007
6 0	-5.587472	-0.731889	0.830674
6 0	-3.003175	-2.606522	2.455003

1 0	3.614119	5.851745	1.154237
6 0	3.269411	-5.166667	0.364985
1 0	3.906551	-3.404475	1.469085
1 0	2.577882	-6.766226	-0.911217
6 0	-4.966098	1.424350	1.856696
6 0	-4.966091	-1.424355	1.856726
6 0	-4.310380	0.692784	2.942119
6 0	-3.099538	-1.424499	3.314894
1 0	3.614475	-5.851571	1.154377
6 0	-4.310377	-0.692762	2.942132
1 0	1.886513	2.331936	-3.536097
1 0	1.886449	-2.332100	-3.536048
6 0	8.589739	-0.707655	1.841450
6 0	7.516724	-1.413660	1.360265
6 0	6.375675	-0.719453	0.849591
6 0	6.375554	0.719544	0.849835
6 0	7.516421	1.413763	1.360895
6 0	8.589527	0.707773	1.841895
1 0	9.470818	-1.238784	2.234403
1 0	7.518158	-2.515425	1.355335
7 0	5.295199	-1.425600	0.358161
7 0	5.295013	1.425680	0.358536
1 0	7.517524	2.515530	1.356685
1 0	9.470595	1.238915	2.234855
6 0	4.264590	0.725868	-0.102975
6 0	4.264681	-0.725795	-0.103154

Linker quinoxaline-2,3-diyl and C₆₀ C

X = quinoxaline-2,3-diyl
PM3 optimized geometry; Nimag=0
E = 1.395876677599

SPE (B3LYP/3-21G**/PM3) =
-3449.93770056 hartrees

SPE (B3LYP/6-31G**/PM3) =
-3469.08451098 hartrees

0 1			
6 0	-0.015436	0.679861	-2.518118
6 0	-1.230443	1.389347	-2.876531
6 0	-0.015435	-0.679862	-2.518119
6 0	0.854307	1.554713	-1.645208
6 0	-2.384390	0.723041	-3.251379
6 0	-1.230443	-1.389347	-2.876531
6 0	1.650060	0.808129	-0.465797
6 0	-0.175856	2.580159	-1.176441
6 0	0.854309	-1.554714	-1.645207
6 0	2.016536	2.270456	-2.438029
6 0	-1.328385	2.570190	-2.042869
6 0	-2.384390	-0.723043	-3.251379
6 0	-1.328383	-2.570192	-2.042868
6 0	3.092185	1.448743	-0.702601
6 0	-0.175853	-2.580162	-1.176441
6 0	-0.328614	3.003447	0.115061
6 0	1.650061	-0.808127	-0.465797
6 0	1.105340	1.163912	0.900191
6 0	-3.688818	1.178443	-2.784764
6 0	2.016539	-2.270456	-2.438028
8 0	3.146713	1.417348	-2.172248
6 0	2.381024	3.488093	-1.611249
6 0	-2.566208	3.017111	-1.603905
6 0	-4.493556	-0.000002	-2.488907
6 0	0.973288	0.000000	1.731525
6 0	3.092188	-1.448738	-0.702601
6 0	0.333016	2.259692	1.194177
6 0	-1.616702	3.459243	0.605176

6 0	-2.717015	3.474856	-0.236882
6 0	-3.777688	2.297517	-1.977388
6 0	1.105339	-1.163910	0.900191
6 0	-0.328611	-3.003449	0.115060
6 0	-2.566205	-3.017116	-1.603907
8 0	3.146715	-1.417346	-2.172250
6 0	3.020502	2.960120	-0.462676
6 0	2.381032	-3.488091	-1.611248
6 0	2.205998	4.840985	-1.787029
6 0	-3.688816	-1.178445	-2.784763
6 0	0.333017	-2.259690	1.194176
6 0	-0.558778	2.277663	2.340034
6 0	-4.016402	3.029295	0.250954
6 0	-4.672783	2.300286	-0.827832
6 0	-1.763652	3.013893	1.982942
6 0	0.142617	0.000000	2.849017
6 0	-3.777685	-2.297520	-1.977387
6 0	-5.342608	-0.000003	-1.394492
6 0	-1.616698	-3.459244	0.605176
6 0	-2.717012	-3.474858	-0.236882
6 0	3.020507	-2.960115	-0.462676
6 0	3.453333	3.796834	0.542543
6 0	2.667514	5.689161	-0.770290
1 0	1.722530	5.242326	-2.682639
6 0	2.206005	-4.840983	-1.787024
6 0	-2.997076	2.596556	2.450299
6 0	-5.433223	1.178938	-0.542488
6 0	-4.151801	2.599612	1.559545
6 0	-4.672780	-2.300290	-0.827833
6 0	-0.647568	-1.172024	3.166365
6 0	-5.433221	-1.178943	-0.542488
6 0	-0.558775	-2.277665	2.340035
6 0	-4.016398	-3.029300	0.250955
6 0	3.267656	5.176800	0.370191
1 0	3.938260	3.410404	1.444676
1 0	2.547114	6.771993	-0.882024
6 0	3.453352	-3.796828	0.542539
6 0	2.667525	-5.689158	-0.770285
1 0	1.722524	-5.242326	-2.682627
6 0	-1.763648	-3.013895	1.982941
6 0	-0.647571	1.172024	3.166363
6 0	-3.091164	1.420350	3.307630
6 0	-5.577081	0.728671	0.836022
6 0	-1.945602	0.728651	3.661652
6 0	-4.151797	-2.599616	1.559545
6 0	-1.945601	-0.728653	3.661652

