Supplementary Information

Intense Excimer CPL of Pyrenes Linked to a Quaternaphthyl

Kazuto Takaishi,* Ryosuke Takehana, and Tadashi Ema*
Division of Applied Chemistry, Graduate School of Natural Science and Technology, Okayama University, Tsushima, Okayama 700-8530, Japan

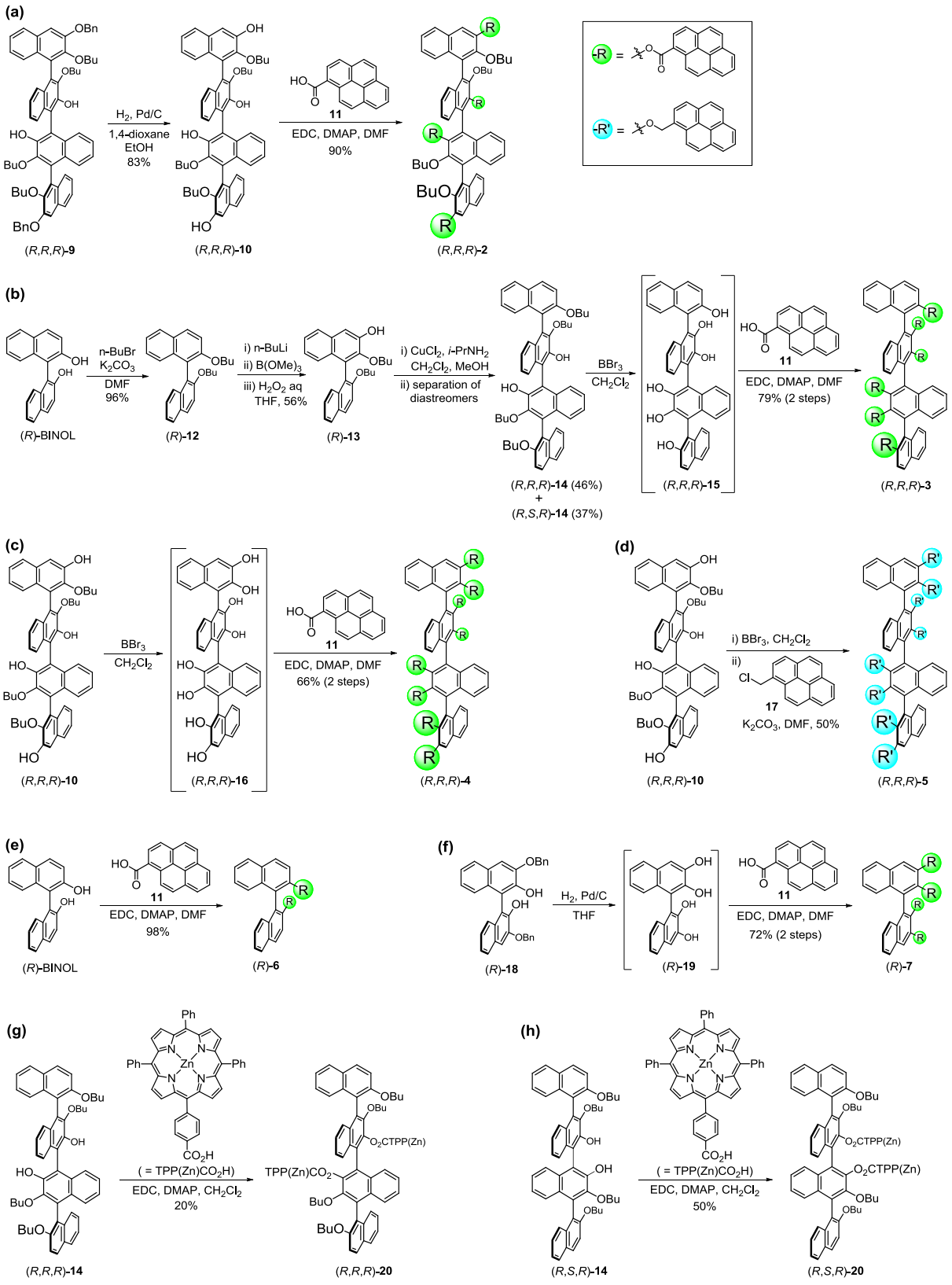
Table of contents

1. General information

Optical rotations were measured on a Horiba SEPA-300. IR spectra were recorded on a Shimadzu IRAffinity-1. ^{1}H and ^{13}C NMR spectra were recorded on a JEOL JNM-ECS400. Data are reported as follows: chemical shifts in ppm using the residual solvent peak as an internal standard, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, sext = sextet, dt = doublet of triplets, td = triplet of doublets, quint = quintet, m = multiplet), coupling constants (Hz). High-resolution mass spectra were performed on an Agilent G6520+G4240 or a Bruker Ultraflextreme. UV-Vis spectra were recorded on a Shimadzu UV-2600. CD spectra were recorded on a JASCO J-720. Fluorescence spectra were recorded on a JASCO FP-750 or a JASCO FP-8500. Absolute fluorescence quantum yields were determined by a JASCO FP-8500 or an Otsuka Electronics QE-2000 with an integrating sphere. CPL spectra were measured on a JASCO CPL-200 or a JASCO CPL-300. TLC analyses were carried out on glass sheets coated with Merck Silica gel 60 F_{254} (0.25 mm), and visualization was accomplished with UV light. Column chromatography was performed on silica gel (Fuji Silysia BW-127 ZH, 100-270 mesh). PTLC was performed on glass sheets coated with Merck Silica gel 60 F_{254} (1 mm). GPC was performed with Bio-Beads™ S-X1 Support (BIO-RAD, 200-400 mesh).

(complete ref. 13) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, revision E.01, Gaussian, Inc., Wallingford, CT, 2013.

2. Synthetic methods and characterization.



Scheme S1. Synthesis of pyrene-tethered binaphthyls and quaternaphthyls.

The synthetic methods for known compound (*R*)-**6**[S1] were improved as shown below. Compounds (*R*,*R*,*R*)-**9**[S2] and (*R*)-**18**[S3] was synthesized according to the literature. (*S*,*S*,*S*)-**4** was synthesized in a similar manner to that for (*R*,*R*,*R*)-**4** with the exception that (*S*,*S*,*S*)-**10** was used as a starting material.

Synthesis of (*R*,*R*,*R*)-10

A mixture of (*R*,*R*,*R*)-**9** (931 mg, 896 μmol) and 10% Pd-C (46.1 mg) in a mixed solvent of 1,4-dioxane (3.5 mL) and EtOH (1.0 mL) was stirred at 60 °C for 16.5 h under H_2 atmosphere. After Pd-C was filtered off, the filtrate was evaporated to give a residue. The residue was purified by column chromatography (SiO_2, hexane/$CHCl_3$/EtOAc (10:9:1)) to afford (*R*,*R*,*R*)-**10** (636 mg, 740 μmol, 83%) as a reddish brown powder.

[α]$_D^{21}$ = +5 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3503, 3063, 2958, 2932, 2872, 1624, 1508, 1463, 1423, 1379, 1240, 1170, 1111, 968, 871, 842, 758 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 0.59 (t, *J* = 7.3 Hz, 6H), 0.72 (t, *J* = 7.6 Hz, 6H), 0.85–1.25 (m, 8H), 1.35 (quint, *J* = 7.0 Hz, 4H), 1.48 (quint, *J* = 7.1 Hz, 4H), 3.48 (dt, *J* = 6.7, 9.2 Hz, 2H), 3.56 (dt, *J* = 6.6, 9.6 Hz, 2H), 3.69 (dt, *J* = 6.4, 9.6 Hz, 4H), 6.20 (s, 2H), 6.34 (s, 2H), 7.15–7.25 (m, 6H), 7.31 (dd, *J* = 1.1, 8.5 Hz, 4H), 7.35–7.45 (m, 4H), 7.52 (s, 2H), 7.81 (d, *J* = 8.2 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 13.8, 13.9, 19.0, 19.3, 32.3, 32.5, 74.1, 74.2, 110.7, 115.7, 124.0, 124.1, 124.5, 124.6, 125.1, 125.8, 125.9, 126.4, 126.6, 127.1, 129.3, 129.4, 130.8, 131.8, 146.0, 146.1, 146.8, 148.5; **HR MS** (ESI^+) Calcd for $C_{56}H_{58}NaO_8$: 881.4024 $[M+Na]^+$. Found: 881.4029.

Synthesis of (*R*,*R*,*R*)-2

A solution of (*R*,*R*,*R*)-**10** (21.5 mg, 25.0 μmol), 1-pyrenecarboxylic acid (**11**) (49.2 mg, 200 μmol), EDC·HCl (77 mg, 0.40 mmol), and DMAP (24.4 mg, 200 μmol) in dry DMF (4.0 mL) was stirred at room temperature for 13 h under N_2 atmosphere. Then a mixed solvent of water and $CHCl_3$ was added. The organic layer was washed successively with water (four times) and brine. After dried over Na_2SO_4, the solvent was evaporated to give a residue. The residue was purified by column chromatography (SiO_2, $CHCl_3$) to afford (*R*,*R*,*R*)-**2** (39.8 mg, 22.5 μmol, 90%) as a yellow powder.

[α]$_D^{22}$ = –197 ($CHCl_3$, *c* 0.11); **IR** (KBr) 3042, 2956, 2931, 2870, 1732, 1597, 1506, 1325, 1246, 1225, 1192, 1180, 1142, 1125, 1078, 1020, 970, 851, 820, 748, 708 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 0.31 (br s, 6H), 0.63 (t, *J* = 7.3 Hz, 6H), 0.80 (br s, 4H), 0.95–1.25 (m, 8H), 1.43 (br s, 4H), 3.61 (br s, 2H), 3.95 (br s, 4H), 4.15 (td, *J* = 6.6, 8.7 Hz, 2H), 6.28 (br s, 2H), 6.83 (br s, 2H), 7.10–7.22 (m, 2H), 7.35 (d, *J* = 6.4 Hz, 4H), 7.43 (d, *J* = 6.8 Hz, 2H), 7.79 (d, *J* = 8.7 Hz, 2H), 7.83 (d, *J* = 8.2 Hz, 2H), 7.98 (s, 2H), 8.02 (d, *J* = 7.3 Hz, 2H), 8.05 (dd, *J* = 2.7, 7.8 Hz, 2H), 8.09 (d, *J* = 7.8 Hz, 2H), 8.10 (d, *J* = 9.2 Hz, 2H), 8.12 (d, *J* = 7.8 Hz, 2H), 8.14–8.32 (m, 18H), 8.57 (br s, 2H), 8.80–9.10 (m, 2H), 9.06 (d, *J* = 8.2 Hz, 2H), 9.50 (d, *J* = 9.2 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 13.6, 14.0, 18.8, 19.2, 32.2, 32.6, 74.03, 74.05, 121.2, 122.5, 123.1, 124.4, 124.5, 124.6, 125.0, 125.26, 125.32, 126.0, 126.6, 126.7, 126.8, 126.87, 126.92, 126.94, 127.2, 127.4, 127.5, 127.9, 129.5, 129.8, 130.17, 130.22, 130.40, 130.45, 130.67, 130.72, 131.2, 131.3, 131.7, 132.4, 132.7, 132.9, 134.8, 135.3, 143.5, 144.4, 149.5, 150.0, 165.2, 166.5; **HR MS** (ESI^+) Calcd for

$C_{124}H_{90}NaO_{12}$: 1793.6324 $[M+Na]^+$. Found: 1793.6328.

Synthesis of (*R*)-12

To a mixture of (*R*)-BINOL (10.1 g, 35.3 mmol), n-BuBr (15.3 mL, 142 mmol), and K_2CO_3 (21.0 g, 152 mmol) in dry DMF (60 mL) was stirred at room temperature for 13.5 h under N_2 atmosphere. After K_2CO_3 was filtered off, a mixed solvent of 1 M HCl aq and $CHCl_3$ was added. The organic layer was separated and washed successively with water (six times) and brine. After dried over Na_2SO_4, the solvent was evaporated to give a residue. The residue was purified by column chromatography (SiO_2, $CHCl_3$) to afford (*R*)-**12** (13.5 g, 33.9 mmol, 96%) as an orange oil.

[α]$_D^{24}$ = +69 ($CHCl_3$, *c* 0.097); **IR** (KBr) 3057, 2957, 2932, 2872, 1622, 1508, 1458, 1429, 1377, 1242, 1217, 1146, 1086, 1018, 806, 746 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 0.63 (t, *J* = 7.3 Hz, 6H), 0.90–1.05 (m, 4H), 1.30–1.45 (m, 4H), 3.85–4.00 (m, 4H), 7.15 (dd, *J* = 0.9, 6.6 Hz, 2H), 7.20 (ddd, *J* = 1.4, 6.4, 8.2 Hz, 2H), 7.30 (ddd, *J* = 1.4, 6.3, 8.0 Hz, 2H), 7.41 (d, *J* = 9.2 Hz, 2H), 7.85 (d, *J* = 7.8 Hz, 2H), 7.94 (d, *J* = 9.2 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 13.9, 19.0, 31.7, 69.7, 116.1, 121.0, 123.7, 125.8, 126.3, 128.1, 129.3, 129.5, 134.5, 154.8; **HR MS** (ESI^+) Calcd for $C_{28}H_{31}O_2$: 399.2319 $[M+H]^+$. Found: 399.2330.

Synthesis of (*R*)-13

To a solution of (*R*)-**12** (4.16 g, 10.4 mmol) in dry THF (40 mL), 1.6 M n-BuLi in hexane (15.6 mL, 25 mmol) was added dropwise at –78 °C under N_2 atmosphere. The solution was stirred at room temperature for 1 h. $B(OMe)_3$ (3.50 mL, 31.7 mmol) was added to the solution at –78 °C, and the reaction mixture was stirred at room temperature for 14 h. H_2O_2 (30 wt% solution in water, 11.6 mL) was added to the solution at 0 °C, and the solution was refluxed for 7 h. Then saturated aqueous Na_2SO_3 was added. The organic solvent was evaporated in vacuo, and $CHCl_3$ was added. The organic layer was separated and washed successively with water and brine. After dried over Na_2SO_4, the solvent was evaporated in vacuo to give a residue. The residue was purified by column chromatography (SiO_2, hexane/EtOAc (5:1)) to afford (*R*)-**13** (2.41 g, 5.81 mmol, 56%) as a yellow powder.

[α]$_D^{20}$ = +38 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3318, 3055, 2959, 2930, 2870, 1622, 1510, 1462, 1379, 1249, 1148, 1105, 966, 806, 771, 752 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 0.59 (t, *J* = 7.2 Hz, 3H), 0.66 (t, *J* = 7.4 Hz, 3H), 0.88–1.10 (m, 4H), 1.28 (quint, *J* = 7.2 Hz, 2H), 1.38–1.48 (m, 2H), 3.48 (t, *J* = 6.6 Hz, 2H), 3.97 (dt, *J* = 6.6, 9.2 Hz, 1H), 4.03 (dt, *J* = 6.6, 9.2 Hz, 1H), 6.17 (s, 1H), 7.01–7.11 (m, 2H), 7.19 (d, *J* = 8.8 Hz, 1H), 7.22–7.36 (m, 3H), 7.41 (s, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 13.8, 13.9, 19.0, 19.1, 31.7, 32.3, 69.4, 73.6, 109.6, 115.3, 119.5, 123.7, 124.0, 124.6, 125.3, 125.6, 128.9, 126.8, 127.0, 128.2, 129.2, 129.3, 130.2, 131.8, 134.3, 145.6, 148.3, 154.9; **HR MS** (ESI^-) Calcd for $C_{28}H_{29}O_3$: 413.2122 $[M–H]^-$. Found: 413.2129.

Synthesis of (*R*,*R*,*R*)-14

To a mixture of $CuCl_2$ (64.5 mg, 480 μmol) in dry MeOH (1.2 mL), *i*-$PrNH_2$ (51 μL, 0.59 mmol) was added under N_2 atmosphere with ice-bath cooling. After 1.5 h, a solution of (*R*)-**13** (104 mg, 251 μmol) in dry CH_2Cl_2 (1.2 mL) was added, and the reaction mixture was stirred at 0 °C for 6 h. Then a mixed solvent of 1 M HCl aq. and EtOAc was added. The organic layer was washed successively with water (twice) and brine (twice). After dried over Na_2SO_4, the solvent was evaporated in vacuo to give a residue. The residue was purified by column chromatography (SiO_2, hexane/EtOAc (7:1)) to afford (*R*,*R*,*R*)-**14** (48.2 mg, 58.3 μmol, 46%) as a colorless powder, (*R*,*S*,*R*)-**14** (38.8 mg, 46.9 μmol, 37%) as a colorless powder, and unreacted (*R*)-**13** (14.6 mg, 35.2 μmol, 14%).

(*R*,*R*,*R*)-**14**: $[\alpha]_D^{20}$ = +76 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3499, 3059, 2957, 2932, 2870, 1622, 1508, 1464, 1422, 1377, 1238, 1152, 1109, 966, 808, 750 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 0.60 (t, *J* = 7.3 Hz, 6H), 0.72 (t, *J* = 7.3 Hz, 6H), 0.85–1.20 (m, 8H), 1.33 (quint, *J* = 7.0 Hz, 4H), 1.45–1.62 (m, 4H), 3.61 (dt, *J* = 6.6, 9.2 Hz, 2H), 3.68 (dt, *J* = 6.6, 9.6 Hz, 2H), 4.05 (dt, *J* = 6.2, 9.2 Hz, 2H), 4.13 (dt, *J* = 6.2, 8.7 Hz, 2H), 6.33 (s, 2H), 7.08 (dt, *J* = 1.2, 7.4 Hz, 2H), 7.20 (dt, *J* = 1.1, 8.5 Hz, 2H), 7.23 (d, *J* = 8.2 Hz, 2H), 7.30–7.42 (m, 6H), 7.49 (d, *J* = 8.7 Hz, 2H), 7.50 (d, *J* = 8.2 Hz, 2H), 7.91 (d, *J* = 7.8 Hz, 2H), 8.03 (d, *J* = 9.2 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 13.8, 14.0, 19.0, 19.3, 31.9, 32.3, 69.6, 73.6, 115.1, 115.7, 120.1, 123.9, 124.1, 125.0, 125.2, 125.6, 126.20, 126.25, 127.0, 128.2, 129.46, 129.50, 130.2, 131.2, 134.5, 145.7, 146.6, 155.2; **HR MS** (ESI^+) Calcd for $C_{56}H_{58}NaO_6$: 849.4126 $[M+Na]^+$. Found: 849.4137.

(*R*,*S*,*R*)-**14**: $[\alpha]_D^{21}$ = +9 ($CHCl_3$, *c* 0.11); **IR** (KBr) 3508, 3061, 2957, 2932, 2872, 1622, 1506, 1464, 1422, 1377, 1242, 1150, 1111, 968, 808, 758 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 0.58 (t, *J* = 7.3 Hz, 6H), 0.71 (t, *J* = 7.3 Hz, 6H), 0.85–1.00 (m, 4H), 1.05–1.20 (m, 4H), 1.30 (quint, *J* = 7.0 Hz, 4H), 1.45–1.55 (m, 4H), 3.69 (td, *J* = 2.6, 6.5 Hz, 4H), 4.03 (dt, *J* = 6.4, 9.2 Hz, 2H), 4.11 (dt, *J* = 6.4, 9.6 Hz, 2H), 6.09 (s, 2H), 7.11 (td, *J* = 1.4, 7.6 Hz, 2H), 7.20–7.30 (m, 4H), 7.35–7.45 (m, 8H), 7.70 (d, *J* = 9.2 Hz, 2H), 7.86–7.94 (m, 2H), 8.02 (d, *J* = 9.1 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 13.8, 13.9, 19.0, 19.2, 31.7, 32.3, 69.6, 73.5, 114.8, 115.6, 120.0, 123.99, 124.02, 125.2, 125.5, 125.7, 125.9, 126.3, 127.0, 128.2, 129.46, 129.48, 130.1, 131.1, 134.5, 145.8, 147.0, 155.1; **HR MS** (ESI^+) Calcd for $C_{56}H_{58}NaO_6$: 849.4126 $[M+Na]^+$. Found: 849.4153.

Synthesis of (*R*,*R*,*R*)-3

To a mixture of (*R*,*R*,*R*)-**14** (16.5 mg, 19.9 μmol) in dry CH_2Cl_2 (0.4 mL), 1.0 M BBr_3 in CH_2Cl_2 (0.48 mL, 0.48 mmol) was added under N_2 atmosphere with ice-bath cooling. After 4.5 h, a mixed solvent of water and CH_2Cl_2 was added. The organic layer was washed successively with 1 M HCl aq, water (twice), brine (twice), and dried over Na_2SO_4. The solvent was evaporated to give a crude hexaol (*R*,*R*,*R*)-**15** (15 mg) as a green powder. A solution of the crude (*R*,*R*,*R*)-**15**, 1-pyrenecarboxylic acid (**11**) (62.3 mg, 253 μmol), EDC·HCl (79.1 mg, 413 μmol), and DMAP (32.5 mg, 266 μmol) in dry DMF (4.0 mL) was stirred at 60 °C for 1 h and then stirred at 40 °C for 18 h under N_2 atmosphere. Then a mixed solvent of water and $CHCl_3$ was added. The organic layer was washed successively with water (five times) and brine (twice).

After dried over Na_2SO_4, the solvent was evaporated to give a residue. The residue was purified by column chromatography (SiO_2, $CHCl_3$) to afford (*R*,*R*,*R*)-**3** (30.9 mg, 15.7 μmol, 79%) as a yellow powder.

[α]$_D^{21}$ = –204 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3040, 2924, 2851, 1732, 1595, 1506, 1325, 1246, 1225, 1192, 1163, 1142, 1123, 1076, 1020, 970, 849, 820, 708 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.80 (t, *J* = 7.6 Hz, 2H), 6.94 (t, *J* = 7.6 Hz, 2H), 7.17 (d, *J* = 9.6 Hz, 2H), 7.21 (d, *J* = 7.3 Hz, 2H), 7.32 (d, *J* = 9.6 Hz, 2H), 7.35–7.80 (m, 28H), 7.88 (d, *J* = 6.9 Hz, 2H), 7.95–8.35 (m, 26H), 8.39 (d, *J* = 8.2 Hz, 2H), 8.93 (br s, 2H), 9.05 (d, *J* = 7.8 Hz, 2H), 9.30 (d, *J* = 9.6 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 122.2, 122.4, 122.6, 122.8, 123.2, 123.5, 123.6, 123.91, 123.94, 124.1, 124.3, 124.9, 125.0, 125.5, 125.86, 125.93, 126.0, 126.2, 126.4, 126.47, 126.54, 126.86, 126.94, 127.1, 127.2, 127.28, 127.31, 127.4, 128.0, 128.3, 128.8, 129.3, 129.5, 129.66, 129.71, 129.74, 129.8, 130.1, 130.3, 130.36, 130.44, 130.5, 130.7, 131.1, 131.8, 132.02, 132.04, 132.11, 132.14, 133.89, 134.1, 134.5, 135.1, 142.1, 142.53, 142.55, 148.0, 165.7, 165.9, 166.4; **HR MS** (MALDI-TOF$^+$; DCTB) Calcd for $C_{142}H_{74}O_{12}$: 1970.5180 [M]$^+$. Found: 1970.5295.

Synthesis of (*R*,*R*,*R*)-4

To a mixture of (*R*,*R*,*R*)-**10** (21.8 mg, 25.4 μmol) in dry CH_2Cl_2 (0.5 mL), 1.0 M BBr_3 in CH_2Cl_2 (0.40 mL, 0.40 mmol) was added under N_2 atmosphere with ice-bath cooling. After 3 h, a mixed solvent of water and CH_2Cl_2 was added. The organic layer was washed successively with water (twice), brine, and dried over Na_2SO_4. The solvent was evaporated to give a crude octaol (*R*,*R*,*R*)-**16** (20.1 mg) as a green powder. A solution of the crude (*R*,*R*,*R*)-**16**, 1-pyrenecarboxylic acid (**11**) (101 mg, 410 μmol), EDC·HCl (238 mg, 1.24 mmol), and DMAP (293 mg, 2.40 mmol) in dry DMF (6.6 mL) was stirred at room temperature for 17 h under N_2 atmosphere. Then a mixed solvent of water and $CHCl_3$ was added. The organic layer was washed successively with water (five times) and brine. After dried over Na_2SO_4, the solvent was evaporated to give a residue. The residue was purified by column chromatography (SiO_2, $CHCl_3$) to afford (*R*,*R*,*R*)-**4** (41.3 mg, 16.8 μmol, 66%) as a yellow powder.

[α]$_D^{21}$ = –246 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3040, 2924, 2851, 1734, 1595, 1506, 1325, 1246, 1225, 1192, 1163, 1141, 1123, 1076, 1020, 970, 849, 819, 708 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.78 (t, *J* = 7.3 Hz, 4H), 6.94 (t, *J* = 7.6 Hz, 4H), 7.05–7.27 (m, 8H), 7.32 (d, *J* = 9.6 Hz, 4H), 7.35–8.35 (m, 54H), 8.36 (s, 2H), 8.45 (d, *J* = 8.7 Hz, 2H), 8.63 (d, *J* = 7.7 Hz, 2H), 8.75 (d, *J* = 8.7 Hz, 2H), 8.94 (d, *J* = 8.2 Hz, 2H), 9.01 (br s, 4H), 9.32 (d, *J* = 9.6 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 122.0, 122.1, 122.6, 122.66, 122.70, 123.28, 123.30, 123.5, 123.6, 123.9, 123.96, 124.01, 124.1, 124.20, 124.23, 124.3, 124.4, 124.5, 124.7, 124.8, 125.3, 125.77, 125.80, 125.9, 126.0, 126.2, 126.3, 126.37, 126.42, 126.5, 126.6, 126.7, 126.9, 126.95, 126.97, 127.05, 127.2, 127.25, 127.30, 127.4, 127.6, 128.3, 128.76, 128.80, 128.86, 129.0, 129.3, 129.6, 129.68, 129.70, 129.8, 129.9, 130.1, 130.19, 130.24, 130.3, 130.47, 130.53, 130.6, 130.8, 130.9, 131.4, 131.77, 131.84, 131.9, 132.0, 132.4, 134.3, 134.5, 134.9, 135.0, 141.5, 142.1, 142.7, 143.1, 165.89, 165.92, 166.0, 166.1; **HR MS** (MALDI-TOF$^+$; DCTB) Calcd for $C_{176}H_{90}O_{16}$: 2458.6223 [M]$^+$. Found: 2458.6313.

Synthesis of (*R*,*R*,*R*)-5

To a mixture of (*R*,*R*,*R*)-**10** (21.5 mg, 25.0 μmol) in dry CH_2Cl_2 (0.5 mL), 1.0 M BBr_3 in CH_2Cl_2 (0.40 mL, 0.40 mmol) was added under N_2 atmosphere with ice-bath cooling. After 4.5 h, a mixed solvent of water and EtOAc was added. The organic layer was washed successively with water (twice), brine, and dried over Na_2SO_4. The solvent was evaporated to give a crude octaol (*R*,*R*,*R*)-**16** (17 mg) as a green powder. A mixture of the crude (*R*,*R*,*R*)-**16**, 1-chloromethylpyrene (**17**) (100 mg, 399 μmol), and K_2CO_3 (166 mg, 1.20 mmol) in dry DMF (4.0 mL) was stirred at room temperature for 16 h under N_2 atmosphere. Then a mixed solvent of water and EtOAc was added. The organic layer was separated and washed successively with water (three times) and brine. After dried over Na_2SO_4, the solvent was evaporated in vacuo to give a residue. The residue was purified by column chromatography (SiO_2, $CHCl_3$) to afford (*R*,*R*,*R*)-**5** (29.1 mg, 12.4 μmol, 50%) as a yellow powder.

[α]$_D^{21}$ = –118 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3040, 2924, 2868, 1603, 1458, 1437, 1242, 1165, 1113, 997, 843, 754, 710 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.39 (d, *J* = 11.0 Hz, 4H), 5.48 (d, *J* = 11.0 Hz, 2H), 5.69 (d, *J* = 11.0 Hz, 4H), 5.85 (d, *J* = 11.5 Hz, 2H), 6.02 (d, *J* = 10.5 Hz, 2H), 6.09 (d, *J* = 10.5 Hz, 2H), 6.48 (d, *J* = 9.2 Hz, 2H), 6.71 (t, *J* = 7.8 Hz, 2H), 6.93 (d, *J* = 1.4 Hz, 2H), 6.95 (d, *J* = 3.2 Hz, 2H), 7.11 (d, *J* = 7.8 Hz, 2H), 7.15 (d, *J* = 9.2 Hz, 2H), 7.19 (d, *J* = 2.3 Hz, 2H), 7.21 (d, *J* = 2.3 Hz, 2H), 7.25–7.35 (m, 8H), 7.37 (d, *J* = 7.8 Hz, 2H), 7.47 (d, *J* = 9.2 Hz, 2H), 7.49 (d, *J* = 7.3 Hz, 2H), 7.52 (d, *J* = 7.3 Hz, 2H), 7.55–7.95 (m, 42H), 8.01 (d, *J* = 9.2 Hz, 2H), 8.02–8.06 (m, 6H), 8.08 (d, *J* = 7.8 Hz, 2H), 8.13 (d, *J* = 7.3 Hz, 2H), 8.17 (d, *J* = 7.8 Hz, 2H), 8.27 (d, *J* = 9.2 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 70.0, 72.9, 73.2, 74.1, 109.2, 122.78, 122.83, 123.3, 123.6, 124.36, 124.39, 124.6, 124.7, 124.80, 124.83, 124.9, 125.0, 125.08, 125.1, 125.2, 125.3, 125.69, 125.74, 125.8, 126.2, 127.0, 127.2, 127.30, 127.33, 127.4, 127.5, 127.57, 127.59, 127.61, 127.9, 128.1, 128.2, 128.4, 129.5, 130.2, 130.6, 130.73, 130.74, 130.81, 130.85, 130.88, 130.90, 131.2, 131.3, 131.4, 131.6, 131.9, 148.1, 150.8, 152.7; **HR MS** (MALDI-TOF$^+$; DCTB) Calcd for $C_{176}H_{106}AgO_8$: 2453.6933 $[M+Ag]^+$. Found: 2453.6988.

Synthesis of (*R*)-6

A solution of (*R*)-BINOL (10.2 mg, 35.6 μmol), 1-pyrenecarboxylic acid (**11**) (26.3 mg, 107 μmol), EDC·HCl (29.8 mg, 155 μmol), and DMAP (13.1 mg, 107 μmol) in dry DMF (1.5 mL) was stirred at room temperature for 15 h under N_2 atmosphere. Then a mixed solvent of water and CH_2Cl_2 was added. The organic layer was washed successively with water (five times) and brine. After dried over Na_2SO_4, the solvent was evaporated to give a residue. The residue was purified by column chromatography (SiO_2, $CHCl_3$) to afford (*R*)-**6** (26.0 mg, 35.0 μmol, 98%) as a yellow powder. The NMR data of (*R*)-**6** were in agreement with those reported previously.[S1]

Synthesis of (*R*)-7

A mixture of (*R*)-**18** (12.5 mg, 25.1 μmol) and 10% Pd-C (6.0 mg) in dry THF (2.0 mL) was stirred and refluxed for 2 h under H_2 atmosphere. After Pd-C was filtered off, the filtrate was evaporated to give a

crude tetraol (*R*)-**19**[S4] as a light pink powder (8.1 mg). A solution of the crude (*R*)-**19**, 1-pyrenecarboxylic acid (**11**) (49.2 mg, 200 μmol), EDC·HCl (77 mg, 0.40 mmol), and DMAP (24 mg, 0.20 mmol) in dry DMF (2.0 mL) was stirred at room temperature for 13.5 h under N_2 atmosphere. Then a mixed solvent of water and $CHCl_3$ was added. The organic layer was washed successively with water (five times) and brine. After dried over Na_2SO_4, the solvent was evaporated to give a residue. The residue was purified by column chromatography (SiO_2, $CHCl_3$) to afford (*R*)-**7** (22 mg, 0.018 mmol, 72%) as a yellow powder.

[α]$_D^{21}$ = –311 ($CHCl_3$, *c* 0.052); **IR** (KBr) 3040, 2957, 2924, 2851, 1734, 1595, 1506, 1325, 1246, 1225, 1190, 1163, 1142, 1123, 1076, 1020, 970, 849, 820, 746, 710 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40–7.90 (m, 32H), 7.93 (dd, *J* = 1.8, 6.4 Hz, 2H), 8.03 (d, *J* = 7.8 Hz, 2H), 8.28 (s, 2H), 8.38 (br s, 2H), 8.59 (d, *J* = 9.2 Hz, 2H), 8.66 (d, *J* = 8.3 Hz, 2H), 9.02 (d, *J* = 9.2 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 121.55, 121.57, 122.5, 123.5, 123.6, 124.0, 124.1, 124.2, 124.3, 124.4, 124.5, 126.0, 126.1, 126.2, 126.3, 126.4, 126.5, 126.7, 126.8, 126.99, 127.04, 127.3, 128.4, 128.8, 129.1, 129.4, 129.5, 129.69, 129.71, 129.98, 130.0, 130.58, 130.6, 131.1, 131.6, 131.9, 132.4, 134.5, 134.7, 141.6, 142.8, 165.6, 165.8; **HR MS** (ESI^+) Calcd for $C_{88}H_{46}NaO_8$: 1253.3085 $[M+Na]^+$. Found: 1253.3090.

Synthesis of (*R,R,R*)-20

A solution of (*R,R,R*)-**14** (22.2 mg, 26.8 μmol), TPP(Zn)CO_2H (55.4 mg, 76.7 μmol), EDC·HCl (16.3 mg, 85.0 μmol), and DMAP (10.7 mg, 87.6 μmol) in dry CH_2Cl_2 (4.0 mL) was stirred and refluxed for 22 h under N_2 atmosphere. Then a mixed solvent of water and CH_2Cl_2 was added. The organic layer was washed successively with water (twice) and brine (twice). After dried over Na_2SO_4, the solvent was evaporated to give a residue (55.4 mg), a crude mono-TPP(Zn) adduct, as a purple powder. A solution of the residue, TPP(Zn)CO_2H (55.4 mg, 76.7 μmol), EDC·HCl (49.8 mg, 260 μmol), and DMAP (31.8 mg, 260 μmol) in dry CH_2Cl_2 (4.0 mL) was stirred at room temperature for 13 h under N_2 atmosphere. Then a mixed solvent of water and CH_2Cl_2 was added. The organic layer was washed successively with water (twice) and brine (twice). After dried over Na_2SO_4, the solvent was evaporated to give a residue. The residue was chromatographed (SiO_2, $CHCl_3$) and recrystallized from $CHCl_3$/hexane to afford (*R,R,R*)-**20** (12.0 mg, 5.37 μmol, 20%) as a purple powder.

IR (KBr) 3055, 2955, 2930, 2870, 1747, 1595, 1508, 1244, 1206, 1070, 1003, 995, 796, 754, 729, 719, 702 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 0.55 (t, *J* = 6.6 Hz, 6H), 0.88 (t, *J* = 7.3 Hz, 6H), 0.80–1.05 (m, 4H), 1.15–1.42 (m, 8H), 1.55–1.85 (m, 4H), 3.80 (br s, 2H), 3.91 (br s, 2H), 4.10–4.20 (m, 2H), 4.22–4.34 (m, 2H), 6.84 (br s, 2H), 7.07 (br s, 2H), 7.30–7.50 (m, 10H), 7.57 (d, *J* = 9.2 Hz, 2H), 7.70–7.90 (m, 20H), 8.03 (d, *J* = 8.7 Hz, 2H), 8.18–8.28 (m, 12H), 8.31 (d, *J* = 7.8 Hz, 4H), 8.46 (br s, 4H), 8.75–8.82 (m, 4H), 8.85 (d, *J* = 4.1 Hz, 4H), 8.99 (s, 8H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 13.9, 14.2, 19.1, 19.5, 32.0, 32.5, 70.0, 74.1, 119.9, 120.2, 121.6, 121.8, 123.8, 125.4, 125.8, 126.3, 126.4, 126.9, 127.4, 127.7, 127.9, 128.1, 128.6, 129.3, 129.5, 130.2, 130.7, 132.0, 132.4, 132.5, 132.7, 133.0, 134.5, 134.8, 143.0, 143.1, 143.2, 148.2, 149.7, 149.9, 150.5, 150.6, 155.3, 164.6; **HR MS** (MALDI-TOF^+; DCTB) Calcd for $C_{146}H_{110}N_8NaO_8Zn_2$: 2253.6922 $[M+Na]^+$. Found: 2253.6871.

Synthesis of (*R*,*S*,*R*)-20

A solution of (*R*,*S*,*R*)-**14** (21.9 mg, 26.4 μmol), TPP(Zn)CO_2H (62.6 mg, 86.7 μmol), EDC·HCl (15.4 mg, 80.3 μmol), and DMAP (9.9 mg, 81 μmol) in dry CH_2Cl_2 (4.0 mL) was stirred and refluxed for 22 h under N_2 atmosphere. Then a mixed solvent of water and CH_2Cl_2 was added. The organic layer was washed successively with water (twice) and brine (twice). After dried over Na_2SO_4, the solvent was evaporated to give a residue (61.6 mg), a crude mono-TPP(Zn) adduct, as a purple powder. A solution of the residue, TPP(Zn)CO_2H (62.6 mg, 86.7 μmol), EDC·HCl (46.2 mg, 241 μmol), and DMAP (29.7 mg, 243 μmol) in dry CH_2Cl_2 (4.0 mL) was stirred at room temperature for 13 h under N_2 atmosphere. Then a mixed solvent of water and CH_2Cl_2 was added. The organic layer was washed successively with water (twice) and brine (twice). After dried over Na_2SO_4, the solvent was evaporated to give a residue. The residue was purified by column chromatography (SiO_2, $CHCl_3$) to afford (*R*,*S*,*R*)-**20** (29.8 mg, 13.3 μmol, 50%) as a purple powder.

IR (KBr) 3055, 2955, 2931, 2870, 1744, 1595, 1508, 1244, 1206, 1069, 1003, 995, 796, 756, 729, 719, 702 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 0.42 (t, *J* = 7.1 Hz, 6H), 0.55 (t, *J* = 7.3 Hz, 6H), 0.84 (sext, *J* = 7.3 Hz, 4H), 0.95 (sext, *J* = 7.4 Hz, 4H), 1.20–1.45 (m, 8H), 3.75–4.15 (m, 8H), 7.20–7.30 (m, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.40–7.50 (m, 8H), 7.54 (t, *J* = 9.1 Hz, 2H), 7.65–7.80 (m, 20H), 7.96 (d, *J* = 7.8 Hz, 2H), 8.04 (d, *J* = 9.2 Hz, 2H), 8.10–8.25 (m, 12H), 8.26 (d, *J* = 7.8 Hz, 4H), 8.53 (d, *J* = 6.4 Hz, 4H), 8.83 (d, *J* = 3.7 Hz, 4H), 8.88 (d, *J* = 4.6 Hz, 4H), 8.90–9.00 (m, 8H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 13.6, 14.0, 18.8, 19.1, 31.5, 32.4, 69.0, 74.0, 120.0, 121.6, 121.9, 124.1, 125.9, 126.0, 126.1, 126.2, 126.4, 126.9, 127.4, 127.5, 127.9, 128.2, 128.69, 128.73, 129.4, 129.5, 130.2, 130.8, 131.8, 132.4, 132.5, 132.9, 134.6, 134.7, 134.8, 143.0, 143.4, 148.1, 149.4, 149.9, 150.5, 150.61, 150.64, 150.67, 155.1; **HR MS** (MALDI-TOF$^+$; DCTB) Calcd for $C_{146}H_{110}N_8NaO_8Zn_2$: 2253.6922 $[M+Na]^+$. Found: 2253.6874.

references

(S1) P. Rajakumar and Visalakshi, K. *Synth. Commun.* 2013, **43**, 2226−2235.

(S2) K. Tsubaki, H. Tanaka, K. Takaishi, M. Miura, H. Morikawa, T. Furuta, K. Tanaka, K. K Fuji and T. Kawabata, *J. Org. Chem.* 2006, **71**, 6579−6587.

(S3) K. Tsubaki, H. Morikawa, H. Tanaka and K. Fuji, *Tetrahedron: Asymmetry* 2003, **14**, 1393−1396.

(S4) H. Danjo, K. Hirata, S. Yoshigai, I. Azumaya, and K. Yamaguchi, *J. Am. Chem. Soc*. 2009, **131**, 1638−1639.

3. Determination of absolute configuration.

To determine the absolute configuration of the newly formed axis of quarternaphthyls **14**, we applied the CD exciton chirality method to the quaternaphthyls with two TPP(Zn)s (**20**). Thus, the sense of the CD derived from the B band of the two TPP(Zn)s should reflect the direction of torsion of the chromophores, which then reveals the configuration of the target central axis. A positive split Cotton effect indicates that the absolute configuration of the target axis should be *S*. Conversely, a negative split Cotton effect indicates *R*-axis.

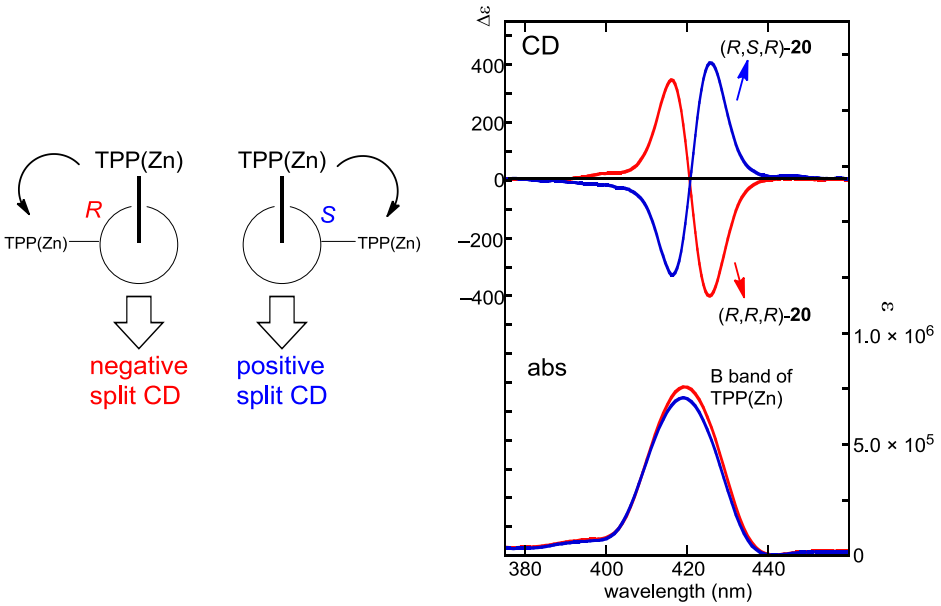


Fig. S1 CD and absorption spectra of (*R*,*R*,*R*)-**20** and (*R*,*S*,*R*)-**20**. Conditions: CH_2Cl_2, 1.0×10^{-6} M, 20 °C, light path length = 1 cm.

4. DFT calculations of optimized structures.

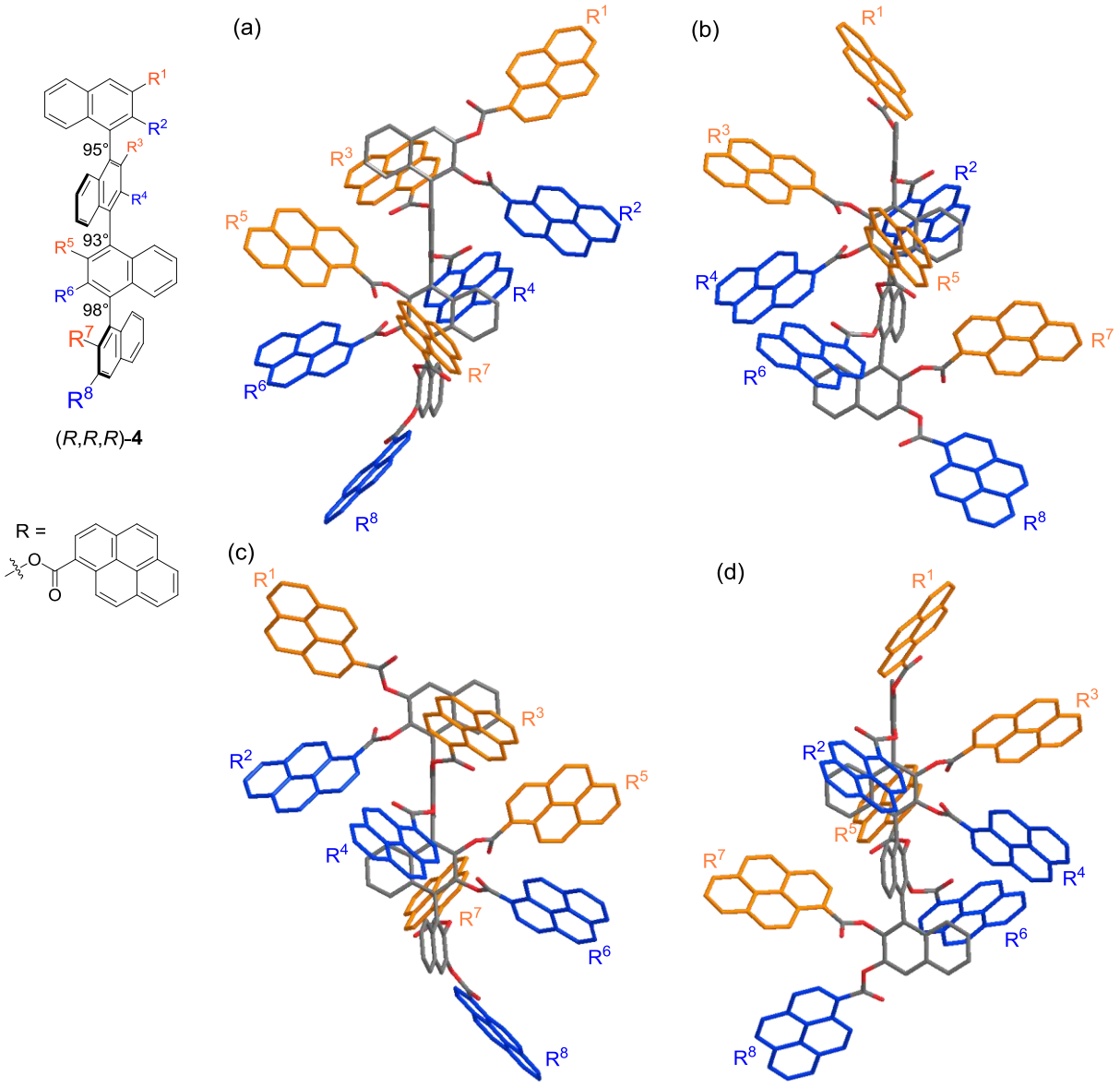


Fig. S2 Four side views of DFT-optimized structure of (*R*,*R*,*R*)-**4** by 90° at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

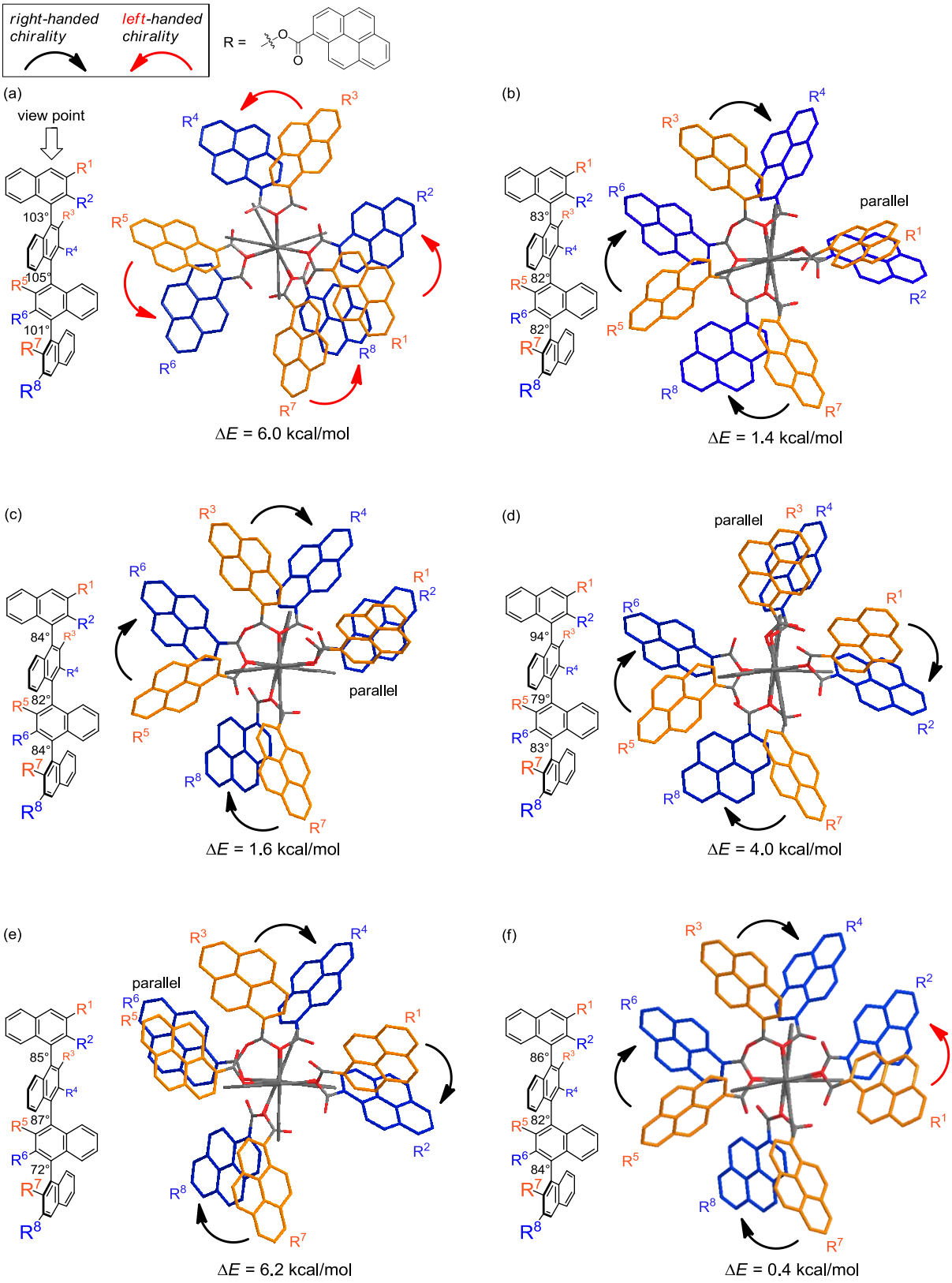


Fig. S3 DFT-optimized metastable structures of (*R*,*R*,*R*)-**4** at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

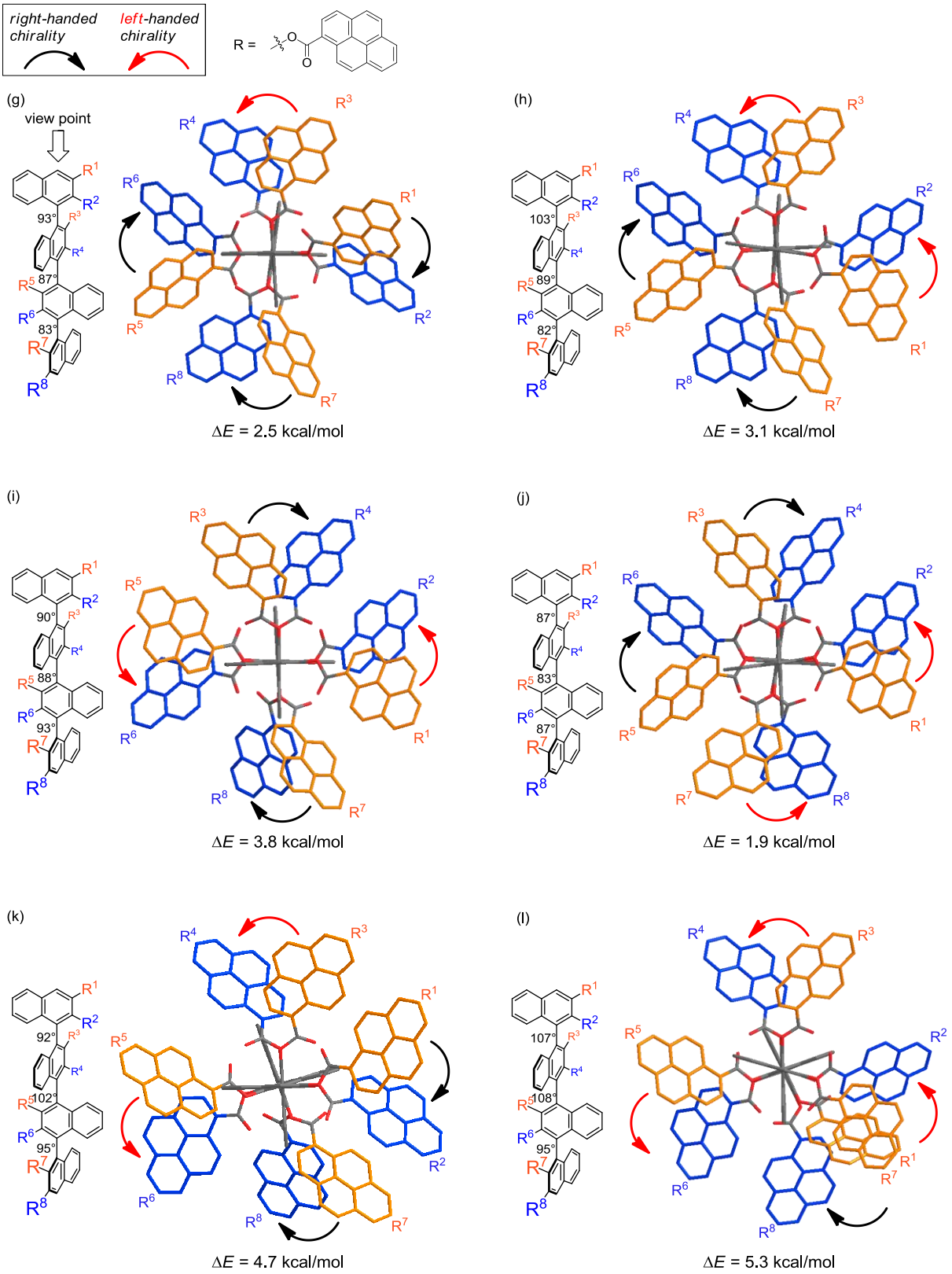


Fig. S3 (Continued).