6 0	-5.577080	-0.728677	0.836022
6 0	-2.997072	-2.596559	2.450298
1 0	3.611379	5.860007	1.154361
6 0	3.267683	-5.176796	0.370186
1 0	3.938301	-3.410398	1.444660
1 0	2.547135	-6.771990	-0.882021
6 0	-4.953156	1.420651	1.859873
6 0	-4.953155	-1.420655	1.859872
6 0	-4.297556	0.692393	2.939185
6 0	-3.091163	-1.420353	3.307630
1 0	3.611406	-5.860000	1.154359
6 0	-4.297555	-0.692398	2.939184
1 0	1.870952	2.385502	-3.524585
1 0	1.870954	-2.385503	-3.524584
6 0	8.585940	-0.706769	1.845876
6 0	7.516121	-1.414664	1.359637
6 0	6.396281	-0.706604	0.850405
6 0	6.396280	0.706609	0.850406
6 0	7.516126	1.414670	1.359624
6 0	8.585930	0.706775	1.845897
1 0	9.460255	-1.235215	2.241824
1 0	7.514193	-2.511121	1.355418
7 0	5.299480	-1.397749	0.346003
7 0	5.299481	1.397755	0.346000
1 0	7.514170	2.511127	1.355467
1 0	9.460278	1.235221	2.241772
6 0	4.260514	0.718608	-0.123362
6 0	4.260517	-0.718603	-0.123367

Linker -CH₂OCH₂- and C₆₀ A

AM1 optimized geometry; Nimag=0
E=0.028935874387

0 1

6 0	-2.738929	1.591748	-0.218283
1 0	-1.721702	2.005423	-0.165887

6 0	-3.844908	2.389839	-0.249291
1 0	-3.745459	3.485417	-0.225412
6 0	-5.167601	1.839970	-0.310967
1 0	-6.014553	2.541956	-0.333096
6 0	-5.380784	0.492891	-0.340029
1 0	-6.392182	0.065324	-0.385964
6 0	-4.259660	-0.381268	-0.309087
6 0	-2.909097	0.180068	-0.247186
6 0	-2.034391	-0.901085	-0.235265
6 0	-4.108262	-1.762293	-0.324708
1 0	-4.783255	-2.611795	-0.360739
8 0	-2.763284	-2.090362	-0.278431
6 0	-0.565986	-1.030520	-0.205816
1 0	-0.231203	-1.871855	-0.872119
6 0	2.078505	-0.433284	0.935145
6 0	3.196008	-0.300144	0.115542
6 0	3.642688	1.087255	0.246348
6 0	2.764674	1.697201	1.134180
1 0	2.658503	2.693704	1.552397
8 0	1.814534	0.784367	1.560357
6 0	3.907614	-1.185531	-0.739982
1 0	3.568565	-2.226980	-0.833740
6 0	4.993494	-0.716051	-1.419603
1 0	5.564189	-1.377704	-2.088657
6 0	4.780711	1.529115	-0.482534
1 0	5.111455	2.572180	-0.378829
6 0	5.431033	0.643067	-1.290787
1 0	6.314937	0.954570	-1.867365
8 0	-0.177291	-1.303942	1.145152
6 0	1.207895	-1.574813	1.283979
1 0	1.312219	-1.826771	2.377645
1 0	1.502208	-2.455924	0.650262
1 0	-0.093428	-0.065026	-0.535070