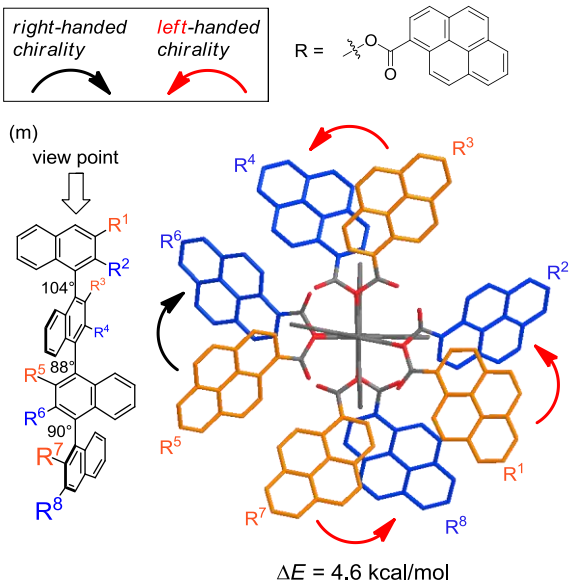


Fig. S3 (Continued).

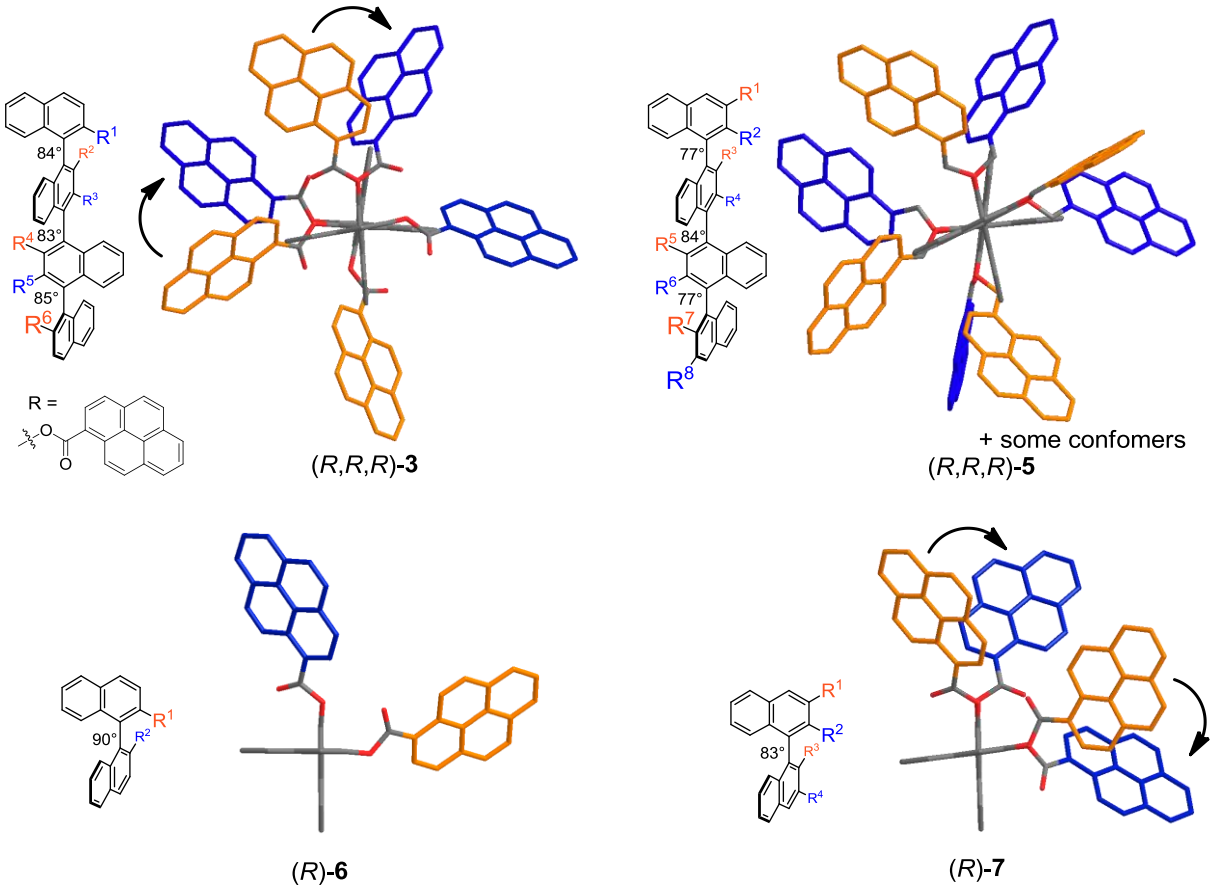


Fig. S4 DFT-optimized structures of (*R*,*R*,*R*)-**3**, (*R*,*R*,*R*)-**5**, (*R*)-**6**, and (*R*)-**7** at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

5. UV-Vis, CD, FL, and CPL spectra.

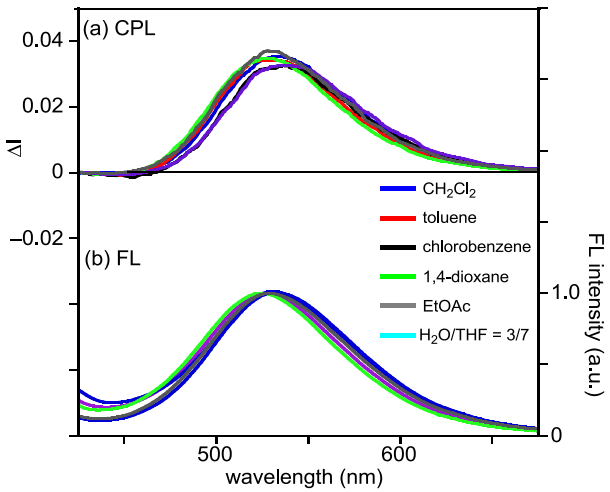


Fig. S5 (a) CPL and (b) FL spectra of (*R*,*R*,*R*)-**4** in solution. Conditions: 5.0×10^{-6} M, 20 °C, light path length = 10 mm, λ_{ex} = 355 nm.

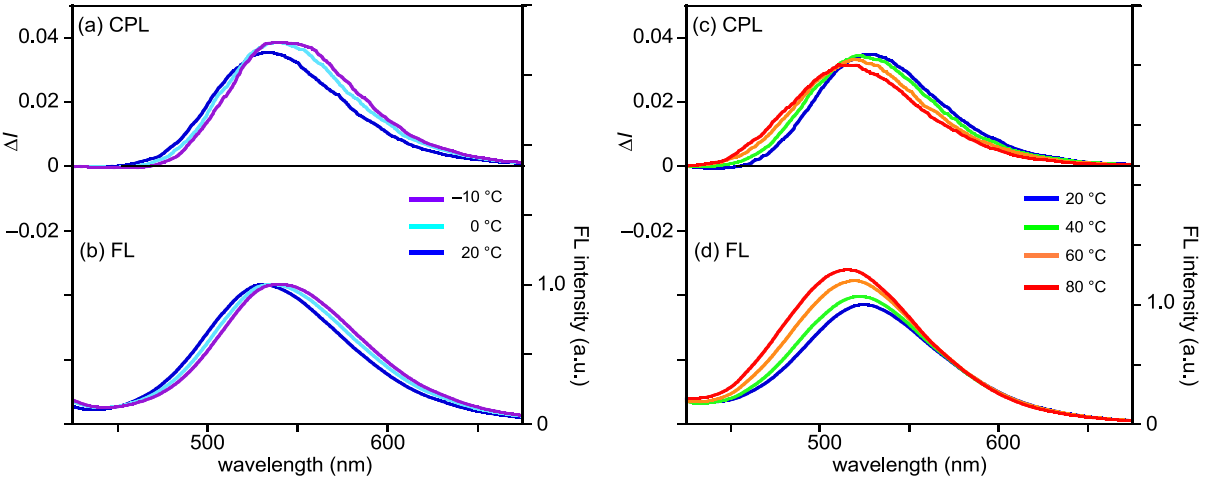


Fig. S6 (a) VT CPL and (b) VT FL spectra of (*R*,*R*,*R*)-**4** in CH_2Cl_2 at –10 °C (purple), 0 °C (light blue), and 20 °C (blue). (c) VT CPL and (d) VT FL spectra of (*R*,*R*,*R*)-**4** in 1,4-dioxane at 20 °C (blue), 40 °C (green), 60 °C (orange), and 80 °C (red). Conditions: 5.0×10^{-6} M, light path length = 10 mm, λ_{ex} = 355 nm.

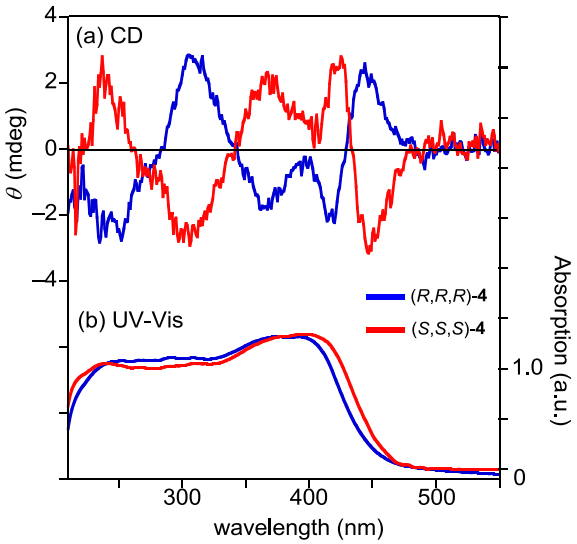


Fig. S7 (a) CD and (b) UV-Vis spectra of (*R*,*R*,*R*)-**4** (blue) and (*S*,*S*,*S*)-**4** (red) in the solid state. Conditions: 20 ℃, KBr.

6. ^{1}H and ^{13}C NMR spectra.

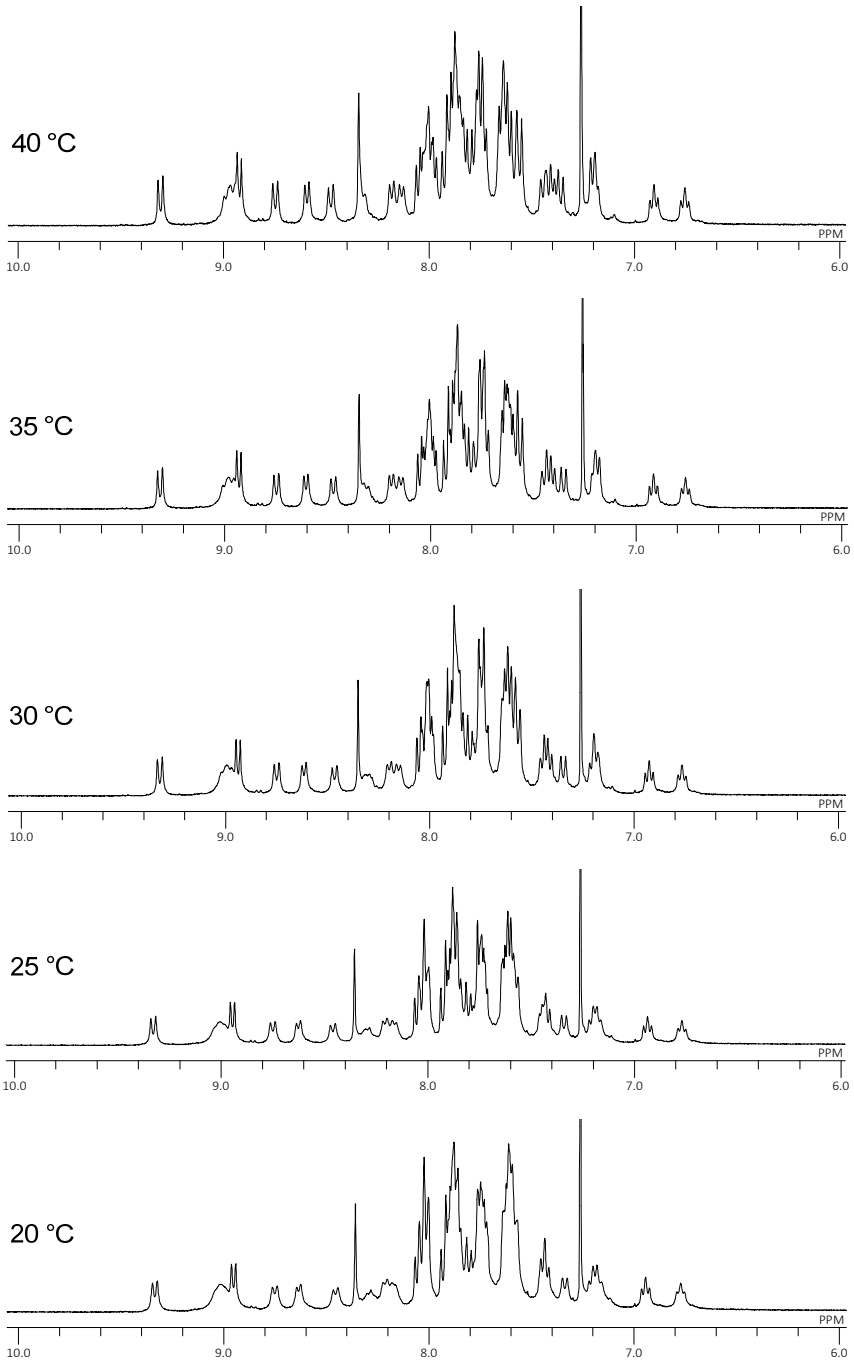
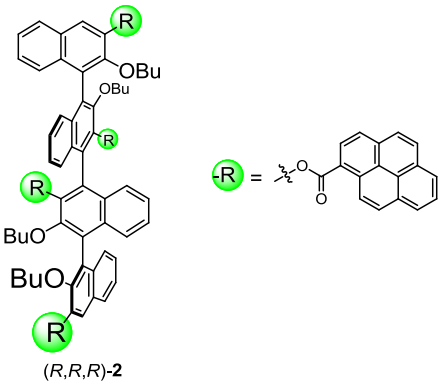
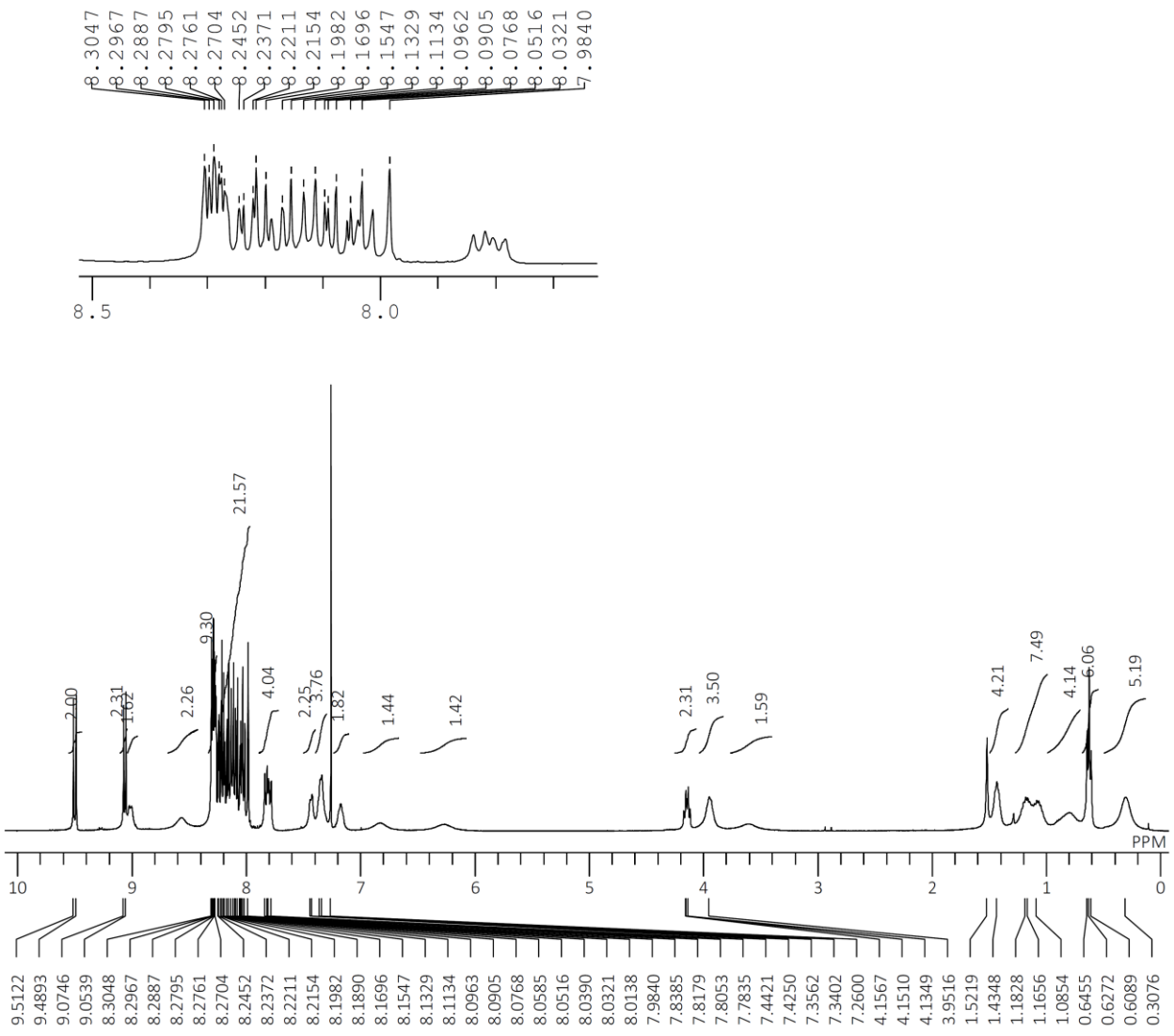
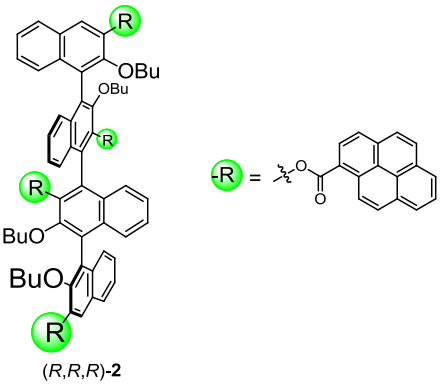


Fig. S8 VT ^{1}H NMR of (*R*,*R*,*R*)-**4** (400 MHz, $CDCl_3$).

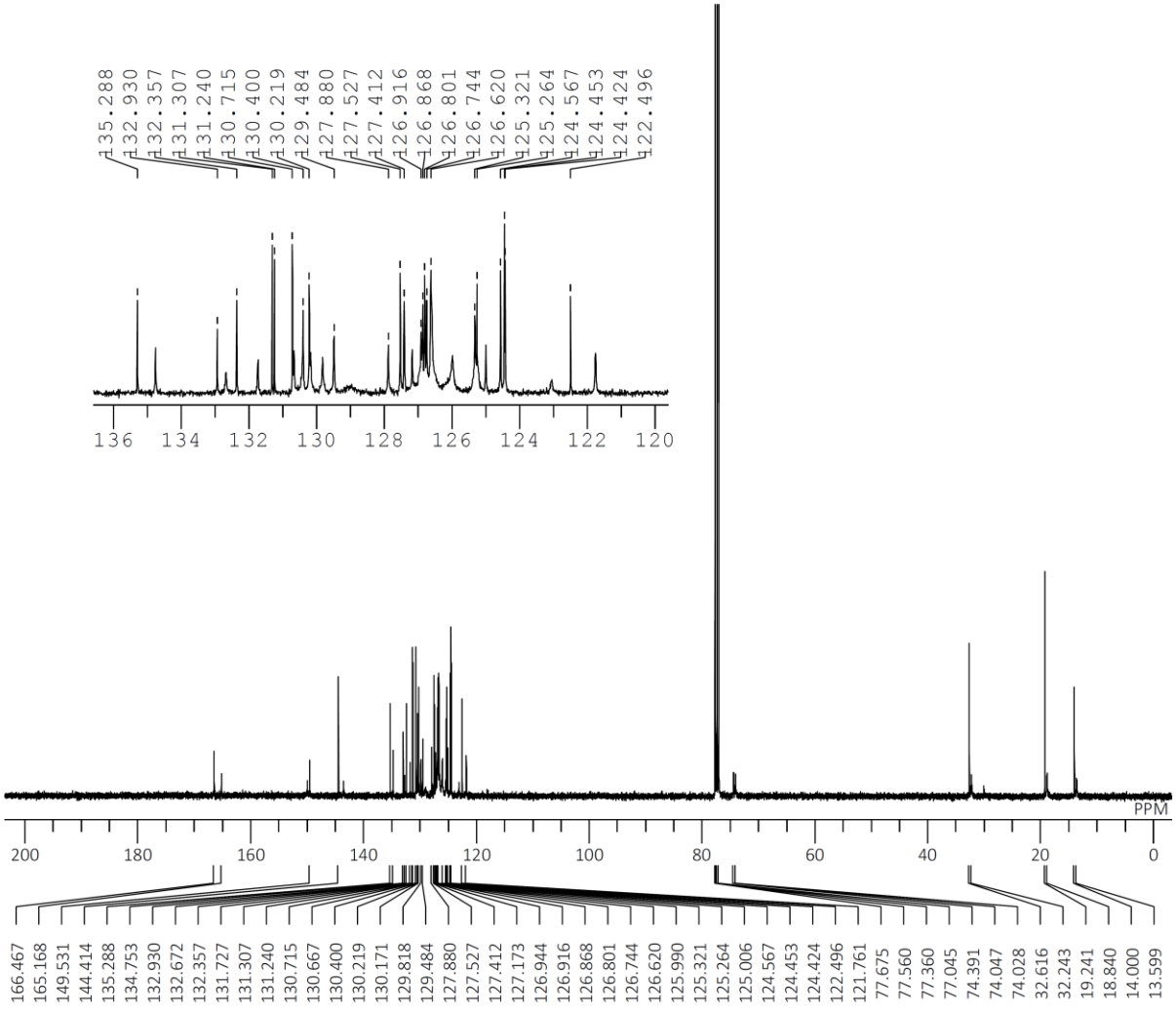




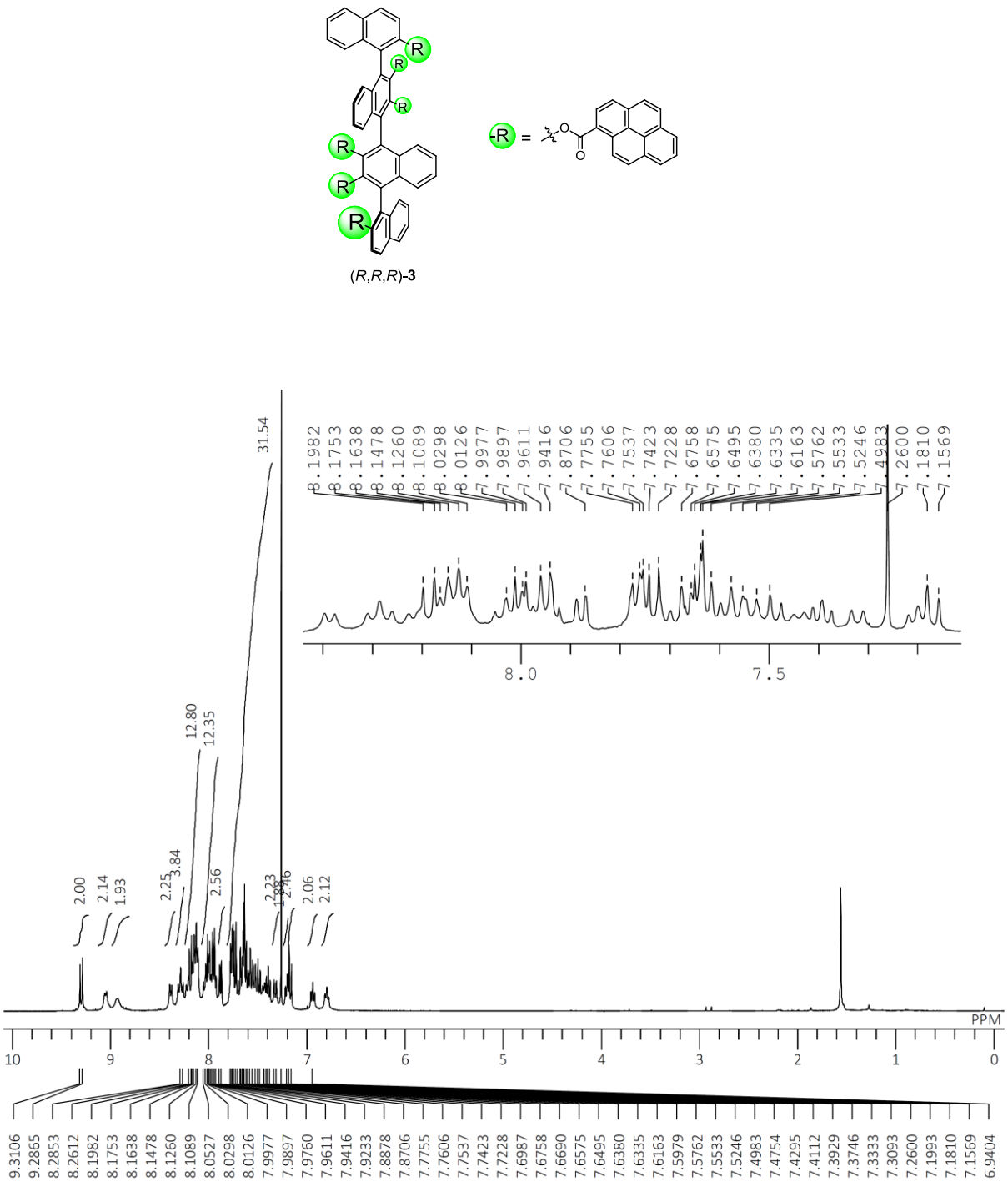
^{1}H NMR spectrum of (*R*,*R*,*R*)-**2** (400 MHz, $CDCl_3$).