PM3 optimized geometry; Nimag=0
E = 0.008126545202

SPE (B3LYP/3-21G*//PM3) =
-914.865177942 hartrees

SPE (B3LYP/6-31G*//PM3) =
-919.937936054 hartrees

0 1

6 0	-2.361681	1.611709	-0.141689
1 0	-1.300076	1.878591	-0.147751
6 0	-3.347183	2.541098	-0.031693
1 0	-3.099026	3.604190	0.054185
6 0	-4.734894	2.174726	-0.022449
1 0	-5.474273	2.977155	0.069766
6 0	-5.134110	0.879542	-0.123191
1 0	-6.189161	0.590809	-0.116574
6 0	-4.134288	-0.129512	-0.240113
6 0	-2.734064	0.240026	-0.248780
6 0	-2.021224	-0.943556	-0.375397
6 0	-4.171491	-1.509135	-0.358493
1 0	-4.968648	-2.244999	-0.394939
8 0	-2.901474	-2.004976	-0.439230
6 0	-0.564976	-1.224994	-0.452297
1 0	-0.336690	-1.959150	-1.250648
6 0	2.084565	-0.813473	0.917504
6 0	2.999227	-0.323196	-0.004641
6 0	3.555527	0.880488	0.576258
6 0	2.939870	1.035338	1.808133
1 0	3.013153	1.769979	2.604274
8 0	2.055217	0.017944	2.017969
6 0	3.439808	-0.759979	-1.287831
1 0	3.015525	-1.673585	-1.716187
6 0	4.379181	-0.020333	-1.934227
1 0	4.741761	-0.325693	-2.921492
6 0	4.538427	1.625403	-0.137769
1 0	4.952377	2.533943	0.309408
6 0	4.928693	1.174127	-1.359060
1 0	5.681710	1.719901	-1.937280
8 0	-0.163760	-1.739711	0.815724
6 0	1.214213	-2.022441	0.914086
1 0	1.259051	-2.563301	1.876068
1 0	1.548418	-2.700508	0.103906

1 0 -0.017588 -0.288413 -0.678546

Linker -CH₂OCH₂- and C₆₀ B

X = CH₂OCH₂

AM1 optimized geometry; Nimag=0

E=1.533518837393

0 1

6 0 -0.401899 -1.070001 -2.172154
 6 0 0.746832 -1.727289 -2.790509
 6 0 -0.530407 0.293501 -2.202940
 6 0 -0.738257 -1.814527 -0.944188
 6 0 1.728537 -0.975501 -3.416676
 6 0 0.515552 1.081013 -2.833732
 6 0 -1.179015 -1.142605 0.166019
 6 0 0.208924 -2.919624 -0.823594
 6 0 -1.235022 1.124483 -1.140182
 6 0 -8.142574 -2.954167 0.630171
 6 0 1.126302 -2.870345 -1.961383
 6 0 1.608107 0.476228 -3.437710
 6 0 0.699354 2.294232 -2.047018
 6 0 -6.245788 -2.069091 -0.189431
 6 0 -0.234770 2.250254 -0.934409
 6 0 0.678541 -3.306120 0.421724
 6 0 -1.610945 0.317378 0.192739
 6 0 -0.659756 -1.529954 1.467476
 6 0 3.141597 -1.313590 -3.236820
 6 0 -2.646173 1.606320 -1.620686
 8 0 -6.800755 -3.205448 0.399495
 6 0 -8.465076 -1.671939 0.201419
 6 0 2.461620 -3.195908 -1.793744
 6 0 3.895905 -0.061646 -3.150225
 6 0 -0.478904 -0.317941 2.256348

6 0 -3.175396 0.500780 0.231414
 6 0 0.228866 -2.585782 1.605302
 6 0 2.090863 -3.645829 0.603363
 6 0 2.958712 -3.590349 -0.474015
 6 0 3.498042 -2.392533 -2.445770
 6 0 -0.889769 0.812118 1.438688
 6 0 0.173149 2.718513 0.287194
 6 0 1.966167 2.840724 -1.903359
 8 0 -3.479834 0.480315 -1.205786
 6 0 -7.230550 -1.095985 -0.331931
 6 0 -3.104318 2.677525 -0.650629
 6 0 -9.659240 -0.900138 0.187660
 6 0 2.947579 1.046129 -3.278262
 6 0 -0.164200 1.972915 1.514801
 6 0 1.358372 -2.482107 2.531289
 6 0 4.297195 -3.023261 -0.307148
 6 0 4.630563 -2.283080 -1.525678
 6 0 2.511840 -3.134629 1.909423
 6 0 0.586074 -0.222132 3.140160
 6 0 3.122051 2.197454 -2.531383
 6 0 4.966588 0.042899 -2.277608
 6 0 1.506423 3.287214 0.464078
 6 0 2.384329 3.355523 -0.606189
 6 0 -4.033754 -0.477700 1.005974
 6 0 -3.434686 1.970760 0.548335
 6 0 -7.241136 0.225738 -0.857415
 6 0 -9.621800 0.363169 -0.326288
 1 0 -10.584385 -1.336988 0.589276
 6 0 -3.253697 4.042987 -0.733252
 6 0 3.778159 -2.595965 2.066988
 6 0 5.344153 -1.098853 -1.443360
 6 0 4.695516 -2.539257 0.927969
 6 0 4.255041 2.310297 -1.611417
 6 0 1.334250 1.024410 3.232282
 6 0 5.151076 1.261304 -1.487086
 6 0 0.968105 2.093009 2.429530
 6 0 3.799027 3.028315 -0.419624
 6 0 -8.411577 0.926550 -0.849769
 1 0 -6.305087 0.646247 -1.255929
 1 0 -10.529664 0.984390 -0.351787
 6 0 -3.909031 2.638377 1.654747
 6 0 -3.740405 4.720796 0.400779
 1 0 -3.004864 4.597866 -1.648678
 6 0 2.000603 2.903836 1.785586
 6 0 1.532394 -1.331054 3.278568
 6 0 3.962518 -1.377547 2.857585