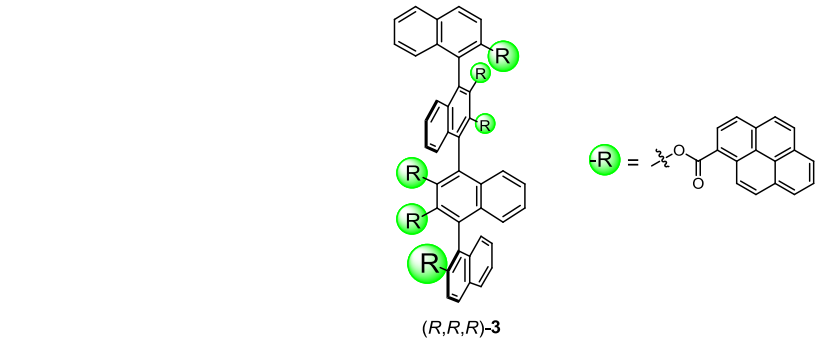
(*R*,*R*,*R*)-**2**



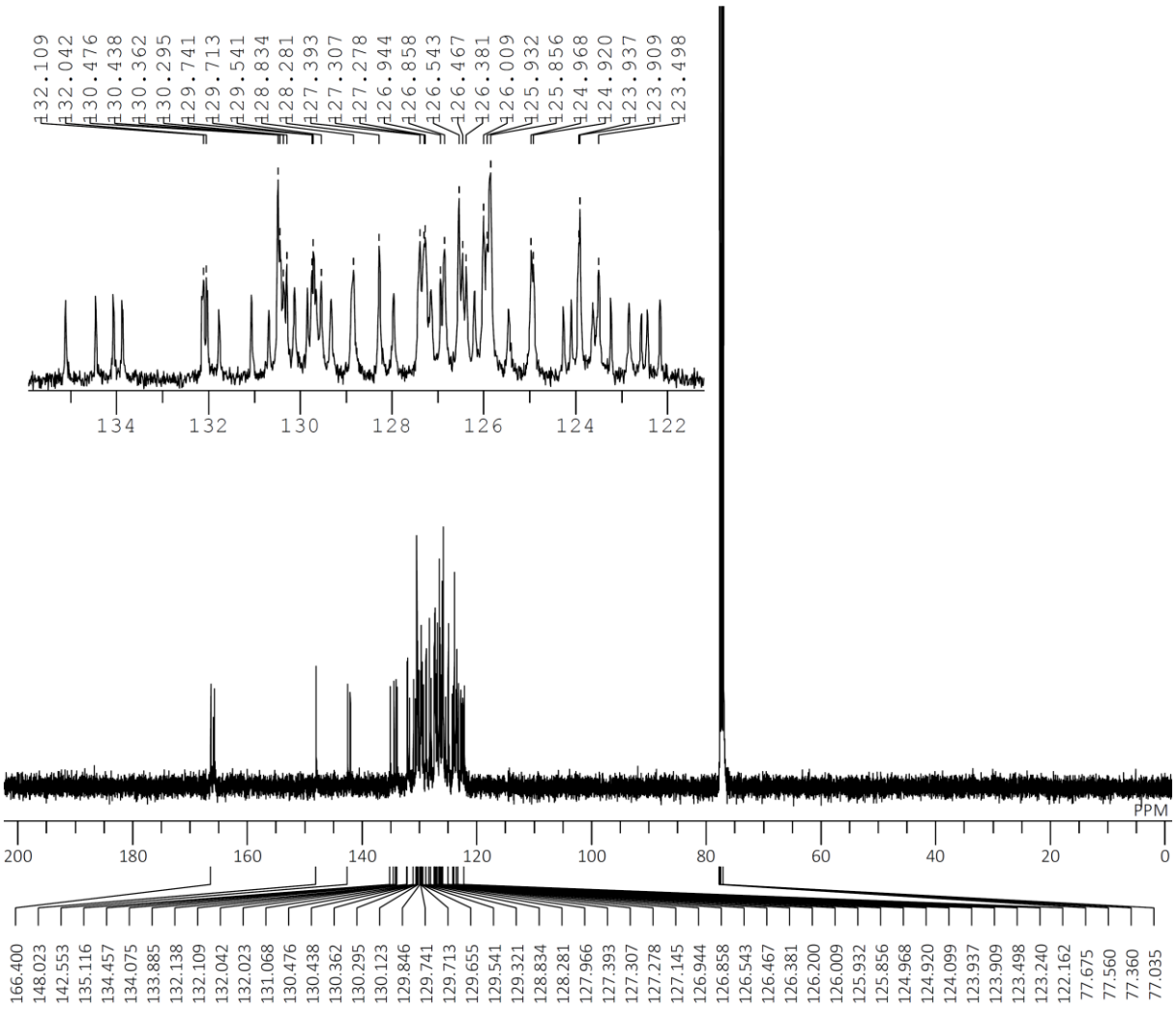
^{13}C NMR spectrum of (*R*,*R*,*R*)-**2** (100 MHz, $CDCl_3$).



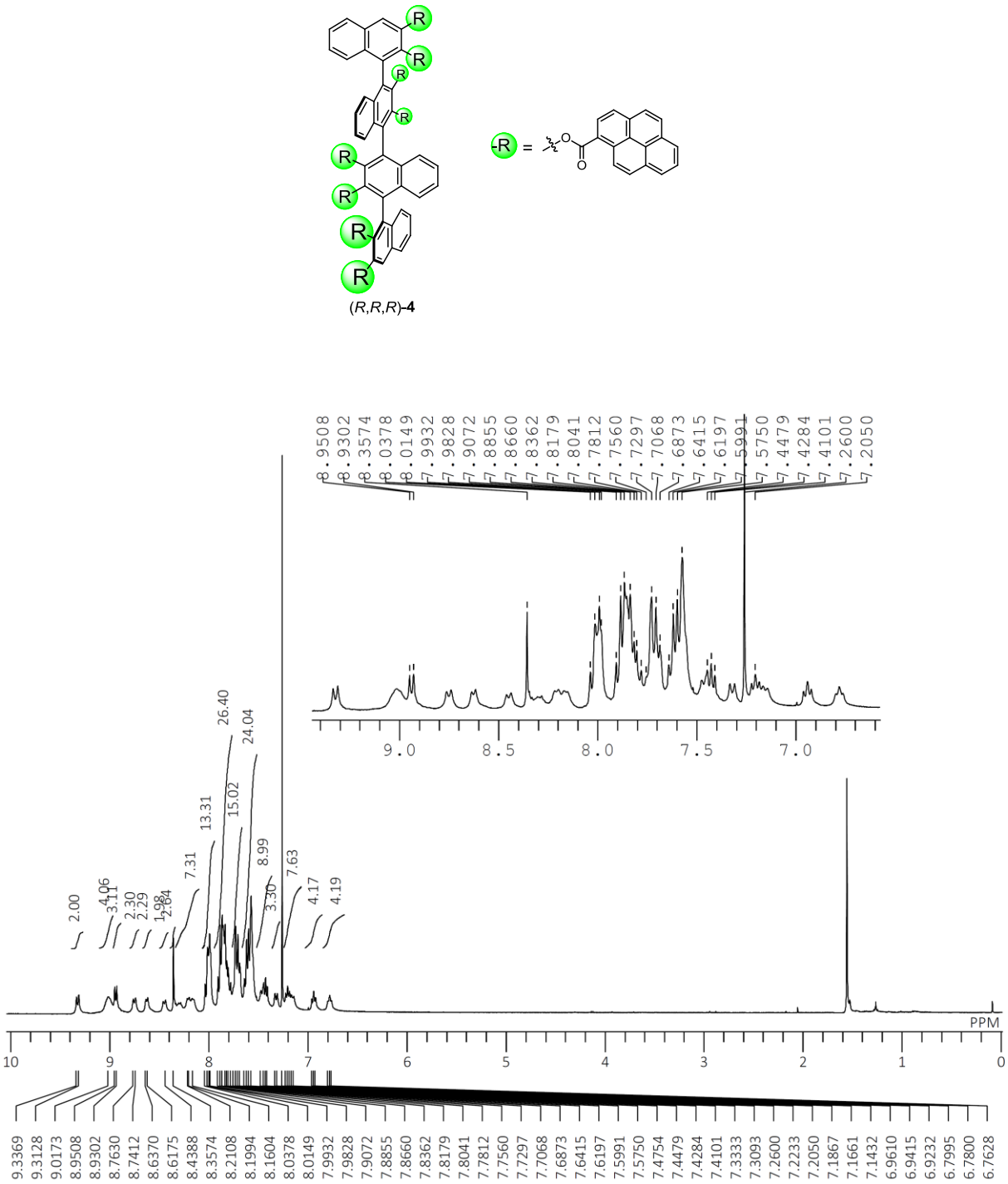
^{1}H NMR spectrum of (*R*,*R*,*R*)-**3** (400 MHz, $CDCl_3$).



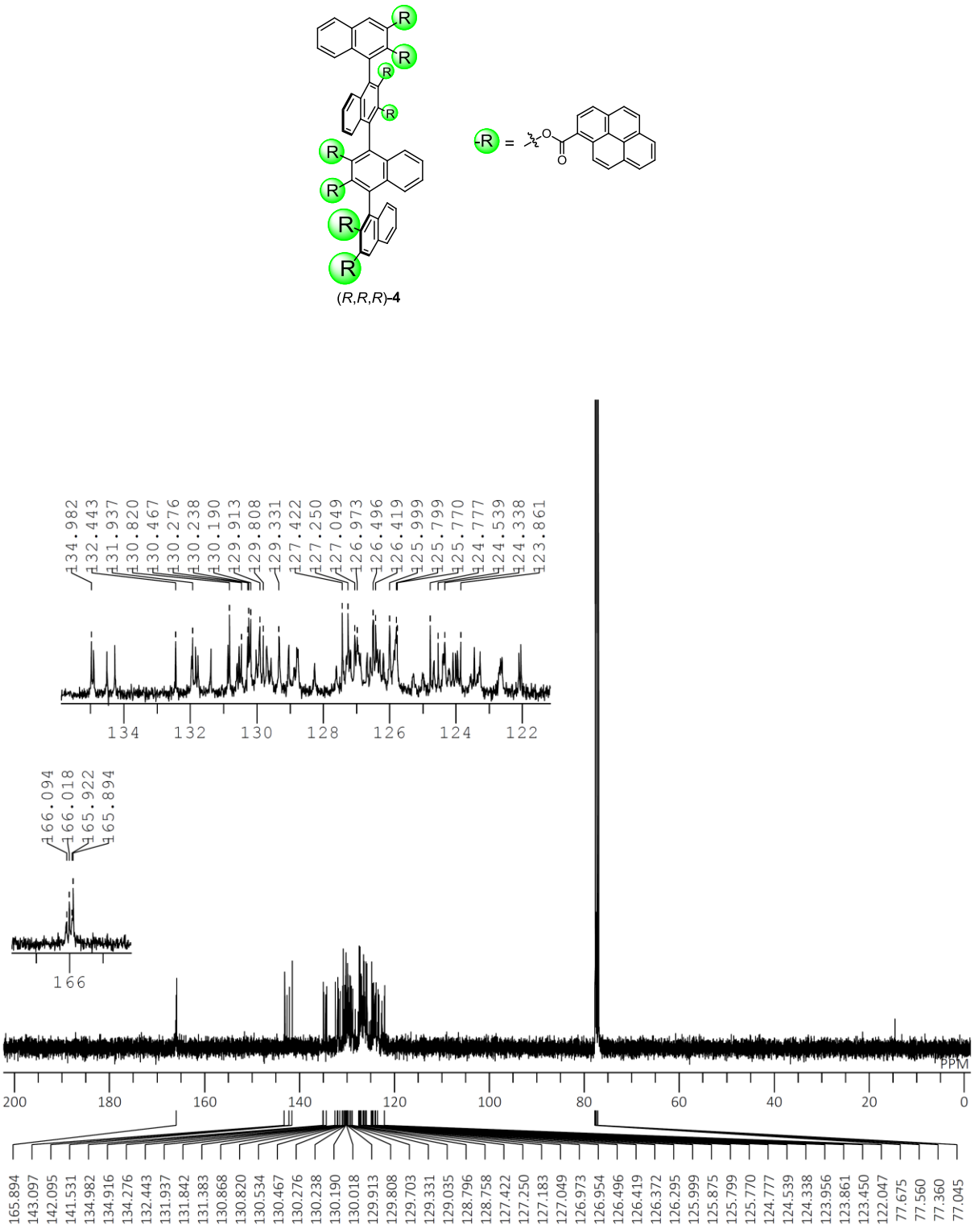
(*R*,*R*,*R*)-**3**



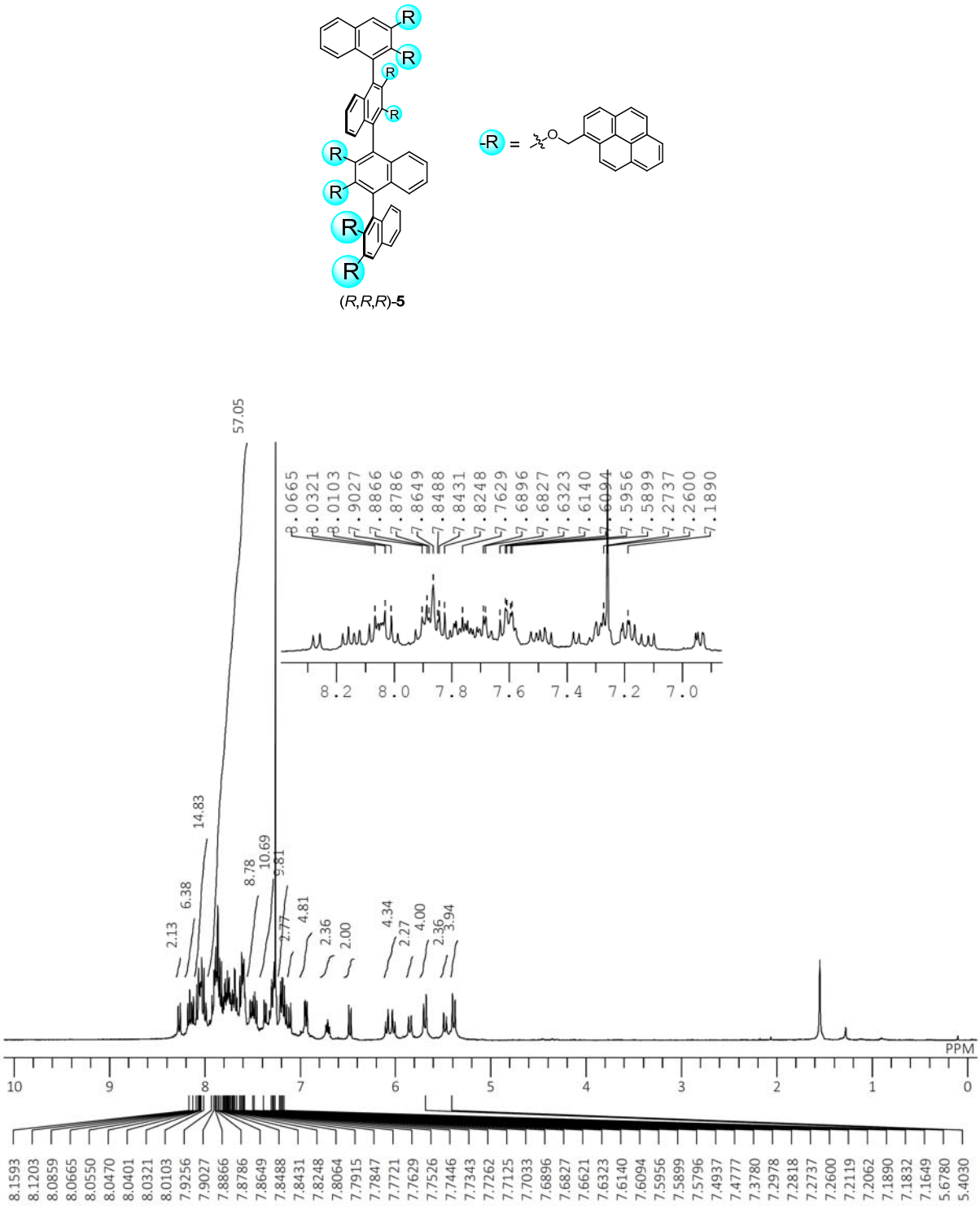
^{13}C NMR spectrum of (*R*,*R*,*R*)-**3** (100 MHz, $CDCl_3$).



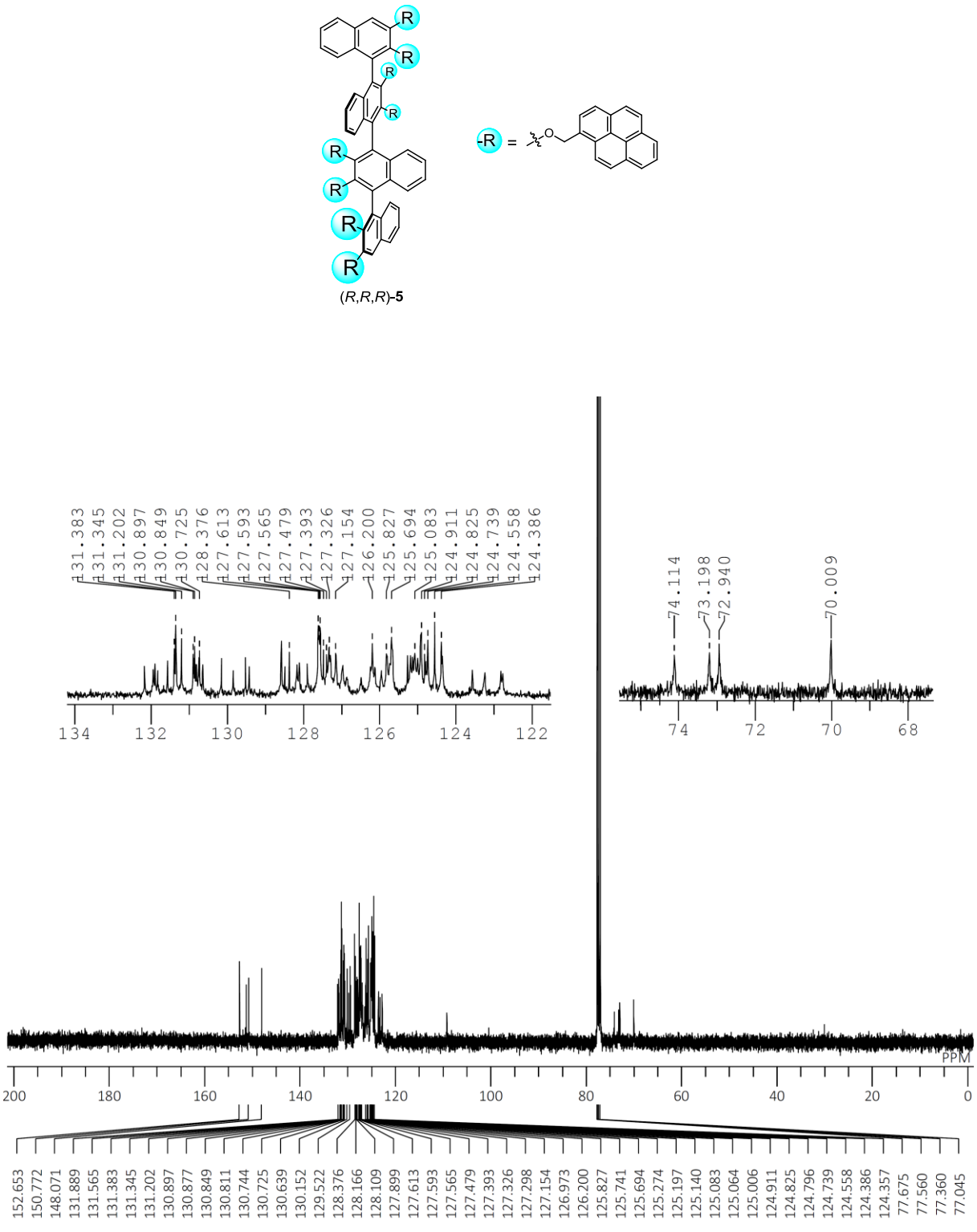
^{1}H NMR spectrum of (*R*,*R*,*R*)-**4** (400 MHz, $CDCl_3$).