6 0	5.762965	-0.586462	-0.137621
6 0	2.870731	-0.762972	3.448480
6 0	4.262786	2.658360	0.831413
6 0	2.748446	0.695812	3.420926
6 0	5.642521	0.872215	-0.164489
6 0	3.339035	2.599029	1.966282
1 0	-8.453309	1.950748	-1.250021
6 0	-4.059243	4.035385	1.566342
1 0	-4.168475	2.107176	2.581503
1 0	-3.869697	5.812868	0.354656
6 0	5.447663	-1.286418	1.014719
6 0	5.211258	1.551930	0.962635
6 0	4.993776	-0.568143	2.206872
6 0	3.723504	1.460643	2.803423
1 0	-4.439863	4.586687	2.439687
6 0	4.877974	0.811830	2.181203
1 0	-8.687907	-3.773812	1.088454
1 0	-2.764361	1.775450	-2.706645
1 0	-3.655511	-0.527677	2.064711
8 0	-3.953535	-1.811574	0.544002
6 0	-4.814198	-2.133844	-0.545636
1 0	-4.620514	-1.444625	-1.412195
1 0	-4.514611	-3.188918	-0.800482
1 0	-5.096737	-0.109755	0.986303

PM3 optimized geometry; Nimag=0
 E = 1.256768512295
 SPE (B3LYP/3-21G*//PM3) =
 -3188.43123304 hartrees

SPE (B3LYP/6-31G*//PM3) =
 -3206.12792621 hartrees

0 1			
6 0	-0.186608	-0.827792	-2.413110
6 0	0.995261	-1.444707	-2.991313
6 0	-0.295870	0.534794	-2.332391
6 0	-0.629727	-1.673651	-1.292763
6 0	2.033544	-0.659335	-3.465857
6 0	0.802828	1.351873	-2.796457
6 0	-1.153334	-1.103724	-0.162605
6 0	0.287489	-2.796831	-1.201422
6 0	-1.081185	1.274639	-1.258420
6 0	-8.155254	-3.074850	0.539804
6 0	1.290596	-2.661203	-2.248010
6 0	1.933899	0.782821	-3.362164
6 0	0.935835	2.479074	-1.890942
6 0	-6.478654	-1.996459	-0.445905
6 0	-0.081690	2.353447	-0.871869
6 0	0.648328	-3.308057	0.034780
6 0	-1.574946	0.354659	-0.038890
6 0	-0.748399	-1.616398	1.127437
6 0	3.416906	-1.039383	-3.206272
6 0	-2.449715	1.819555	-1.801213
8 0	-6.891060	-3.217943	0.045673
6 0	-8.579532	-1.765362	0.380999
6 0	2.602525	-3.027948	-2.006246
6 0	4.173953	0.178341	-2.944259
6 0	-0.619037	-0.490713	2.035290
6 0	-3.141336	0.571560	-0.115361
6 0	0.115118	-2.695846	1.235158
6 0	2.031358	-3.688943	0.294469
6 0	2.983946	-3.550856	-0.699688
6 0	3.693905	-2.192741	-2.493624
6 0	-0.947621	0.711754	1.301997
6 0	0.229385	2.692752	0.418312
6 0	2.193175	2.982859	-1.593693
8 0	-3.324060	0.687160	-1.563473
6 0	-7.488510	-1.062237	-0.260314
6 0	-2.977192	2.809226	-0.780365
6 0	-9.779792	-1.068791	0.705589
6 0	3.257179	1.306716	-3.043799
6 0	-0.215183	1.845693	1.537979
6 0	1.162473	-2.699889	2.249770
6 0	4.305387	-3.030642	-0.375665
6 0	4.744107	-2.191483	-1.484173
6 0	2.349527	-3.311360	1.666041