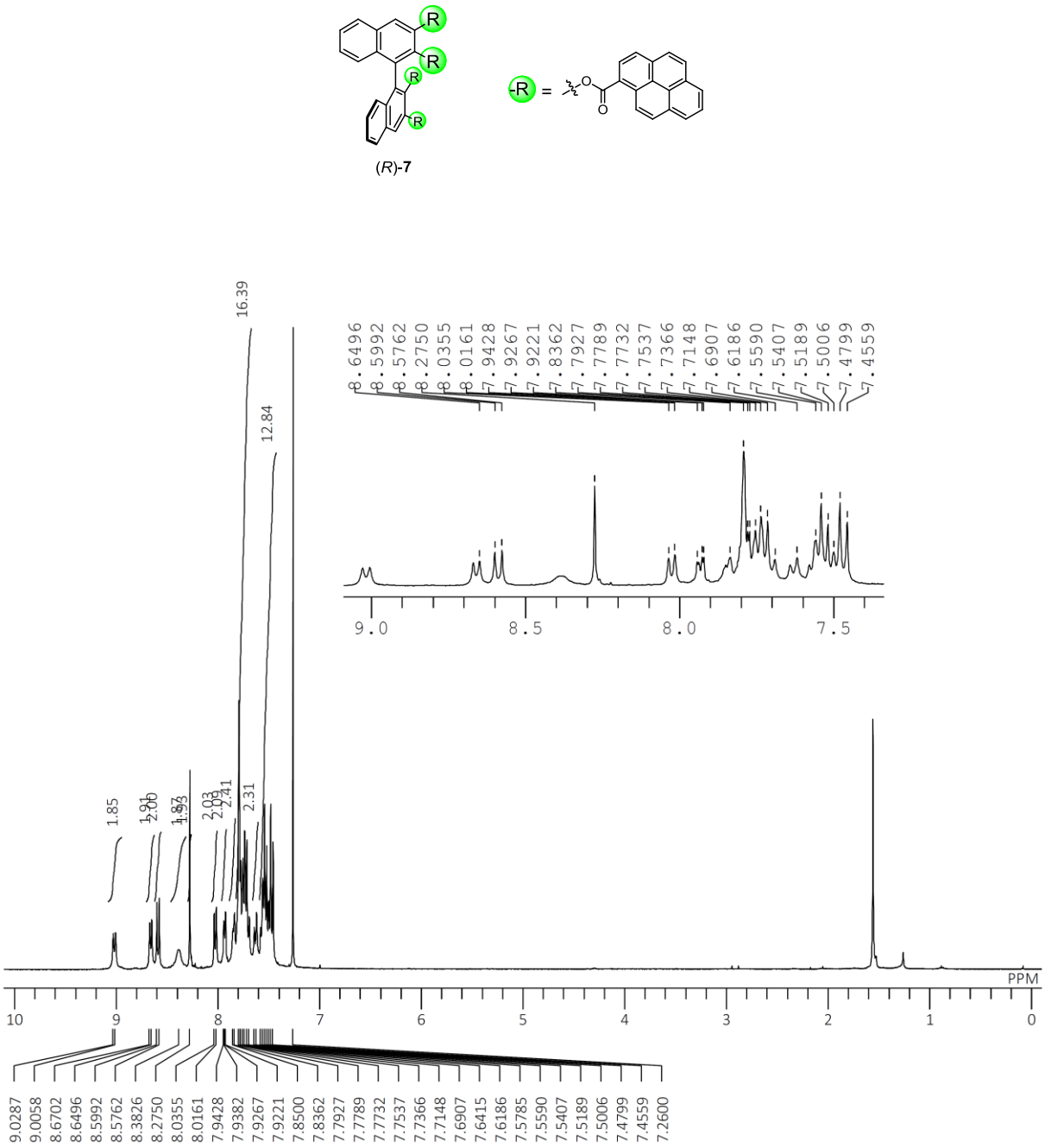
^{13}C NMR spectrum of (*R*,*R*,*R*)-**4** (100 MHz, $CDCl_3$).



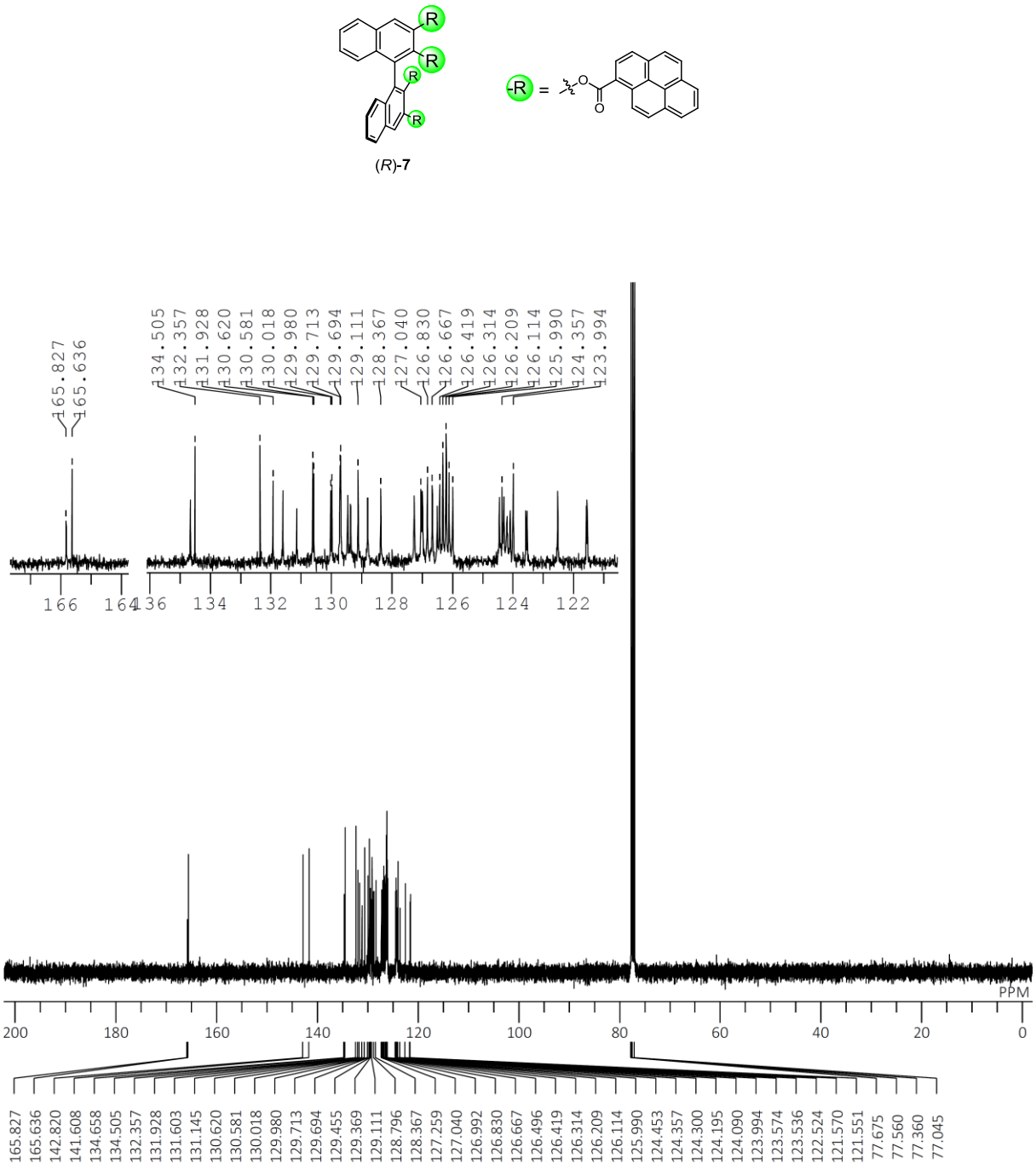
^{1}H NMR spectrum of (*R*,*R*,*R*)-**5** (400 MHz, $CDCl_3$).



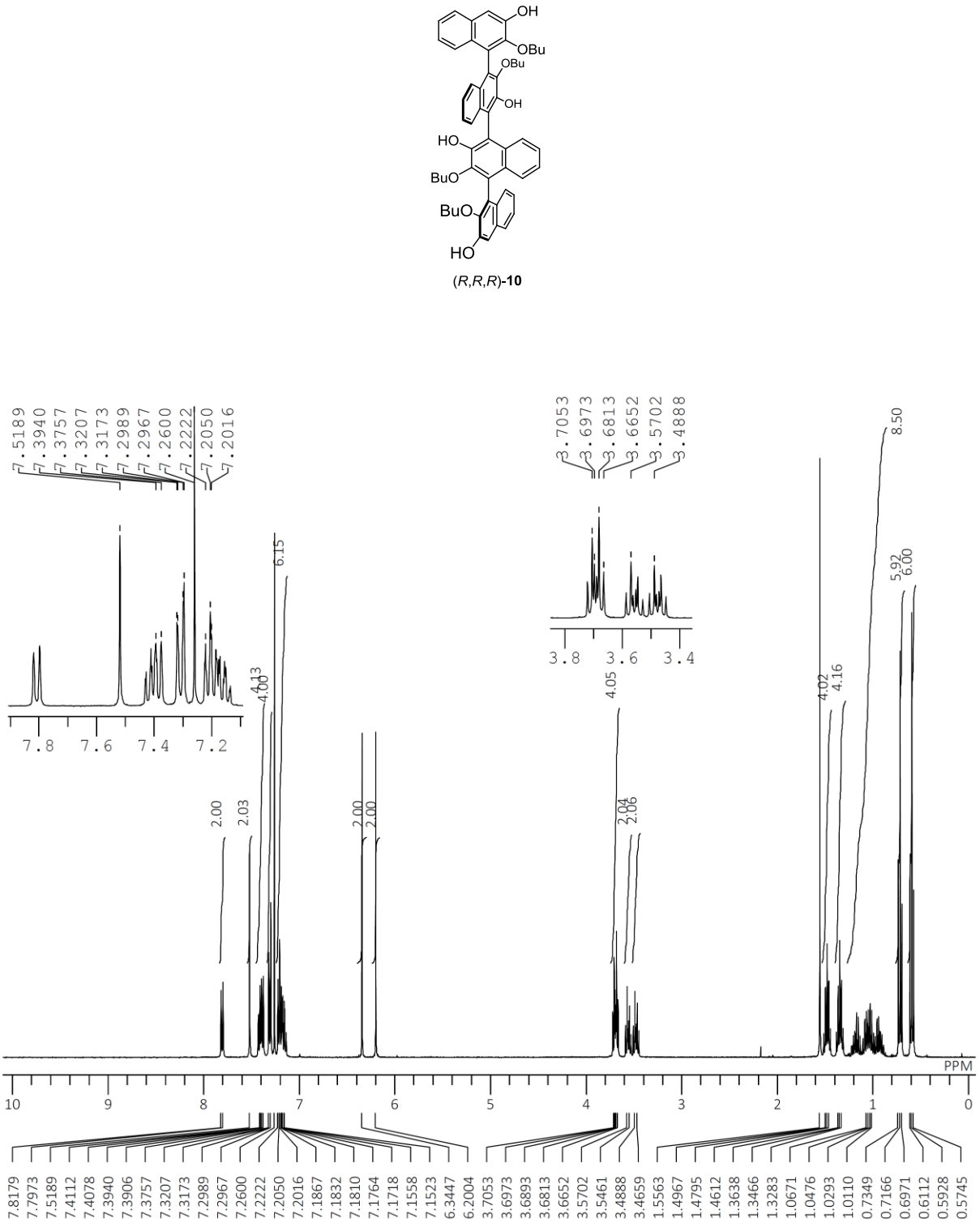
^{13}C NMR spectrum of (*R*,*R*,*R*)-**5** (100 MHz, $CDCl_3$).



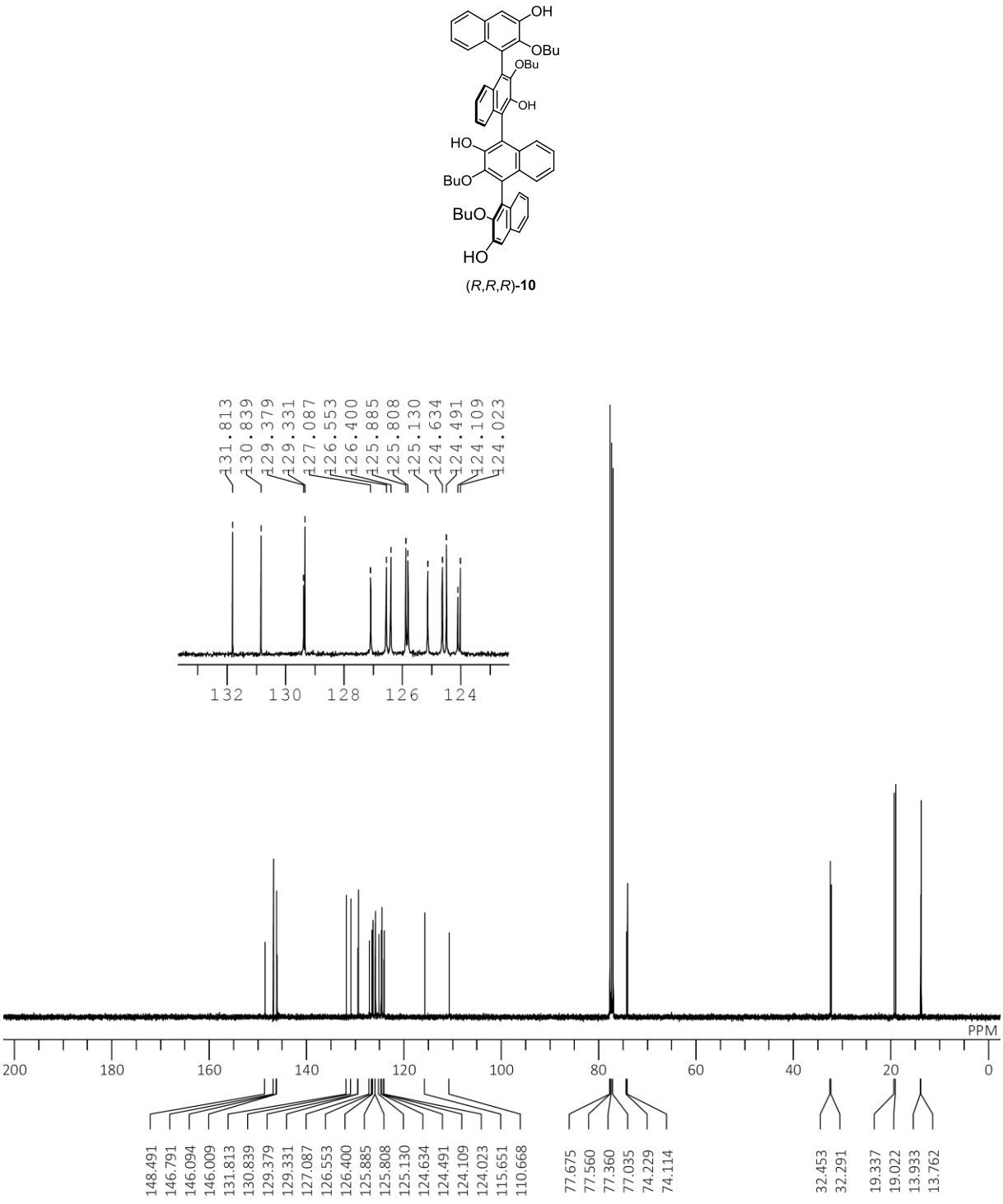
^{1}H NMR spectrum of (*R*)-**7** (400 MHz, $CDCl_3$).



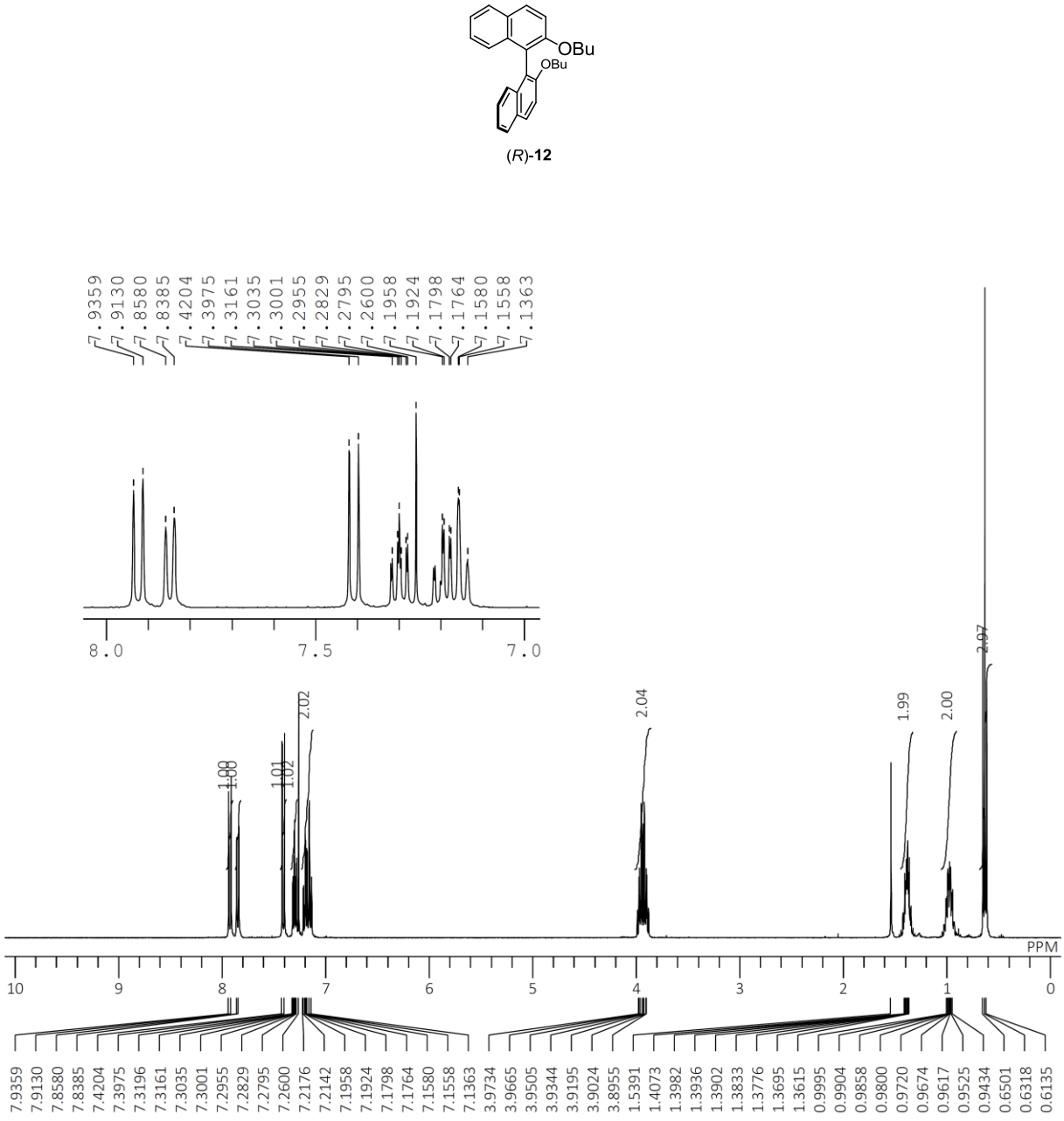
^{13}C NMR spectrum of (*R*)-**7** (100 MHz, $CDCl_3$).



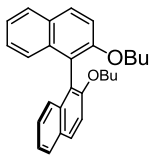
^{1}H NMR spectrum of (*R*,*R*,*R*)-**10** (400 MHz, $CDCl_3$).



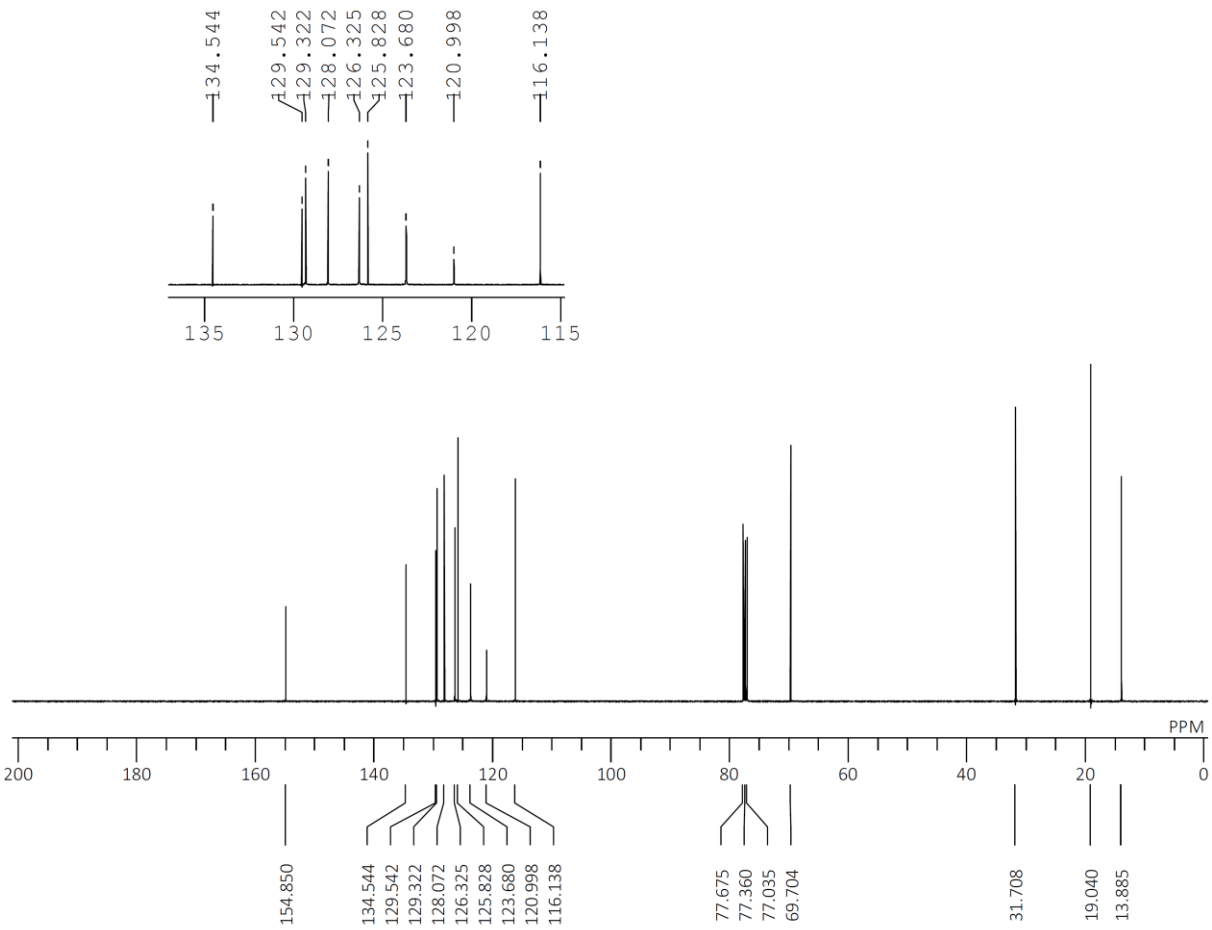
^{13}C NMR spectrum of (*R*,*R*,*R*)-**10** (100 MHz, $CDCl_3$).



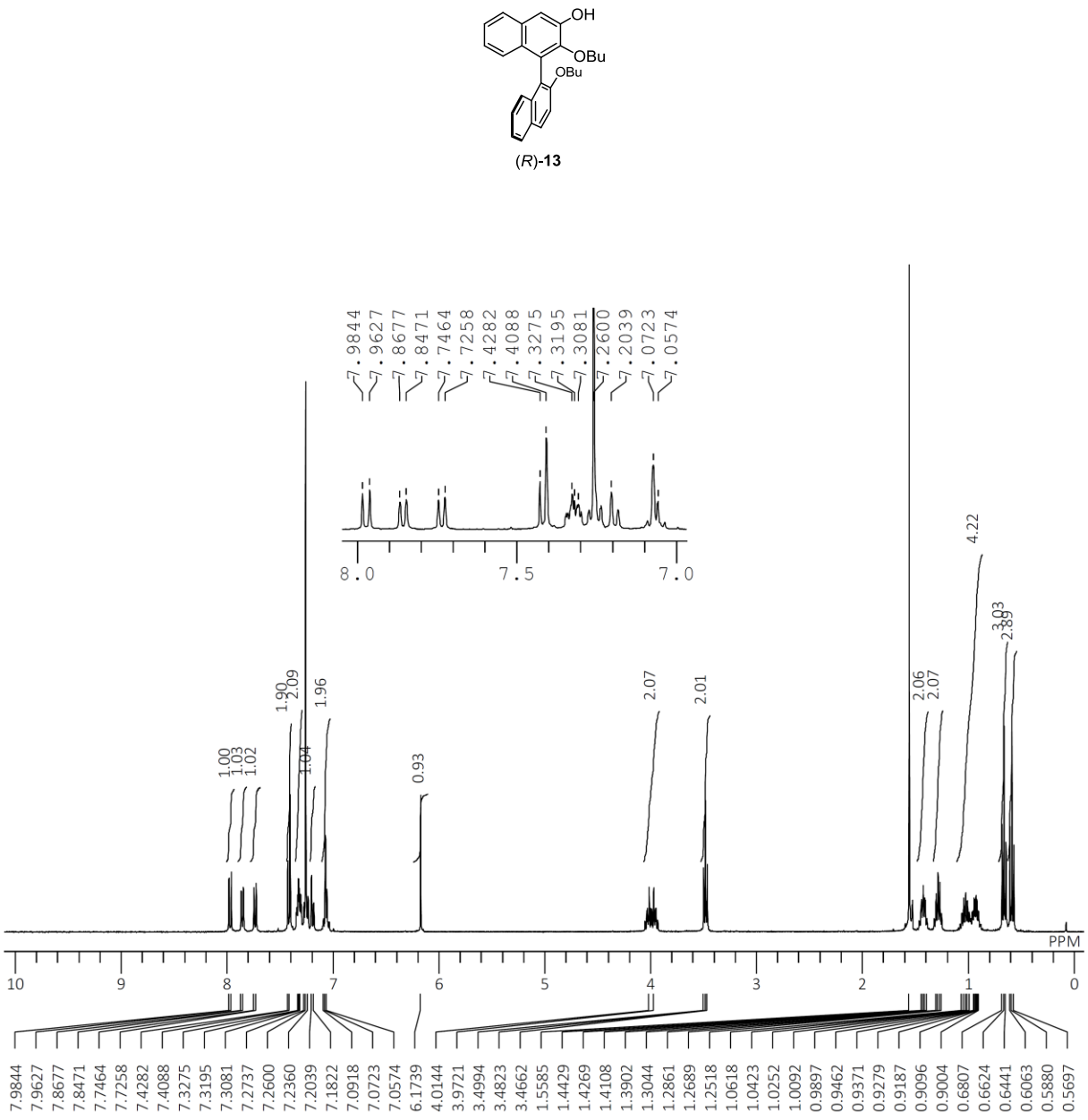
^{1}H NMR spectrum of (*R*)-**12** (400 MHz, $CDCl_3$).