6 0	0.373277	-0.496823	3.004190
6 0	3.383803	2.379922	-2.181485
6 0	5.170309	0.180600	-1.982883
6 0	1.544122	3.212185	0.752837
6 0	2.507492	3.364505	-0.231355
6 0	-4.062593	-0.454336	0.546096
6 0	-3.409455	2.014773	0.308336
6 0	-7.619689	0.323910	-0.566439
6 0	-9.862449	0.252367	0.397284
1 0	-10.598883	-1.608480	1.189909
6 0	-3.100117	4.179505	-0.760808
6 0	3.604607	-2.814516	1.973734
6 0	5.462950	-1.035040	-1.234696
6 0	4.607673	-2.671192	0.926567
6 0	4.433899	2.384885	-1.171139
6 0	1.122235	0.715150	3.269283
6 0	5.303591	1.312017	-1.073610
6 0	0.835932	1.858453	2.541010
6 0	3.892186	2.995468	0.036505
6 0	-8.781573	0.949019	-0.240143
1 0	-6.788260	0.843510	-1.054728
1 0	-10.769027	0.820510	0.630846
6 0	-3.964972	2.587793	1.429983
6 0	-3.667462	4.761743	0.382068
1 0	-2.768615	4.794821	-1.602719
6 0	1.922267	2.701262	2.062376
6 0	1.288546	-1.627082	3.112545
6 0	3.737774	-1.683089	2.883062
6 0	5.778410	-0.655406	0.136669
6 0	2.609256	-1.105160	3.439413
6 0	4.246977	2.502686	1.279977
6 0	2.506787	0.345477	3.537562
6 0	5.678456	0.795262	0.236235
6 0	3.236834	2.356684	2.321393
1 0	-8.919094	2.012669	-0.461681
6 0	-4.088348	3.984575	1.451926
1 0	-4.302198	1.976758	2.273569
1 0	-3.779154	5.850574	0.426095
6 0	5.361920	-1.451965	1.188900
6 0	5.164412	1.375973	1.382926
6 0	4.823125	-0.840843	2.397507
6 0	3.537143	1.144579	3.074176
1 0	-4.528215	4.466289	2.331979
6 0	4.725779	0.536848	2.491497
1 0	-8.603855	-3.970655	0.958267
1 0	-2.474375	2.102606	-2.866978

1 0	-3.669227	-0.697403	1.549791
8 0	-4.098110	-1.713678	-0.086627
6 0	-5.120687	-1.896822	-1.049396
1 0	-5.123055	-1.093891	-1.811104
1 0	-4.804538	-2.842685	-1.523619
1 0	-5.079014	-0.022526	0.658137

Linker -CH₂OCH₂- and C₆₀ C

X = CH₂OCH₂

AM1 optimized geometry; Nimag=0

E=1.531903312108

0 1

6 0	-1.086899	-0.678040	-2.220130
6 0	0.037859	-1.394185	-2.811068
6 0	-1.086919	0.678069	-2.220124
6 0	-1.775510	-1.541354	-1.196688
6 0	1.098548	-0.727141	-3.400492
6 0	0.037838	1.394231	-2.811043
6 0	-2.343312	-0.812081	0.123353
6 0	-0.683684	-2.581148	-0.927498
6 0	-1.775575	1.541356	-1.196702
6 0	-3.058696	-2.240616	-1.789235
6 0	0.289529	-2.577229	-2.003998
6 0	1.098538	0.727210	-3.400477
6 0	0.289488	2.577264	-2.003954
6 0	-3.752348	-1.544466	0.188407
6 0	-0.683747	2.581156	-0.927464
6 0	-0.282744	-3.009735	0.308916

6 0	-2.343281	0.812057	0.123391	1 0	-3.989752	-3.625097	2.361355
6 0	-1.535426	-1.166963	1.350429	1 0	-3.122477	-6.848600	-0.399992
6 0	2.473200	-1.184100	-3.189141	6 0	-3.718713	3.958698	1.349726
6 0	-3.058902	2.240491	-1.789121	6 0	-3.230958	5.771033	-0.204682
8 0	-4.137602	-1.446425	-1.221707	1 0	-2.775841	5.222342	-2.266603
6 0	-3.182347	-3.521322	-0.987522	6 0	1.491655	3.024555	1.875808
6 0	1.588942	-3.025045	-1.810764	6 0	0.618391	-1.177903	3.252203
6 0	3.323217	0.000042	-3.051338	6 0	3.049809	-1.424445	2.925619
6 0	-1.246291	-0.000054	2.146812	6 0	5.023974	-0.731851	0.016153
6 0	-3.752164	1.544535	0.188687	6 0	1.992589	-0.732118	3.492173
6 0	-0.725471	-2.266231	1.498759	6 0	3.759616	2.608579	0.999074
6 0	1.081484	-3.470582	0.545263	6 0	1.992579	0.732049	3.492185
6 0	2.001149	-3.485035	-0.491289	6 0	5.023966	0.731894	0.016165
6 0	2.712412	-2.303460	-2.411676	6 0	2.792511	2.606117	2.098955
6 0	-1.535370	1.166874	1.350456	1 0	-3.701107	-6.057817	1.883712
6 0	-0.282780	3.009699	0.308962	6 0	-3.557117	5.329123	1.071612
6 0	1.588899	3.025077	-1.810706	1 0	-3.989305	3.625368	2.361477
8 0	-4.137753	1.446366	-1.221315	1 0	-3.122689	6.848630	-0.400348
6 0	-3.532860	-3.064405	0.318125	6 0	4.607401	-1.424299	1.141045
6 0	-3.182493	3.521288	-0.987532	6 0	4.607384	1.424313	1.141072
6 0	-3.035818	-4.861898	-1.261587	6 0	4.168439	-0.692787	2.330835
6 0	2.473184	1.184175	-3.189117	6 0	3.049790	1.424406	2.925648
6 0	-0.725474	2.266172	1.498802	1 0	-3.700983	6.058065	1.883493
6 0	0.372872	-2.285060	2.459296	6 0	4.168431	0.692771	2.330848
6 0	3.375843	-3.038271	-0.260194	1 0	-3.149784	-2.263385	-2.889418
6 0	3.815616	-2.305972	-1.449826	1 0	-3.150184	2.263121	-2.889289
6 0	1.491688	-3.024590	1.875753	6 0	-4.870257	1.173837	1.135646
6 0	-0.221770	-0.000048	3.089825	1 0	-5.665382	1.973153	1.078329
6 0	2.712380	2.303521	-2.411629	1 0	-4.455174	1.118809	2.178736
6 0	4.365189	0.000038	-2.137933	6 0	-4.871040	-1.174047	1.134709
6 0	1.081440	3.470562	0.545325	1 0	-4.457272	-1.120981	2.178456
6 0	2.001105	3.485048	-0.491222	1 0	-5.666447	-1.973072	1.076228
6 0	-3.532714	3.064479	0.318230	8 0	-5.568813	0.000228	0.795387
6 0	-3.718976	-3.958520	1.349682				
6 0	-3.230800	-5.770990	-0.204434				
1 0	-2.775438	-5.222499	-2.266351				
6 0	-3.036091	4.861847	-1.261769				
6 0	2.792540	-2.606142	2.098903				
6 0	4.617288	-1.184229	-1.315196				
6 0	3.759645	-2.608571	0.999023				
6 0	3.815585	2.306027	-1.449782				
6 0	0.618374	1.177820	3.252221				
6 0	4.617274	1.184293	-1.315173				
6 0	0.372857	2.284999	2.459348				
6 0	3.375805	3.038300	-0.260133				
6 0	-3.557243	-5.328970	1.071744

PM3 optimized geometry; Nimag=0

E = 1.248020719621

SPE (B3LYP/3-21G**/PM3) =

-3188.43736067 hartrees

SPE (B3LYP/6-31G**/PM3) =

-3206.11143835 hartrees

0 1

6 0	1.078712	0.678448	-2.215821
6 0	-0.043715	1.389268	-2.800642
6 0	1.078700	-0.678442	-2.215821
6 0	1.773032	1.544318	-1.195414
6 0	-1.104834	0.723206	-3.389136
6 0	-0.043728	-1.389250	-2.800652
6 0	2.347807	0.819762	0.129766
6 0	0.671431	2.573083	-0.928727
6 0	1.773010	-1.544333	-1.195425
6 0	3.059436	2.248674	-1.784733
6 0	-0.296378	2.568139	-1.998490
6 0	-1.104839	-0.723177	-3.389145
6 0	-0.296399	-2.568130	-1.998512
6 0	3.758725	1.566906	0.183046
6 0	0.671406	-2.573087	-0.928744
6 0	0.273667	2.997174	0.309464
6 0	2.347850	-0.819773	0.129752
6 0	1.534690	1.162923	1.358169
6 0	-2.473901	1.178571	-3.178399
6 0	3.059359	-2.248737	-1.784787
8 0	4.138110	1.467870	-1.225681
6 0	3.189876	3.531305	-0.988217
6 0	-1.594997	3.015793	-1.803855
6 0	-3.320241	0.000019	-3.040910
6 0	1.244968	-0.000024	2.148668
6 0	3.758779	-1.566861	0.182924
6 0	0.716735	2.256480	1.496697
6 0	-1.083445	3.455707	0.545030