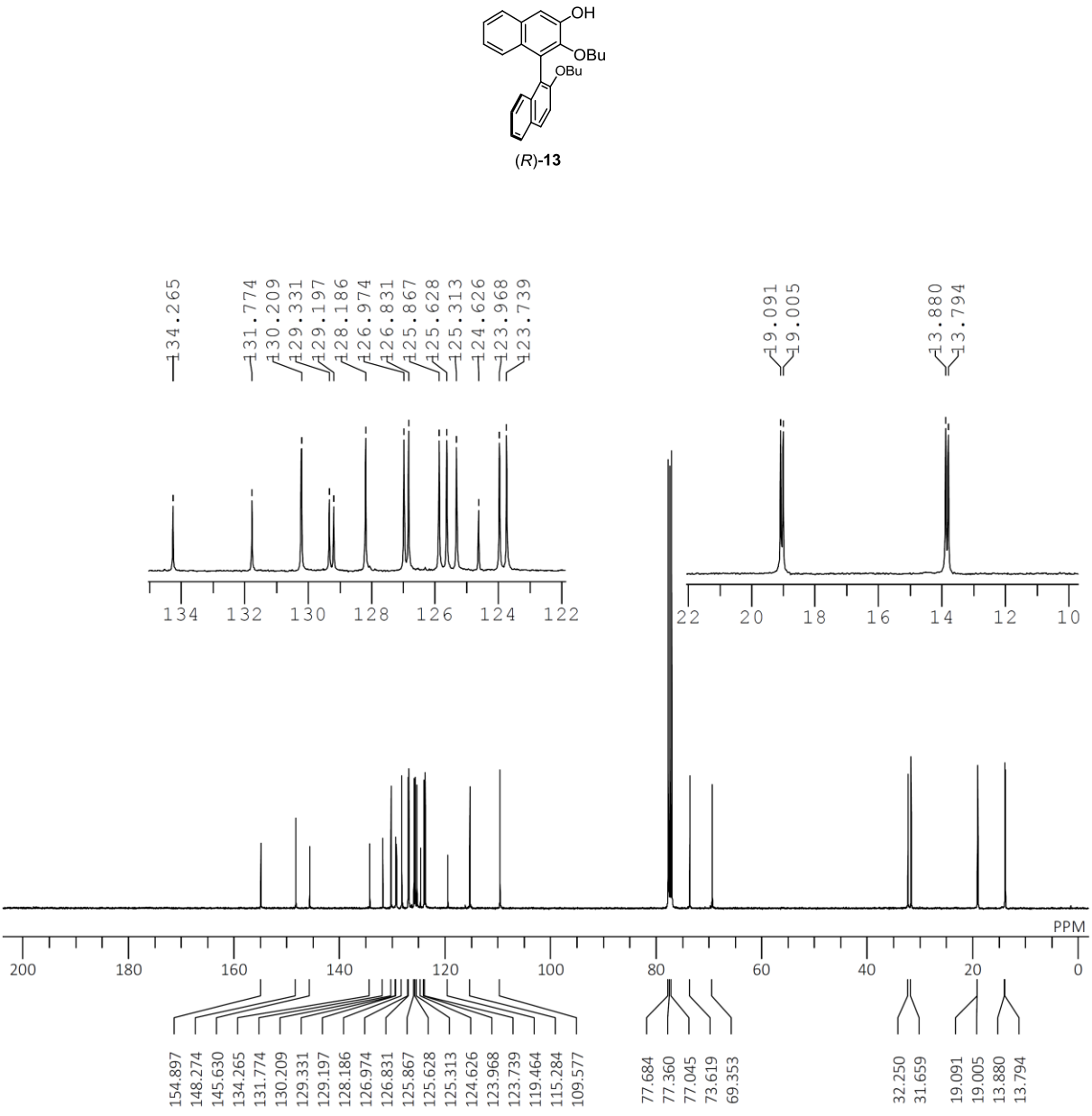
(*R*)-**12**



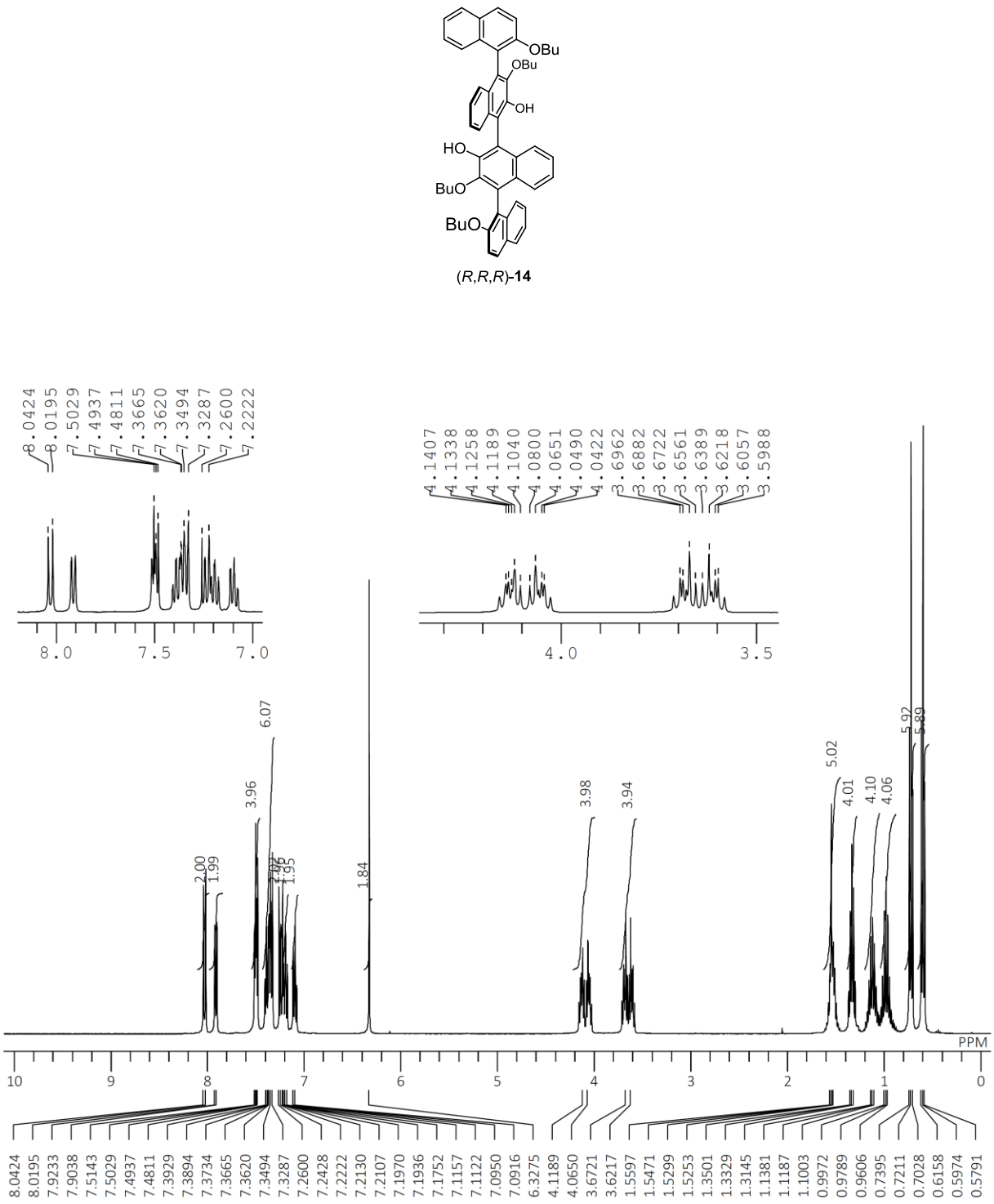
^{13}C NMR spectrum of (*R*)-**12** (100 MHz, $CDCl_3$).



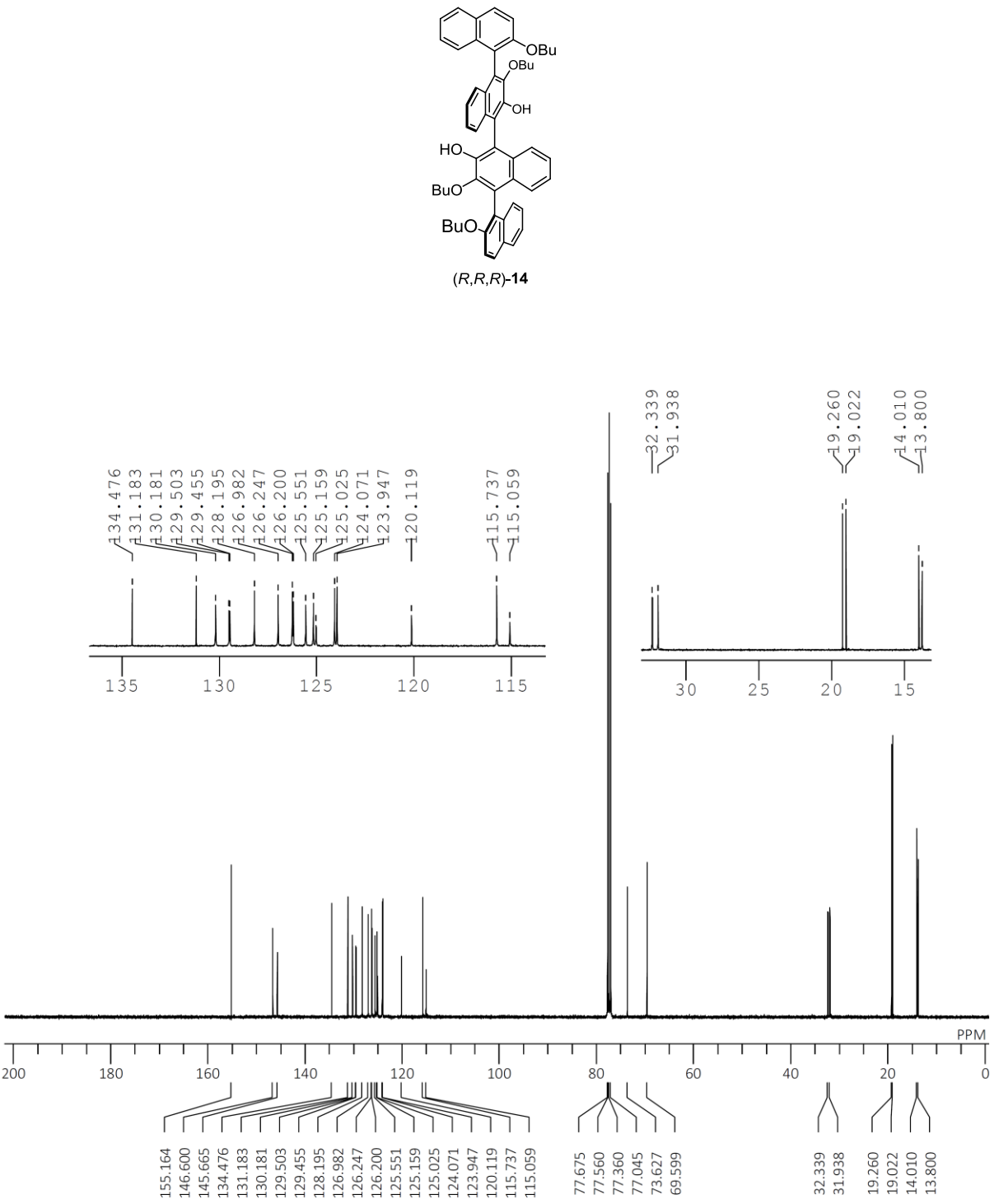
^{1}H NMR spectrum of (*R*)-**13** (400 MHz, $CDCl_3$).



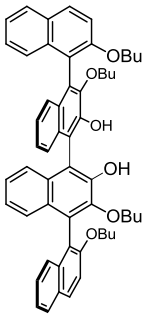
^{13}C NMR spectrum of (*R*)-**13** (100 MHz, $CDCl_3$).



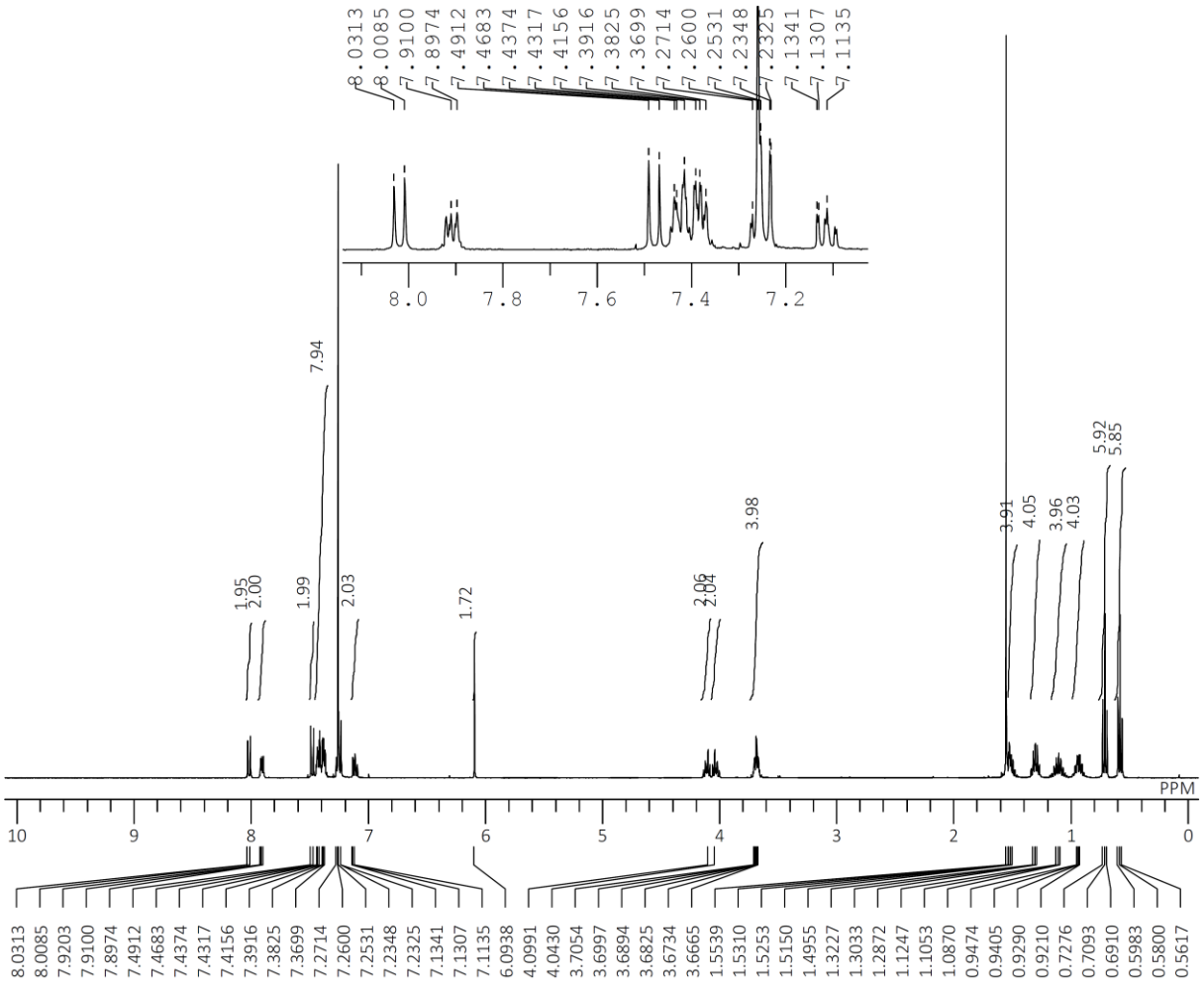
^{1}H NMR spectrum of (*R*,*R*,*R*)-**14** (400 MHz, $CDCl_3$).



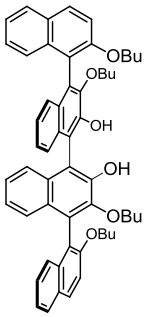
^{13}C NMR spectrum of (*R*,*R*,*R*)-**14** (100 MHz, $CDCl_3$).



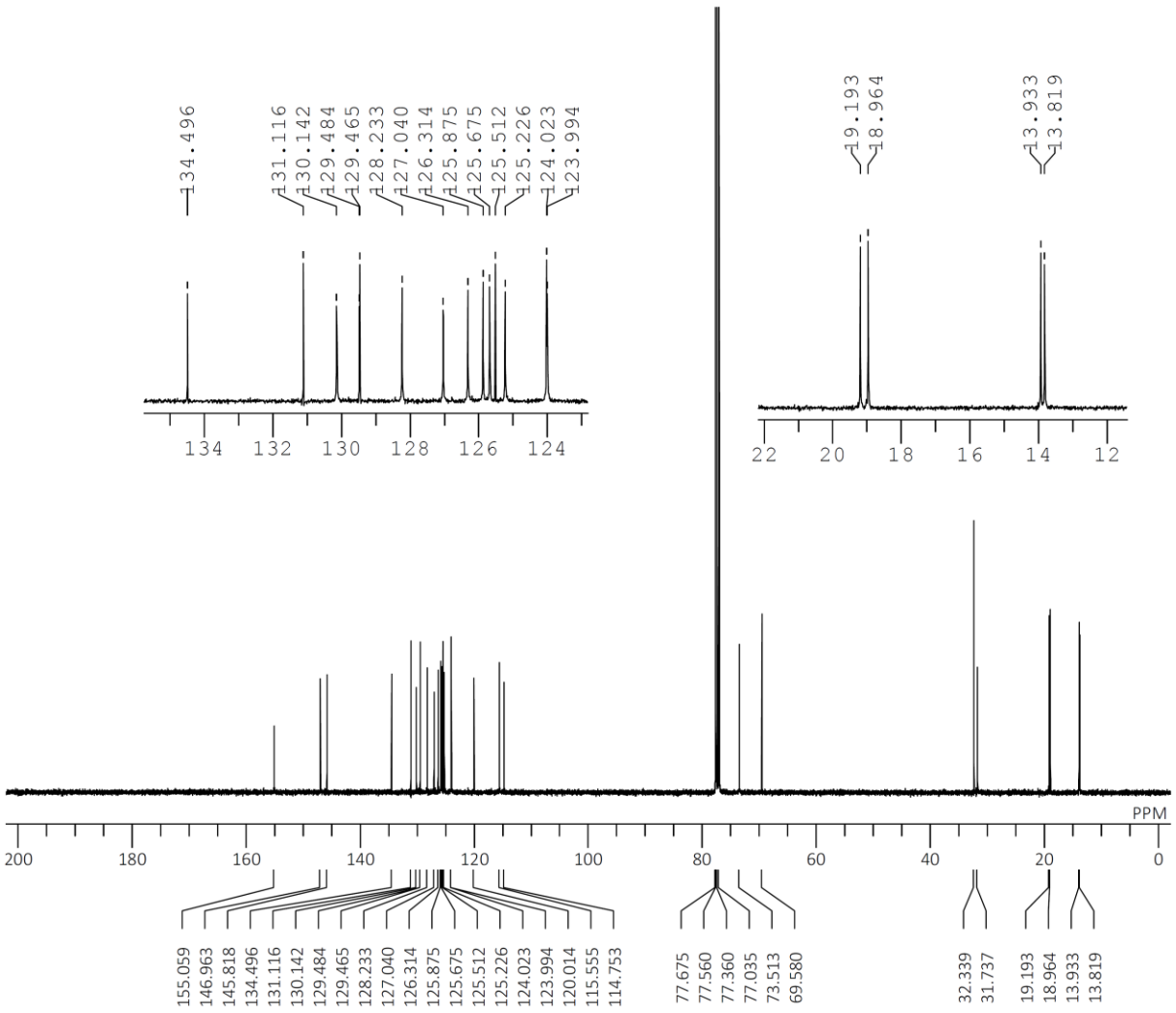
(*R*,*S*,*R*)-**14**



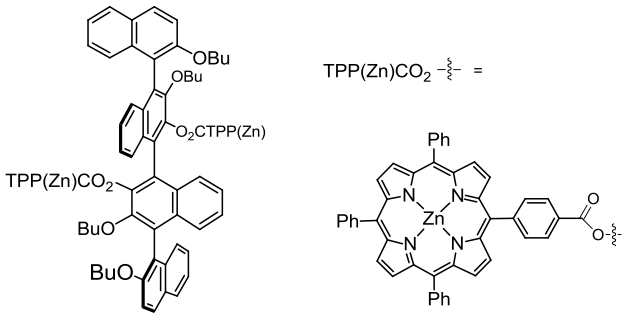
^{1}H NMR spectrum of (*R*,*S*,*R*)-**14** (400 MHz, $CDCl_3$).



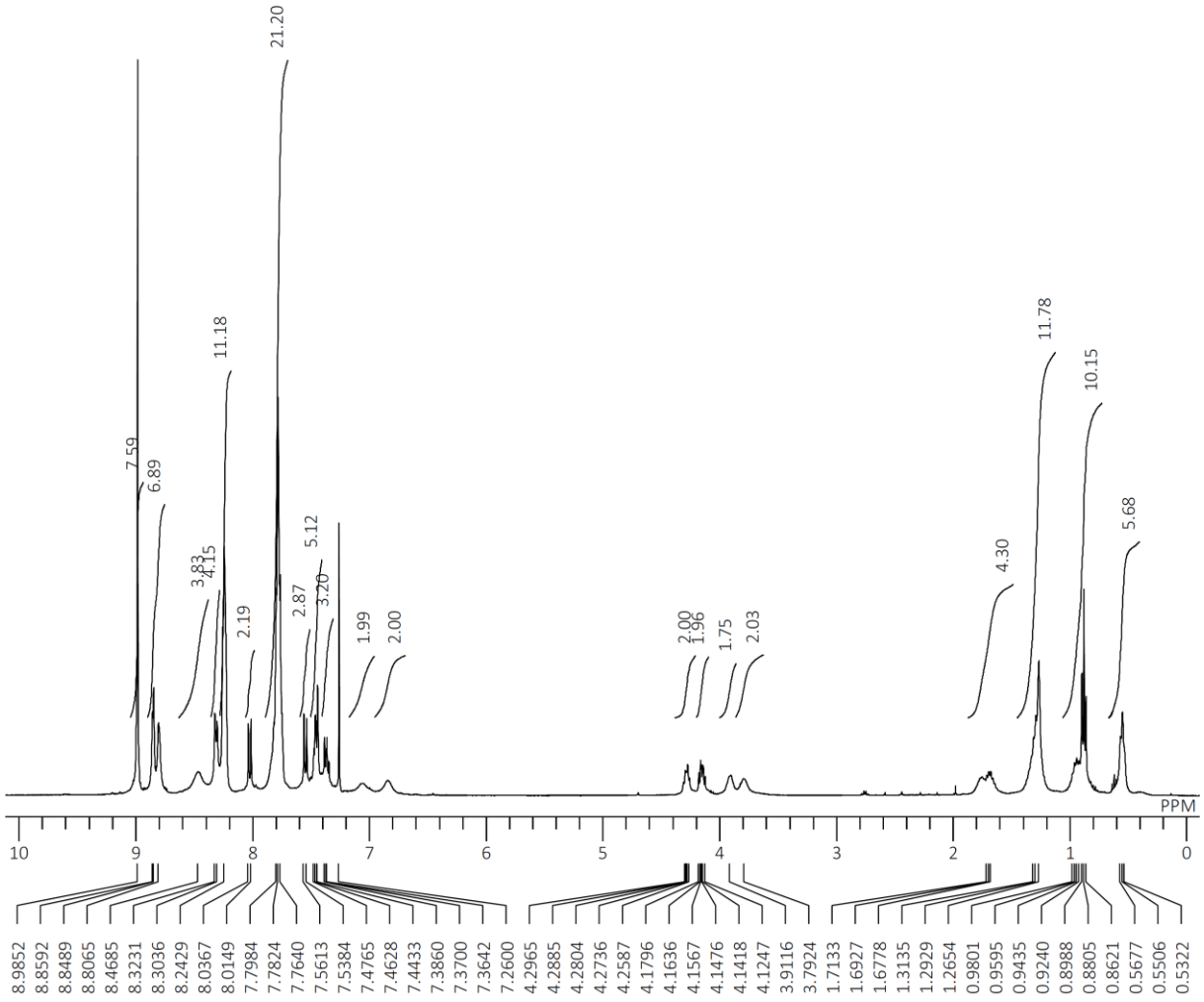
(*R*,*S*,*R*)-**14**



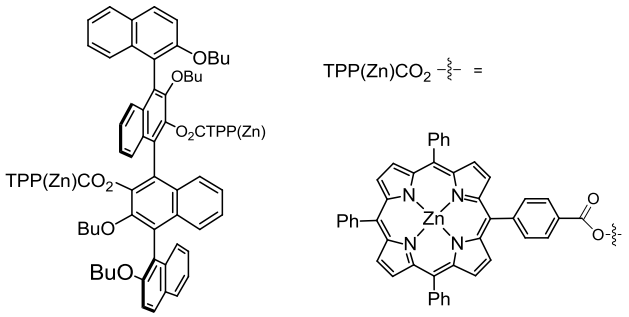
^{13}C NMR spectrum of (*R*,*S*,*R*)-**14** (100 MHz, $CDCl_3$).