6 0	-2.003475	3.473276	-0.490688
6 0	-2.713753	2.297372	-2.401826
6 0	1.534721	-1.162962	1.358158
6 0	0.273653	-2.997192	0.309445
6 0	-1.595018	-3.015785	-1.803884
8 0	4.138049	-1.467905	-1.225855
6 0	3.551294	3.089171	0.304413
6 0	3.189830	-3.531323	-0.988200
6 0	3.035212	4.866961	-1.279897
6 0	-2.473906	-1.178534	-3.178404
6 0	0.716739	-2.256504	1.496677
6 0	-0.377224	2.276142	2.450893
6 0	-3.372344	3.028857	-0.259434
6 0	-3.811368	2.300167	-1.443651
6 0	-1.491187	3.012453	1.869880
6 0	0.214511	-0.000019	3.085716
6 0	-2.713767	-2.297342	-2.401841
6 0	-4.361638	0.000017	-2.127674
6 0	-1.083464	-3.455713	0.545001
6 0	-2.003494	-3.473265	-0.490716
6 0	3.551333	-3.089132	0.304386
6 0	3.735184	3.989908	1.330704
6 0	3.232315	5.781391	-0.235148
1 0	2.766364	5.205296	-2.285035
6 0	3.035127	-4.866990	-1.279810
6 0	-2.791353	2.596175	2.093916
6 0	-4.612513	1.178986	-1.308403
6 0	-3.755036	2.599436	0.999380
6 0	-3.811385	-2.300144	-1.443669
6 0	-0.622067	-1.171610	3.246336
6 0	-4.612523	-1.178959	-1.308414
6 0	-0.377229	-2.276166	2.450868
6 0	-3.372364	-3.028844	-0.259458
6 0	3.566222	5.351503	1.041286
1 0	4.010162	3.659568	2.337741
1 0	3.118882	6.852433	-0.434584
6 0	3.735246	-3.989823	1.330710
6 0	3.232261	-5.781375	-0.235027
1 0	2.766230	-5.205365	-2.284921
6 0	-1.491200	-3.012462	1.869853
6 0	-0.622058	1.171576	3.246348
6 0	-3.047609	1.420300	2.918078
6 0	-5.016411	0.728702	0.017452
6 0	-1.990909	0.728601	3.484817
6 0	-3.755051	-2.599431	0.999361
6 0	-1.990913	-0.728629	3.484810

6 0	-5.016417	-0.728683	0.017447
6 0	-2.791365	-2.596184	2.093893
1 0	3.707780	6.086628	1.840922
6 0	3.566234	-5.351429	1.041369
1 0	4.010268	-3.659452	2.337725
1 0	3.118797	-6.852425	-0.434406
6 0	-4.599160	1.420650	1.141500
6 0	-4.599171	-1.420643	1.141489
6 0	-4.161531	0.692407	2.326152
6 0	-3.047618	-1.420316	2.918064
1 0	3.707808	-6.086517	1.841037
6 0	-4.161537	-0.692412	2.326148
1 0	3.141975	2.285529	-2.883078
1 0	3.141819	-2.285676	-2.883136
6 0	4.855677	-1.174622	1.163860
1 0	5.671965	-1.921317	1.139446
1 0	4.429420	-1.154297	2.188045
6 0	4.855228	1.174480	1.164332
1 0	4.428430	1.153420	2.188281
1 0	5.671297	1.921474	1.140927
8 0	5.554611	0.000123	0.863406

C₆₀; Nimag=0
 AM1 optimized geometry; Nimag=0
 E=1.549593041776

0 1			
6 0	-3.477546	-0.746062	-0.051030
6 0	-3.003427	-1.438609	-1.250363
6 0	-3.499324	0.637978	-0.013617
6 0	-3.024197	-1.502833	1.117173
6 0	-2.576399	-0.709339	-2.347347
6 0	-3.048238	1.408880	-1.173396
6 0	-2.617205	-0.834681	2.259576
6 0	-2.269757	-2.662977	0.639710
6 0	-3.069010	1.344415	1.194152
6 0	-2.256758	-2.622907	-0.823331
6 0	-2.599456	0.753722	-2.307825
6 0	-2.338917	2.591388	-0.682397
6 0	-2.351808	2.551787	0.780694
6 0	-1.148906	-3.091630	1.330511
6 0	-2.640222	0.628646	2.299125

6 0	-1.432140	-1.288133	2.990302
6 0	-1.378677	-1.123298	-3.080181
6 0	-1.123592	-3.014384	-1.516513
6 0	-0.661480	0.084023	-3.493433
6 0	-0.723256	-0.105499	3.480787
6 0	-0.718624	-2.385392	2.538187
6 0	0.048879	-3.505789	0.597759
6 0	0.060972	-3.468231	-0.786422
6 0	-0.672533	-2.243897	-2.676311
6 0	-1.469411	1.079030	3.054339
6 0	-1.244450	2.977583	1.494624
6 0	-1.219215	3.055199	-1.352468
6 0	-1.415938	1.244080	-3.016128
6 0	-0.791139	2.221020	2.662758
6 0	0.745175	-2.362806	2.551941
6 0	1.244334	-2.977646	-1.494645
6 0	0.791009	-2.221065	-2.662742
6 0	1.219559	-3.055215	1.352515
6 0	0.661637	-0.084035	3.493352
6 0	-0.745052	2.362873	-2.551692
6 0	0.723016	0.105484	-3.480575
6 0	-0.060922	3.468145	0.786330
6 0	-0.048844	3.505820	-0.597854
6 0	2.338944	-2.591316	0.682293
6 0	1.469434	-1.079020	-3.053697
6 0	2.351662	-2.551426	-0.780821
6 0	0.718497	2.385449	-2.538191
6 0	1.378693	1.123139	3.080258
6 0	1.432178	1.288108	-2.989713
6 0	0.672652	2.243759	2.676477
6 0	1.148785	3.091709	-1.330559
6 0	1.123982	3.014515	1.516622
6 0	1.415976	-1.244000	3.016309
6 0	3.048203	-1.408628	1.173147
6 0	2.640041	-0.628472	-2.299178
6 0	2.599520	-0.753741	2.307666
6 0	2.269574	2.662590	-0.639857
6 0	2.576498	0.709368	2.347228
6 0	2.617018	0.834497	-2.259629
6 0	2.256835	2.622940	0.823265
6 0	3.068997	-1.344311	-1.194202
6 0	3.024158	1.502723	-1.117222
6 0	3.499300	-0.637961	0.013346
6 0	3.003399	1.438374	1.250126
6 0	3.477514	0.746058	0.050764

C₆₀
 PM3 optimized geometry; Nimag=0
 E = 1.292121233889
 SPE (B3LYP/3-21G*//PM3) =
 -2273.52687753 hartrees
 SPE (B3LYP/6-31G*//PM3) =
 S -2286.17993906 hartrees
 0 1
 6 0 -2.075771 1.374041 2.525549
 6 0 -1.012583 0.761386 3.312174
 6 0 -2.976067 0.577497 1.839768
 6 0 -1.536547 2.572900 1.895870
 6 0 -0.903406 -0.616910 3.373256
 6 0 -2.861092 -0.874101 1.904109
 6 0 -1.924833 2.914655 0.612244
 6 0 -0.140087 2.701170 2.293383
 6 0 -3.385016 0.937451 0.487839
 6 0 0.183706 1.581593 3.168690
 6 0 -1.851583 -1.455819 2.651000
 6 0 -3.198996 -1.411290 0.591981
 6 0 -3.522805 -0.291725 -0.283336
 6 0 0.797512 3.164750 1.387110
 6 0 -2.873022 2.075734 -0.110020
 6 0 -0.937371 3.402902 -0.342272
 6 0 0.407916 -1.248293 3.294074
 6 0 1.428823 0.982091 3.093493
 6 0 0.270179 -2.477433 2.522880
 6 0 -1.275316 2.865758 -1.654384
 6 0 0.388539 3.524700 0.035193
 6 0 2.108823 2.533352 1.307912
 6 0 2.416285 1.470295 2.139021
 6 0 1.543816 -0.469506 3.157820
 6 0 -2.471556 2.045518 -1.510906
 6 0 -3.141626 -0.320446 -1.613451
 6 0 -2.510302 -2.503093 0.092939
 6 0 -1.126274 -2.605686 2.125436
 6 0 -2.602412 0.878422 -2.243104
 6 0 1.447087 3.115763 -0.879523
 6 0 3.141601 0.320430 1.613442
 6 0 2.602376 -0.878439 2.243101
 6 0 2.510292 2.503074 -0.092931
 6 0 -0.270167 2.477450 -2.522918
 6 0 -1.447105 -3.115757 0.879546
 6 0 1.275285 -2.865706 1.654362
 6 0 -2.416297 -1.470297 -2.139013

6 0 -2.108830 -2.533348 -1.307898
 6 0 3.198963 1.411281 -0.591948
 6 0 2.471598 -2.045497 1.510844
 6 0 3.522804 0.291674 0.283335
 6 0 -0.388530 -3.524674 -0.035162
 6 0 -0.407953 1.248324 -3.294070
 6 0 0.937401 -3.402892 0.342201
 6 0 -1.543841 0.469509 -3.157804
 6 0 -0.797500 -3.164728 -1.387090
 6 0 -1.428817 -0.982094 -3.093473
 6 0 1.126241 2.605718 -2.125426
 6 0 2.861059 0.874083 -1.904112
 6 0 2.873066 -2.075775 0.109992
 6 0 1.851560 1.455826 -2.650967
 6 0 0.140123 -2.701183 -2.293354
 6 0 0.903377 0.616910 -3.373229
 6 0 1.924891 -2.914687 -0.612263
 6 0 -0.183726 -1.581587 -3.168646
 6 0 3.385062 -0.937450 -0.487870
 6 0 1.536573 -2.572914 -1.895915
 6 0 2.976093 -0.577503 -1.839772
 6 0 1.012595 -0.761366 -3.312147
 6 0 2.075783 -1.374061 -2.525563

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