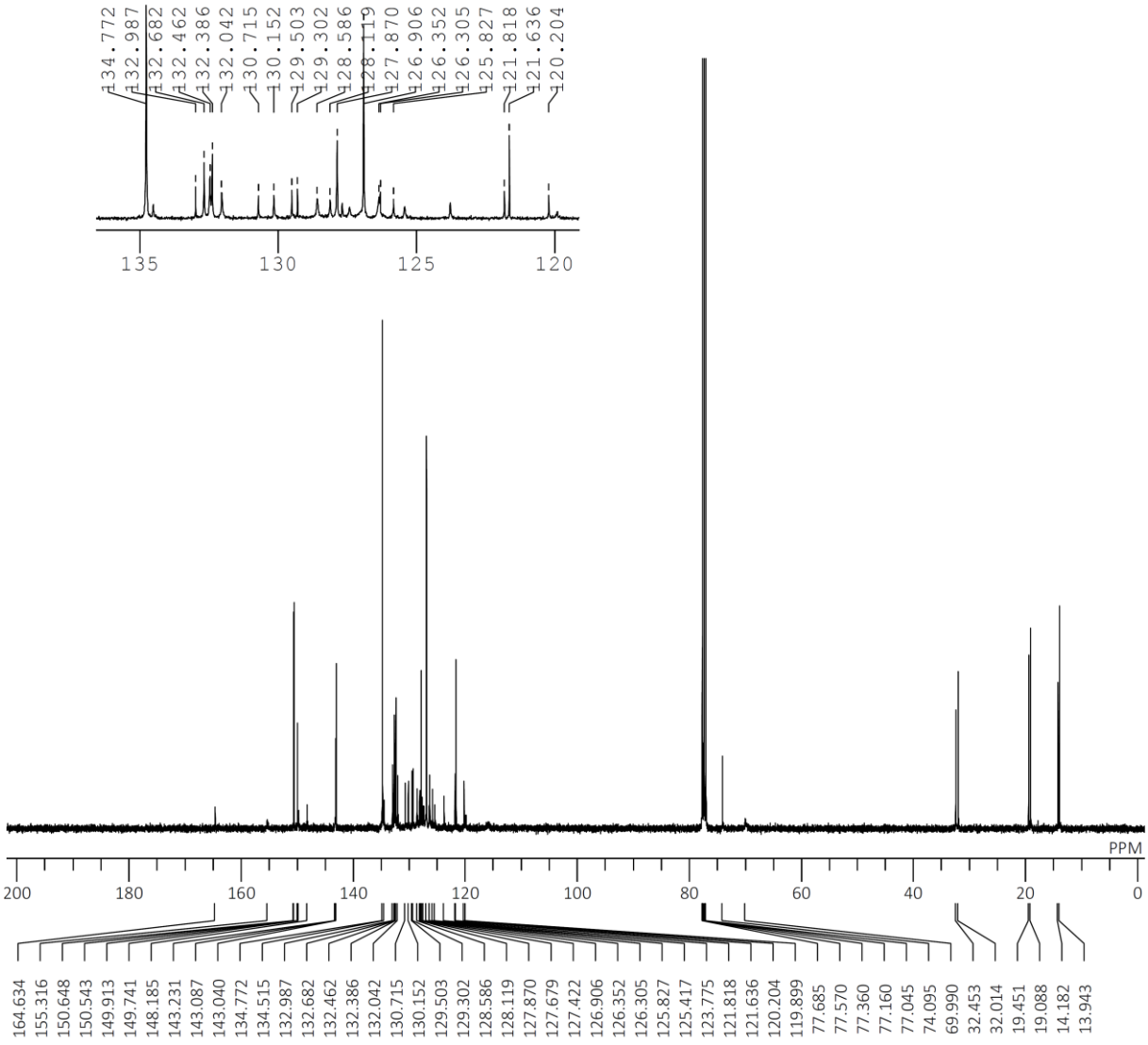
(*R*,*R*,*R*)-**20**



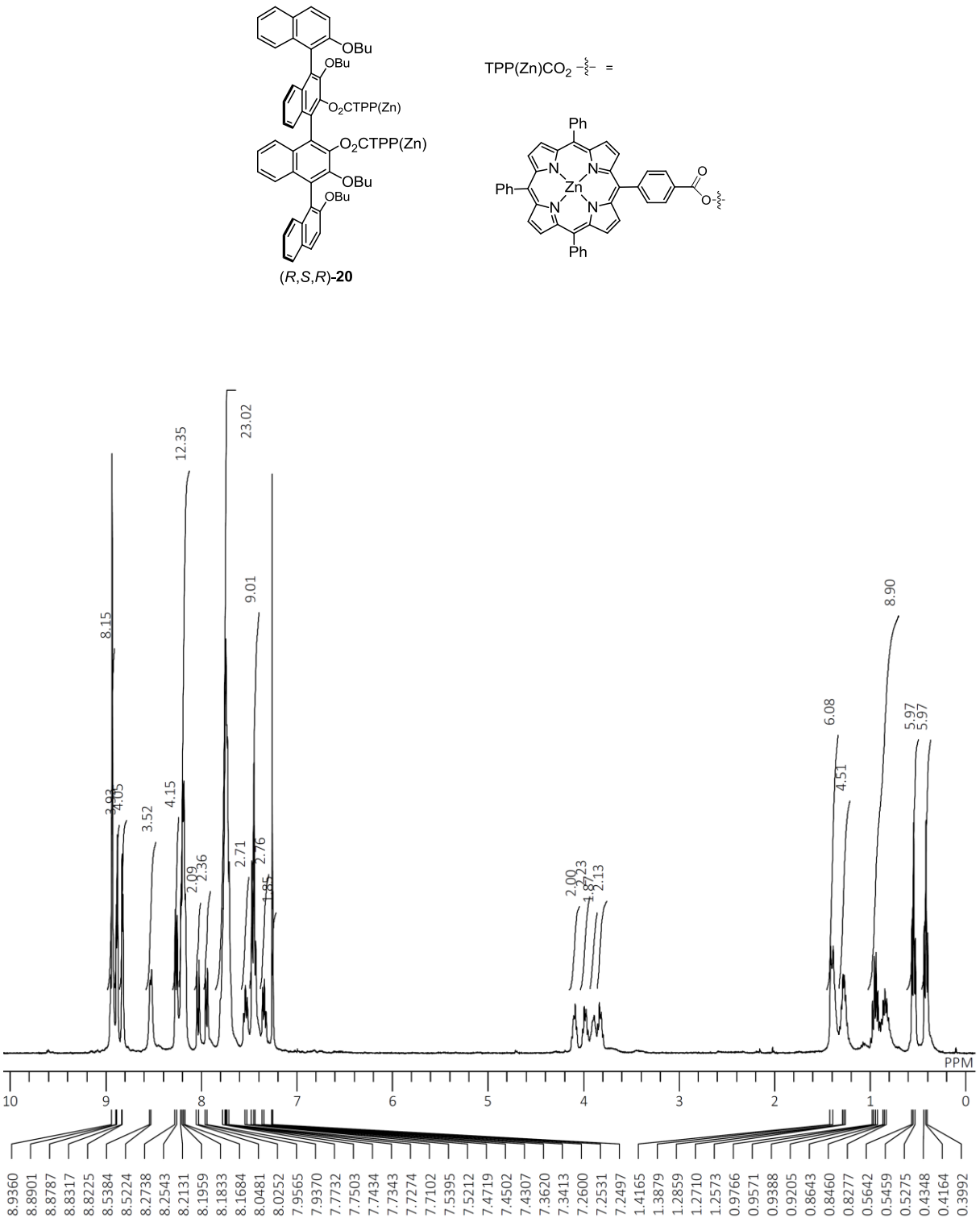
^{1}H NMR spectrum of (*R*,*R*,*R*)-**20** (400 MHz, $CDCl_3$).



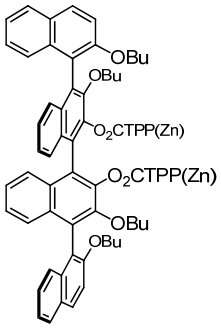
(*R*,*R*,*R*)-**20**



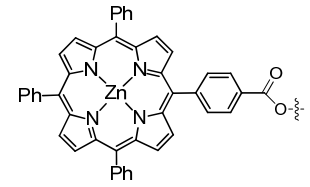
^{13}C NMR spectrum of (*R*,*R*,*R*)-**20** (100 MHz, $CDCl_3$).

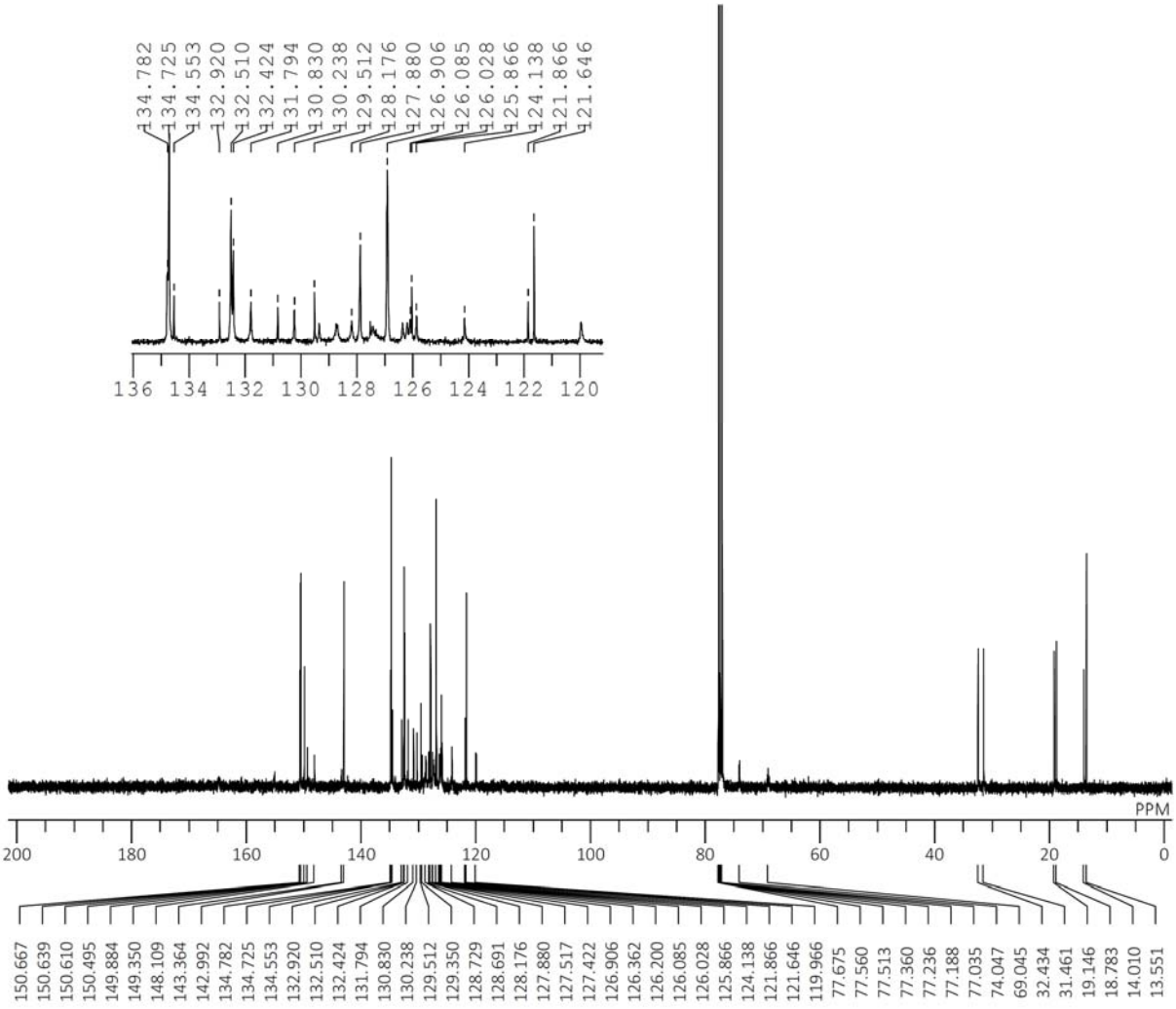


^{1}H NMR spectrum of (*R*,*S*,*R*)-**20** (400 MHz, $CDCl_3$).



(*R*,*S*,*R*)-**20**





^{13}C NMR spectrum of (*R*,*S*,*R*)-**20** (100 MHz, $CDCl_3$).

7. Coordinates of optimized structures.

Coordinates of (*R*,*R*,*R*)-**4** in Figure 2.

–7965.21585914 hartree

C	-0.027740	-3.205889	2.886809
C	-0.215703	-2.329524	1.852470
C	1.604785	0.425272	0.151313
C	1.983078	-1.341552	2.279709
C	0.783593	-1.382213	1.513676
C	0.615537	-0.479452	0.419884
C	0.027826	-3.205713	-2.886859
C	-2.150904	-2.273543	-3.335056
C	-0.783531	-1.382121	-1.513626
C	2.151004	-2.273757	3.335017
C	1.171323	-3.183333	3.629053
C	2.775717	0.490242	0.933583
C	2.985189	-0.368169	1.976955
C	-1.982997	-1.341406	-2.279685
C	-2.985105	-0.368031	-1.976899
C	0.215769	-2.329415	-1.852459
C	-1.171220	-3.183105	-3.629129
C	-2.775653	0.490311	-0.933468
C	-1.604745	0.425282	-0.151168
C	-0.615495	-0.479430	-0.419773
C	-3.590440	2.694178	-0.960892
C	-2.017113	1.081777	2.069962
C	2.017047	1.081914	-2.069797
C	3.590543	2.694096	0.961101
C	-4.739788	3.530778	-0.540851
C	-4.667549	4.943831	-0.526388
C	-5.925622	2.884936	-0.176438
C	-5.827523	5.674950	-0.139551
C	-3.479503	5.690033	-0.856603
C	-7.047994	3.600111	0.187861
C	-5.802940	7.103264	-0.103994
C	-7.023559	4.995625	0.213311
C	-3.463852	7.041500	-0.815206

C	-4.619853	7.803689	-0.444706
C	-6.961140	7.832301	0.273646
C	-8.181593	5.758182	0.590368
C	-4.612176	9.200516	-0.405326
C	-6.912937	9.227830	0.299721
C	-8.152737	7.108204	0.618942
C	-5.748815	9.905200	-0.036855
C	-1.530933	2.007809	3.119074
C	-2.252784	2.220725	4.316329
C	-0.292408	2.625989	2.923948
C	-1.680638	3.068739	5.306724
C	-3.548654	1.649539	4.581350
C	0.263991	3.435762	3.894955
C	-2.373861	3.317440	6.531078
C	-0.411417	3.671139	5.093861
C	-4.202243	1.897265	5.738991
C	-3.643447	2.732366	6.761727
C	-1.797784	4.151020	7.525670
C	0.148632	4.509663	6.118803
C	-4.308275	2.986080	7.964571
C	-2.493870	4.378291	8.714818
C	-0.509925	4.737312	7.276297
C	-3.737960	3.801160	8.931312
C	1.530788	2.008005	-3.118820
C	2.252553	2.221002	-4.316112
C	0.292272	2.626163	-2.923567
C	1.680332	3.069074	-5.306412
C	3.548409	1.649842	-4.581260
C	-0.264202	3.435993	-3.894484
C	2.373467	3.317860	-6.530799
C	0.411121	3.671451	-5.093423
C	4.201915	1.897648	-5.738931
C	3.643042	2.732810	-6.761574
C	1.797315	4.151501	-7.525296
C	-0.149005	4.510038	-6.118271
C	4.307785	2.986609	-7.964448
C	2.493317	4.378856	-8.714477

C	0.509470	4.737767	-7.275796
C	3.737397	3.801748	-8.931095
C	4.739903	3.530693	0.541091
C	4.667694	4.943748	0.526702
C	5.925721	2.884845	0.176637
C	5.827680	5.674862	0.139895
C	3.479666	5.689957	0.856964
C	7.048106	3.600016	-0.187632
C	5.803126	7.103179	0.104412
C	7.023699	4.995531	-0.213011
C	3.464042	7.041427	0.815636
C	4.620056	7.803610	0.445168
C	6.961339	7.832211	-0.273199
C	8.181747	5.758083	-0.590036
C	4.612408	9.200440	0.405861
C	6.913165	9.227743	-0.299200
C	8.152918	7.108107	-0.618540
C	5.749059	9.905119	0.037419
O	-2.614094	3.044629	-1.581358
H	-0.804623	-3.922482	3.132648
H	-1.138858	-2.347757	1.285600
H	0.804711	-3.922294	-3.132725
H	-3.074673	-2.262144	-3.901062
H	3.074786	-2.262400	3.901002
H	1.318239	-3.891165	4.437944
H	1.138911	-2.347689	-1.285569
H	-1.318122	-3.890884	-4.438069
O	-3.755651	1.395455	-0.568819
O	-1.428730	1.348017	0.864212
O	1.428737	1.348078	-0.863996
O	3.755720	1.395390	0.568957
H	0.258019	2.455947	2.008885
O	-2.803794	0.173680	2.201536
O	2.803703	0.173811	-2.201483
O	2.614218	3.044533	1.581607
H	-5.958148	1.803507	-0.193212
H	-2.593640	5.143575	-1.142558

H	-7.960967	3.077788	0.454679
H	-2.553793	7.578583	-1.066042
H	-9.085283	5.217455	0.853565
H	-3.701351	9.730360	-0.667416
H	-7.801802	9.780770	0.588241
H	-9.034308	7.673560	0.905907
H	-5.728271	10.989659	-0.011004
H	-3.991536	1.010066	3.832144
H	1.238540	3.878890	3.718797
H	-5.180229	1.458036	5.912587
H	1.118786	4.960739	5.934125
H	-5.281471	2.535457	8.134605
H	-2.048765	5.015478	9.473099
H	-0.076950	5.373841	8.042213
H	-4.265867	3.988577	9.860496
H	-0.258090	2.456057	-2.008476
H	3.991348	1.010323	-3.832127
H	-1.238742	3.879101	-3.718230
H	5.179893	1.458438	-5.912624
H	-1.119150	4.961095	-5.933496
H	5.280972	2.536005	-8.134578
H	2.048155	5.016089	-9.472686
H	0.076437	5.374343	-8.041641
H	4.265238	3.989231	-9.860303
H	5.958225	1.803414	0.193355
H	2.593793	5.143503	1.142896
H	7.961067	3.077686	-0.454482
H	2.553995	7.578516	1.066507
H	9.085424	5.217351	-0.853267
H	3.701595	9.730289	0.667985
H	7.802039	9.780679	-0.587698
H	9.034499	7.673460	-0.905482
H	5.728537	10.989580	0.011625
C	8.916287	-1.356528	2.367938
C	5.724793	1.137163	5.876321
C	3.273839	1.122209	4.535390
C	4.261613	-0.300075	2.744096

C	4.648333	1.799581	6.400824
C	3.410715	1.793302	5.721136
C	5.363134	-0.942906	2.248090
C	6.608829	-0.923076	2.923501
C	5.617289	0.431058	4.651901
C	4.369080	0.419761	3.972230
C	5.224657	-2.921271	0.971154
C	6.732710	-0.254979	4.107547
C	4.946884	-3.401666	-0.405248
C	5.218278	-4.732855	-0.799117
C	4.366755	-2.506487	-1.308644
C	4.903825	-5.119315	-2.133433
C	5.816008	-5.718907	0.066314
C	4.038606	-2.895030	-2.593000
C	5.183597	-6.445740	-2.585818
C	4.303905	-4.194034	-3.029560
C	6.084443	-6.970242	-0.372455
C	5.782344	-7.385874	-1.711097
C	4.863768	-6.833507	-3.913932
C	3.984934	-4.615901	-4.366488
C	6.051552	-8.678095	-2.170085
C	5.149025	-8.134524	-4.333923
C	4.251840	-5.871164	-4.788094
C	5.738173	-9.047690	-3.469849
C	9.714227	-2.369649	1.627427
C	11.080719	-2.164833	1.317801
C	9.079217	-3.552758	1.233337
C	11.770057	-3.182221	0.595059
C	11.817972	-0.979216	1.677602
C	9.753974	-4.535253	0.538716
C	13.147626	-3.018241	0.250873
C	11.099483	-4.371899	0.205319
C	13.120959	-0.832805	1.346742
C	13.839873	-1.840186	0.624260
C	13.834531	-4.031631	-0.468413
C	11.818190	-5.380867	-0.522606
C	15.186644	-1.694866	0.280756

C	15.180619	-3.848402	-0.792641
C	13.120231	-5.220017	-0.843390
C	15.850207	-2.690465	-0.421082
O	5.271236	-1.555904	1.011503
O	7.589590	-1.667869	2.309829
O	9.328124	-0.382170	2.950498
H	6.681444	1.142024	6.389544
H	2.325457	1.131603	4.011247
H	4.744099	2.334816	7.339863
H	2.561795	2.324357	6.139557
H	3.525652	-3.892365	-5.032931
O	5.382953	-3.587950	1.965862
H	7.681354	-0.230358	4.623960
H	4.152060	-1.492350	-1.001146
H	6.022440	-5.443085	1.090007
H	3.570526	-2.177507	-3.258805
H	6.529706	-7.695871	0.302260
H	6.508962	-9.393631	-1.493370
H	4.902080	-8.426539	-5.350227
H	4.008727	-6.177235	-5.801213
H	5.952226	-10.054687	-3.812414
H	8.038315	-3.698248	1.489081
H	11.304755	-0.206804	2.229598
H	9.232190	-5.439540	0.241605
H	13.651646	0.070866	1.632144
H	11.283226	-6.280439	-0.810515
H	15.709973	-0.788901	0.571279
H	15.700982	-4.626891	-1.342443
H	13.652969	-5.989388	-1.394224
H	16.895991	-2.564133	-0.680954
C	-15.850194	-2.690676	0.420510
C	-13.120136	-5.220134	0.842853
C	-15.180574	-3.848595	0.792067
C	-15.186646	-1.695037	-0.281286
C	-11.818078	-5.380927	0.522107
C	-13.834469	-4.031767	0.467878
C	-13.839859	-1.840299	-0.624751

C	-13.120960	-0.832876	-1.347190
C	-11.099386	-4.371916	-0.205773
C	-13.147580	-3.018336	-0.251367
C	-9.753858	-4.535210	-0.539127
C	-11.817958	-0.979232	-1.678013
C	-11.769994	-3.182257	-0.595512
C	-9.079115	-3.552672	-1.233702
C	-11.080673	-2.164831	-1.318214
C	-9.714163	-2.369584	-1.627793
C	-5.738315	-9.047690	3.469508
C	-4.251819	-5.871273	4.787834
C	-5.149108	-8.134580	4.333602
C	-6.051715	-8.678033	2.169767
C	-3.984873	-4.616005	4.366268
C	-4.863811	-6.833558	3.913652
C	-5.782467	-7.385805	1.710821
C	-6.084586	-6.970110	0.372202
C	-4.303865	-4.194074	3.029365
C	-5.183660	-6.445728	2.585562
C	-4.038523	-2.895065	2.592847
C	-5.816115	-5.718768	-0.066526
C	-4.903848	-5.119296	2.133219
C	-4.366694	-2.506460	1.308516
C	-5.218322	-4.732773	0.798927
C	-4.946888	-3.401579	0.405103
C	-6.732566	-0.254638	-4.107589
C	-5.224680	-2.921116	-0.971273
C	-4.368917	0.420030	-3.972177
C	-5.617108	0.431391	-4.651879
C	-6.608737	-0.922795	-2.923569
C	-5.363056	-0.942691	-2.248130
C	-3.410470	1.793630	-5.720990
C	-4.648070	1.799973	-6.400711
C	-4.261505	-0.299869	-2.744075
C	-3.273643	1.122477	-4.535273
C	-5.724561	1.137557	-5.876268
C	-8.916243	-1.356421	-2.368269

H	-9.232049	-5.439483	-0.242018
H	-16.895991	-2.564388	0.680352
H	-13.652862	-5.989536	1.393654
H	-15.700925	-4.627114	1.341836
H	-15.710001	-0.789086	-0.571807
H	-11.283089	-6.280485	0.810016
H	-13.651672	0.070782	-1.632588
H	-6.529896	-7.695695	-0.302528
H	-11.304755	-0.206792	-2.229983
H	-8.038198	-3.698113	-1.489413
H	-5.952399	-10.054691	3.812041
H	-4.008691	-6.177392	5.800934
H	-4.902147	-8.426643	5.349888
H	-6.509171	-9.393525	1.493038
H	-3.570389	-2.177589	3.258665
H	-6.022563	-5.442899	-1.090202
H	-4.151959	-1.492322	1.001049
H	-7.681193	-0.229962	-4.624027
O	-5.383026	-3.587747	-1.966006
H	-3.525543	-3.892513	5.032726
H	-2.561525	2.324684	-6.139362
H	-4.743797	2.335256	-7.339727
H	-2.325275	1.131823	-4.011102
H	-6.681198	1.142466	-6.389517
O	-9.328128	-0.382173	-2.950978
O	-7.589518	-1.667586	-2.309927
O	-5.271204	-1.555746	-1.011566

Coordinates of methyl 1-pyrenecarboxylate in Figure 2.

–843.64883371 hartree

C	-4.405790	-1.316124	-0.000218
C	-3.271030	-2.123424	-0.000192
C	-1.985636	-1.556983	-0.000141
C	-1.845278	-0.138278	-0.000114
C	-3.016265	0.681110	-0.000140
C	-4.281267	0.071714	-0.000192
C	-0.795394	-2.353279	-0.000111

C	-0.544797	0.456164	-0.000059
C	0.631279	-0.366979	-0.000036
C	0.447548	-1.795874	-0.000063
C	1.905795	0.270892	0.000027
C	1.978592	1.674659	0.000068
C	0.841063	2.463823	0.000035
C	-0.435021	1.880844	-0.000027
C	-1.627326	2.680291	-0.000058
C	-2.861711	2.107922	-0.000112
H	-3.755962	2.725502	-0.000135
H	-1.520041	3.761518	-0.000034
H	-0.899520	-3.435327	-0.000129
H	-5.392359	-1.769837	-0.000258
H	-3.370221	-3.205526	-0.000212
H	-5.168579	0.699061	-0.000213
H	1.327923	-2.421198	-0.000055
H	2.954336	2.142602	0.000119
H	0.931479	3.546412	0.000058
C	3.182597	-0.501352	0.000048
O	3.307237	-1.713613	-0.000108
O	4.268705	0.315688	0.000508
C	5.535646	-0.356043	0.000585
H	6.285694	0.434812	0.000501
H	5.640841	-0.984441	0.888402
H	5.640841	-0.984675	-0.887058

Coordinates of **8** in Figure 4.

–1991.08138919 hartree

C	8.907647	-0.705545	0.015416
C	6.485465	-0.709518	0.018334
C	6.485497	0.712151	-0.020084
C	7.725518	-1.395840	0.035241
C	8.907712	0.707741	-0.021760
C	4.067317	0.710806	-0.008530
C	4.066990	-0.708388	0.010266
C	5.245078	1.397261	-0.032577
C	7.725599	1.398244	-0.039230

H	9.851262	-1.242055	0.028136
H	7.720723	-2.481842	0.063355
H	9.851392	1.244070	-0.036363
H	5.217453	2.481410	-0.061735
H	7.720828	2.484223	-0.067227
C	1.867302	1.192443	0.785899
C	0.577192	1.563044	0.184550
C	-0.670267	1.453386	0.888497
C	0.576027	2.042556	-1.140215
C	-1.875454	1.778352	0.195944
C	-0.776249	1.013446	2.236318
C	-0.586140	2.392448	-1.779715
C	-3.140329	1.592324	0.821808
C	-1.840972	2.264893	-1.140820
C	-1.999033	0.848126	2.837648
C	-3.209528	1.102665	2.151940
C	-4.343511	1.864448	0.110566
C	-3.047033	2.580712	-1.807430
C	-4.475394	0.870073	2.737622
C	-5.581592	1.599741	0.729871
C	-4.263712	2.375982	-1.212578
C	-5.639565	1.121755	2.035424
O	2.090269	0.753218	1.894077
O	2.883752	1.395903	-0.127437
H	1.517259	2.116473	-1.664582
H	0.133883	0.796652	2.776311
H	-0.552267	2.761694	-2.800733
H	-2.047244	0.499556	3.865644
H	-2.991187	2.967748	-2.821061
H	-4.518470	0.500700	3.758142
H	-6.495956	1.811817	0.184296
H	-5.183511	2.604358	-1.741647
H	-6.603402	0.941210	2.501155
C	1.870334	-1.209964	-0.780966
C	0.576901	-1.561870	-0.176744
C	-0.666183	-1.467581	-0.886249
C	0.568731	-2.002367	1.161250

C	-1.875163	-1.771899	-0.190571
C	-0.766158	-1.057836	-2.244809
C	-0.596667	-2.332315	1.805724
C	-3.135838	-1.598248	-0.825654
C	-1.847852	-2.220485	1.159343
C	-1.986184	-0.902835	-2.854424
C	-3.198812	-1.138785	-2.167403
C	-4.342462	-1.849492	-0.113652
C	-3.057962	-2.516362	1.828675
C	-4.461612	-0.914985	-2.762777
C	-5.576508	-1.597712	-0.744182
C	-4.270284	-2.326649	1.222511
C	-5.628724	-1.149216	-2.060382
O	2.884815	-1.396317	0.138022
O	2.097493	-0.799070	-1.898726
H	1.509249	-2.066506	1.688956
H	0.146173	-0.858347	-2.787463
H	-0.567614	-2.674857	2.836216
H	-2.028970	-0.578334	-3.890384
H	-3.008670	-2.878082	2.851828
H	-4.499804	-0.568139	-3.791248
H	-6.493262	-1.795502	-0.197421
H	-5.192522	-2.540916	1.752961
H	-6.590275	-0.977501	-2.534001
C	5.245259	-1.394534	0.033768
H	5.218003	-2.478752	0.064209

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3a.

–7965.20632507 hartree

C	-0.175648	-1.826807	-3.164107
C	0.010553	-1.044300	-2.046580
C	-1.939126	1.297055	0.105593
C	-2.334552	-0.317103	-2.155816
C	-1.053667	-0.268546	-1.510895
C	-0.869218	0.569018	-0.360170
C	-0.128045	-1.427277	3.412695
C	2.155761	-0.632165	3.445897

C	0.677006	-0.047216	1.574692
C	-2.489814	-1.137145	-3.306114
C	-1.436812	-1.875068	-3.797917
C	-3.216471	1.208784	-0.500291
C	-3.427812	0.445296	-1.624809
C	1.964372	0.029812	2.202915
C	3.027950	0.751972	1.565769
C	-0.351500	-0.793593	2.211060
C	1.136283	-1.344320	4.036625
C	2.773381	1.381127	0.369267
C	1.483997	1.359839	-0.217819
C	0.449636	0.642342	0.337586
C	4.312098	1.554059	-1.411015
C	1.235813	3.409516	-1.374767
C	-1.732061	3.468573	1.006401
C	-4.791551	1.568866	1.225491
C	5.257729	2.498597	-2.057147
C	6.187112	2.066715	-3.045519
C	5.194093	3.856096	-1.699336
C	7.031123	3.048798	-3.660499
C	6.346314	0.693868	-3.448168
C	6.008242	4.800432	-2.302406
C	7.978595	2.663560	-4.658975
C	6.934150	4.424887	-3.287310
C	7.255031	0.334572	-4.397084
C	8.098326	1.295595	-5.043316
C	8.812938	3.643251	-5.280352
C	7.784739	5.388028	-3.927699
C	9.033310	0.937165	-6.028521
C	9.733109	3.239069	-6.260747
C	8.682107	5.015828	-4.880417
C	9.840651	1.899561	-6.629890
C	0.941386	3.972434	-2.717948
C	1.081443	5.362695	-2.996814
C	0.499998	3.098255	-3.726084
C	0.772659	5.826756	-4.318392
C	1.535297	6.334273	-2.034652

C	0.188227	3.555726	-4.995357
C	0.915453	7.209478	-4.652761
C	0.318650	4.914112	-5.320186
C	1.672287	7.649904	-2.363165
C	1.371133	8.141220	-3.674438
C	0.606675	7.671354	-5.969583
C	0.010612	5.406026	-6.633339
C	1.510151	9.495059	-4.022544
C	0.759642	9.033628	-6.272812
C	0.148507	6.723165	-6.945116
C	1.207359	9.934817	-5.308679
C	-1.649536	4.206010	2.292430
C	-1.303406	5.586843	2.342831
C	-1.946831	3.514494	3.479641
C	-1.283640	6.236767	3.620862
C	-0.948916	6.366601	1.185703
C	-1.928924	4.149710	4.709914
C	-0.945096	7.621925	3.722173
C	-1.603427	5.510781	4.809567
C	-0.623742	7.685193	1.291601
C	-0.614882	8.366431	2.551687
C	-0.933664	8.272521	4.994481
C	-1.583083	6.188994	6.074722
C	-0.288024	9.727468	2.671191
C	-0.600963	9.634678	5.066093
C	-1.264061	7.508726	6.164162
C	-0.282305	10.353271	3.915362
C	-5.884370	2.479590	1.653676
C	-6.477720	2.385376	2.946273
C	-6.340784	3.450557	0.745602
C	-7.533321	3.297333	3.279894
C	-6.070033	1.437175	3.951281
C	-7.366143	4.321804	1.071444
C	-8.153587	3.248951	4.567258
C	-7.980550	4.268141	2.331234
C	-6.663169	1.401575	5.177886
C	-7.722745	2.295842	5.536138

C	-9.208361	4.154943	4.897328
C	-9.043077	5.164955	2.688434
C	-8.341979	2.264635	6.796710
C	-9.799729	4.086699	6.168863
C	-9.631085	5.111572	3.914160
C	-9.369792	3.151029	7.107946
O	3.993154	0.447929	-1.788581
H	0.652673	-2.407850	-3.558078
H	0.984118	-1.006124	-1.571344
H	-0.929388	-1.989200	3.882942
H	3.124460	-0.568260	3.928240
H	-3.458409	-1.185483	-3.790689
H	-1.578243	-2.497351	-4.676587
H	-1.328346	-0.848914	1.744301
H	1.305220	-1.842278	4.986847
O	3.774302	2.104215	-0.259327
O	1.284519	2.027755	-1.417951
O	-1.790801	2.101977	1.224190
O	-4.252148	1.972907	0.017377
H	0.398312	2.045514	-3.497018
O	1.424479	4.014293	-0.340989
O	-1.759875	3.926671	-0.115045
O	-4.369343	0.590026	1.803766
H	4.479337	4.164006	-0.946679
H	5.726141	-0.054729	-2.978426
H	5.928786	5.845313	-2.016842
H	7.351963	-0.711490	-4.676138
H	7.694284	6.429383	-3.631187
H	9.119370	-0.106650	-6.318399
H	10.364805	3.987316	-6.731967
H	9.319293	5.756356	-5.356659
H	10.557979	1.605199	-7.390301
H	1.758337	5.997691	-1.032781
H	-0.158433	2.857726	-5.751811
H	2.022858	8.357079	-1.615422
H	-0.334789	4.695137	-7.378792
H	1.859307	10.199476	-3.272278

H	0.523981	9.380268	-7.275404
H	-0.085847	7.080756	-7.944253
H	1.320187	10.984755	-5.561944
H	-2.204697	2.464729	3.421917
H	-0.943167	5.880917	0.221575
H	-2.172306	3.592898	5.610127
H	-0.356710	8.243669	0.398118
H	-1.830571	5.618999	6.965954
H	-0.038390	10.290163	1.775630
H	-0.594793	10.126019	6.035368
H	-1.253088	8.008928	7.128964
H	-0.027795	11.406399	3.989758
H	-5.879670	3.509816	-0.231502
H	-5.279800	0.742214	3.708778
H	-7.701473	5.057641	0.346352
H	-6.327104	0.677924	5.916501
H	-9.367889	5.893890	1.951192
H	-8.007630	1.536260	7.530674
H	-10.601959	4.777251	6.414693
H	-10.433987	5.797472	4.170952
H	-9.838616	3.113581	8.086744
C	-7.390123	-2.927084	-3.187770
C	-6.793973	2.597022	-4.642971
C	-4.305102	2.680782	-3.352899
C	-4.761294	0.456156	-2.299304
C	-5.959933	3.677233	-4.819491
C	-4.705872	3.717397	-4.167026
C	-5.630276	-0.601242	-2.137756
C	-6.872295	-0.644585	-2.820886
C	-6.413523	1.512330	-3.809420
C	-5.142428	1.550213	-3.147572
C	-5.891470	-1.835439	-0.134022
C	-7.259266	0.386520	-3.631389
C	-5.443748	-3.078164	0.544688
C	-5.709134	-3.312233	1.924312
C	-4.764474	-4.047881	-0.212814
C	-5.276485	-4.552371	2.499556

C	-6.368591	-2.365064	2.785058
C	-4.355373	-5.246231	0.348114
C	-5.519171	-4.832486	3.880187
C	-4.599473	-5.525455	1.701300
C	-6.592552	-2.638446	4.100640
C	-6.187153	-3.875115	4.699092
C	-5.095128	-6.071336	4.452516
C	-4.185101	-6.761959	2.301867
C	-6.418248	-4.169225	6.053155
C	-5.347627	-6.322488	5.810635
C	-4.421639	-7.023963	3.616026
C	-6.002730	-5.380215	6.601264
C	-8.336292	-3.992329	-2.764230
C	-8.415615	-5.240684	-3.445988
C	-9.157283	-3.750039	-1.648881
C	-9.350352	-6.218264	-2.969097
C	-7.624096	-5.575659	-4.601330
C	-10.048664	-4.703516	-1.186583
C	-9.474173	-7.481466	-3.626420
C	-10.168627	-5.944701	-1.829705
C	-7.750722	-6.780927	-5.223656
C	-8.671224	-7.778557	-4.766487
C	-10.402582	-8.457385	-3.149049
C	-11.091363	-6.943910	-1.370222
C	-8.806878	-9.025188	-5.399637
C	-10.504498	-9.690145	-3.813104
C	-11.204259	-8.144697	-2.000103
C	-9.714453	-9.969604	-4.926625
O	-5.255626	-1.682853	-1.354680
O	-7.728574	-1.716934	-2.613262
O	-6.436204	-3.032037	-3.928889
H	-7.759170	2.556518	-5.140685
H	-3.344469	2.728101	-2.852459
H	-6.262548	4.500928	-5.459343
H	-4.051833	4.572561	-4.307531
H	-3.673639	-7.489283	1.677419
O	-6.706474	-1.028134	0.255099

H	-8.217051	0.333820	-4.138695
H	-4.571013	-3.851561	-1.259771
H	-6.685491	-1.422240	2.365266
H	-3.841772	-5.982569	-0.263263
H	-7.089628	-1.898944	4.723148
H	-6.928536	-3.436019	6.671987
H	-5.024649	-7.266381	6.241497
H	-4.101920	-7.964601	4.056649
H	-6.189615	-5.591609	7.649935
H	-9.072674	-2.800674	-1.135444
H	-6.912983	-4.847242	-4.963012
H	-10.662252	-4.493635	-0.315323
H	-7.139195	-7.004129	-6.094175
H	-11.702479	-6.716670	-0.501186
H	-8.191851	-9.245118	-6.268064
H	-11.211313	-10.429613	-3.446490
H	-11.907720	-8.891275	-1.641207
H	-9.807412	-10.928516	-5.427634
C	12.319662	-7.722208	5.847956
C	11.765541	-7.086153	2.187299
C	12.382727	-7.862883	4.462924
C	11.591571	-6.679851	6.415853
C	11.113170	-6.203395	1.383245
C	11.717441	-6.961753	3.616367
C	10.910607	-5.754751	5.607266
C	10.150333	-4.671306	6.153441
C	10.353913	-5.115675	1.931909
C	10.968201	-5.887783	4.189049
C	9.678103	-4.202750	1.108494
C	9.493534	-3.777999	5.361820
C	10.281329	-4.955758	3.350225
C	8.947677	-3.162100	1.655872
C	9.529677	-3.877041	3.925402
C	8.856177	-2.977593	3.047366
C	6.901142	-6.780365	-5.215697
C	3.907594	-7.139837	-2.974271
C	5.733235	-7.288675	-4.650243

C	7.470322	-5.610392	-4.719435
C	3.319895	-6.494560	-1.930577
C	5.110273	-6.635865	-3.574571
C	6.880602	-4.923584	-3.645394
C	7.433238	-3.715925	-3.109225
C	3.877664	-5.286708	-1.390746
C	5.685698	-5.433906	-3.058088
C	3.279896	-4.618931	-0.311698
C	6.850527	-3.052764	-2.070535
C	5.071638	-4.748971	-1.963323
C	3.835487	-3.457259	0.198216
C	5.644458	-3.538788	-1.448771
C	5.003741	-2.899587	-0.348262
C	6.912220	0.962294	3.466752
C	5.529496	-1.638124	0.238308
C	4.742965	2.020811	2.953346
C	6.026333	2.063586	3.589208
C	6.542704	-0.141283	2.741519
C	5.276849	-0.184425	2.096856
C	4.259950	4.239811	3.827354
C	5.525770	4.279716	4.457517
C	4.378465	0.857254	2.198643
C	3.876626	3.138801	3.094275
C	6.388385	3.214601	4.339054
C	8.051449	-1.835420	3.560123
H	9.724393	-4.319295	0.029623
H	12.840654	-8.429042	6.486826
H	12.336277	-7.905321	1.757978
H	12.951551	-8.677603	4.022946
H	11.542969	-6.571902	7.496016
H	11.153623	-6.306197	0.302441
H	10.103133	-4.568202	7.234530
H	8.344500	-3.323306	-3.553853
H	8.932589	-2.968162	5.804065
H	8.435295	-2.468738	1.001775
H	7.368693	-7.299051	-6.047304
H	3.473910	-8.053491	-3.372003

H	5.291204	-8.201605	-5.040127
H	8.380445	-5.215061	-5.162545
H	2.370661	-5.020716	0.125951
H	7.281521	-2.132542	-1.704307
H	3.358691	-2.957332	1.031253
H	7.874662	0.989316	3.961270
O	6.396378	-0.920335	-0.212917
H	2.410434	-6.884342	-1.481847
H	3.584696	5.084990	3.920566
H	5.814801	5.153713	5.033785
H	2.908692	3.124397	2.605799
H	7.362883	3.235711	4.819249
O	7.974389	-1.439276	4.703514
O	7.357458	-1.238117	2.528513
O	4.897171	-1.341405	1.427494

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3b.

–7965.21672663 hartree

C	-0.401171	-2.775868	3.456895
C	-0.482069	-1.988292	2.331290
C	1.682672	0.313420	0.346932
C	1.842051	-1.258900	2.667340
C	0.631729	-1.219479	1.896546
C	0.575470	-0.423081	0.707588
C	-0.362981	-3.429454	-2.274580
C	-2.424798	-2.297073	-2.845594
C	-0.937496	-1.361909	-1.127024
C	1.893475	-2.094742	3.815964
C	0.799867	-2.837189	4.199146
C	2.857276	0.313519	1.134277
C	2.961138	-0.457913	2.271090
C	-2.138291	-1.267851	-1.907700
C	-3.013305	-0.146201	-1.733612
C	-0.060214	-2.458092	-1.347928
C	-1.560153	-3.353393	-3.021410
C	-2.691936	0.803894	-0.789575
C	-1.534819	0.684892	0.015056

C	-0.654501	-0.362899	-0.140524
C	-3.222325	3.097402	-1.072992
C	-1.883887	1.656643	2.151196
C	2.205160	0.671866	-1.938789
C	3.965949	2.401813	0.964382
C	-4.270068	4.105369	-0.769010
C	-4.040745	5.501688	-0.936155
C	-5.525914	3.650372	-0.330265
C	-5.117964	6.406581	-0.657289
C	-2.780670	6.065057	-1.345975
C	-6.563285	4.529276	-0.069636
C	-4.936021	7.816401	-0.808138
C	-6.388119	5.912551	-0.227142
C	-2.613817	7.410332	-1.481129
C	-3.676305	8.336297	-1.226783
C	-6.012042	8.717562	-0.539761
C	-7.451997	6.840017	0.034802
C	-3.516248	9.724521	-1.370129
C	-5.807330	10.097571	-0.697586
C	-7.273630	8.180624	-0.115193
C	-4.571836	10.594334	-1.108512
C	-1.316932	2.671270	3.074031
C	-2.032342	3.123860	4.218785
C	-0.016507	3.142122	2.825284
C	-1.389237	4.056861	5.096629
C	-3.378377	2.722039	4.532961
C	0.606189	4.030886	3.687427
C	-2.069956	4.546272	6.254113
C	-0.057691	4.504491	4.829351
C	-4.023567	3.199228	5.633754
C	-3.400754	4.119653	6.537753
C	-1.425171	5.467056	7.136728
C	0.566622	5.428422	5.734865
C	-4.053767	4.612281	7.679810
C	-2.115836	5.932004	8.267073
C	-0.085578	5.888186	6.837288
C	-3.416553	5.508557	8.534135

C	1.892310	1.571539	-3.076835
C	2.669228	1.565909	-4.269981
C	0.761454	2.399690	-2.977352
C	2.259574	2.412803	-5.351368
C	3.861942	0.779433	-4.445317
C	0.362529	3.205074	-4.032231
C	3.009301	2.443990	-6.567838
C	1.093131	3.230744	-5.230051
C	4.576051	0.820959	-5.604695
C	4.180079	1.642400	-6.709553
C	2.593584	3.277056	-7.652025
C	0.698190	4.057672	-6.336004
C	4.903226	1.685868	-7.913172
C	3.346338	3.287357	-8.837055
C	1.413815	4.079738	-7.493417
C	4.489005	2.499688	-8.964529
C	5.254724	3.009305	0.550613
C	5.382655	4.409982	0.326983
C	6.375552	2.171154	0.425049
C	6.672544	4.926478	-0.024441
C	4.284979	5.338201	0.404884
C	7.621463	2.679824	0.097616
C	6.850509	6.324396	-0.263832
C	7.798010	4.051713	-0.134589
C	4.461392	6.668470	0.169880
C	5.742018	7.215908	-0.165230
C	8.138755	6.841425	-0.603540
C	9.080608	4.599088	-0.477002
C	5.937082	8.586960	-0.401776
C	8.287136	8.218810	-0.830600
C	9.244747	5.931023	-0.701072
C	7.196800	9.081205	-0.730240
O	-2.196511	3.263819	-1.700190
H	-1.264245	-3.354569	3.771810
H	-1.405856	-1.941248	1.766629
H	0.321042	-4.258522	-2.428366
H	-3.345240	-2.244782	-3.415559

H	2.815987	-2.149016	4.382599
H	0.860627	-3.472762	5.077433
H	0.861285	-2.516192	-0.780544
H	-1.799843	-4.131866	-3.739371
O	-3.556215	1.865297	-0.551618
O	-1.246893	1.691804	0.928008
O	1.627054	1.132586	-0.772824
O	3.951432	1.048003	0.698135
H	0.525807	2.790432	1.957967
O	-2.768892	0.859326	2.385765
O	2.850175	-0.355854	-1.966951
O	3.021420	2.957481	1.486856
H	-5.681294	2.586408	-0.207116
H	-1.960050	5.392748	-1.548124
H	-7.526446	4.148349	0.257330
H	-1.648886	7.804775	-1.789080
H	-8.410140	6.443209	0.358606
H	-2.553308	10.114143	-1.689070
H	-6.628703	10.779183	-0.493675
H	-8.088243	8.870963	0.086955
H	-4.431831	11.664893	-1.224451
H	-3.873279	2.022757	3.874465
H	1.620814	4.352275	3.473805
H	-5.041412	2.880240	5.843077
H	1.578217	5.757305	5.513489
H	-5.068036	4.283796	7.890063
H	-1.621559	6.631086	8.936300
H	0.399212	6.588731	7.512144
H	-3.935308	5.879524	9.413060
H	0.170734	2.395976	-2.071184
H	4.183630	0.144325	-3.632464
H	-0.531838	3.811336	-3.927266
H	5.475192	0.218697	-5.706072
H	-0.190488	4.672634	-6.223470
H	5.795028	1.073365	-8.014892
H	3.025952	3.920869	-9.659828
H	1.103326	4.711755	-8.321293

H	5.059088	2.521163	-9.888537
H	6.275752	1.110247	0.612060
H	3.306617	4.957896	0.661213
H	8.468819	2.005015	0.028935
H	3.612570	7.344419	0.234230
H	9.923544	3.917993	-0.553993
H	5.088359	9.261289	-0.325182
H	9.268648	8.608268	-1.087300
H	10.221834	6.330376	-0.959955
H	7.330751	10.143820	-0.909734
C	8.287858	-1.746821	1.771442
C	5.872327	1.141208	6.034061
C	3.420304	1.242102	4.674779
C	4.243638	-0.460514	3.040226
C	4.866605	1.967304	6.480514
C	3.632053	2.019256	5.791530
C	5.277618	-1.269273	2.615778
C	6.524045	-1.285001	3.288240
C	5.689253	0.327293	4.884790
C	4.434250	0.370862	4.191764
C	4.896090	-3.380353	1.600509
C	6.725167	-0.513209	4.400334
C	4.556908	-3.998595	0.294200
C	4.575234	-5.411208	0.105768
C	4.167522	-3.155384	-0.761011
C	4.203773	-5.930443	-1.178270
C	4.961665	-6.352738	1.124216
C	3.790841	-3.665087	-1.993047
C	4.219471	-7.339042	-1.420804
C	3.805482	-5.047778	-2.230389
C	4.978480	-7.693698	0.883369
C	4.610562	-8.240931	-0.387985
C	3.841553	-7.857544	-2.698037
C	3.427623	-5.596476	-3.502856
C	4.619720	-9.622073	-0.644862
C	3.865703	-9.245123	-2.909828
C	3.445348	-6.938514	-3.727408

C	4.251390	-10.117038	-1.893183
C	9.175279	-2.851316	1.321987
C	10.330154	-2.610553	0.525124
C	8.832351	-4.166464	1.680137
C	11.116007	-3.734760	0.107799
C	10.773821	-1.298249	0.133467
C	9.587818	-5.249175	1.261283
C	12.289626	-3.541795	-0.684789
C	10.735082	-5.062322	0.475480
C	11.896864	-1.122132	-0.616928
C	12.694315	-2.226887	-1.059109
C	13.068309	-4.662661	-1.108247
C	11.534245	-6.170325	0.033957
C	13.850705	-2.056948	-1.838154
C	14.216358	-4.445633	-1.886654
C	12.648971	-5.980416	-0.722852
C	14.602280	-3.155820	-2.246789
O	5.120854	-2.021113	1.460447
O	7.517016	-2.147592	2.842403
O	8.205417	-0.629265	1.306632
H	6.825940	1.100703	6.553398
H	2.475996	1.298885	4.145603
H	5.019825	2.584940	7.360505
H	2.844779	2.679457	6.142793
H	3.128997	-4.908062	-4.288519
O	4.974407	-3.921030	2.683400
H	7.684444	-0.547824	4.906359
H	4.137804	-2.085101	-0.609757
H	5.223858	-5.971786	2.100634
H	3.474563	-2.981653	-2.774852
H	5.272397	-8.379622	1.673909
H	4.917421	-10.303759	0.147358
H	3.576637	-9.635078	-3.882072
H	3.158417	-7.339052	-4.696104
H	4.262911	-11.187483	-2.075515
H	7.947003	-4.328436	2.282091
H	10.187415	-0.446081	0.444729

H	9.289986	-6.256215	1.538173
H	12.207533	-0.118562	-0.896042
H	11.225734	-7.171716	0.320890
H	14.153728	-1.052301	-2.120348
H	14.804997	-5.300631	-2.208036
H	13.244166	-6.828936	-1.049569
H	15.493475	-3.007425	-2.849183
C	-15.697520	-4.659873	-1.959390
C	-13.791204	-3.606534	1.101293
C	-15.373136	-4.435701	-0.622762
C	-14.806650	-4.302168	-2.968150
C	-12.600324	-3.033880	1.425671
C	-14.148629	-3.847582	-0.267700
C	-13.570147	-3.711553	-2.658989
C	-12.627769	-3.330306	-3.667372
C	-11.658199	-2.648934	0.413351
C	-13.227268	-3.476597	-1.295363
C	-10.430924	-2.053408	0.740680
C	-11.429412	-2.760658	-3.358515
C	-11.973654	-2.875370	-0.961874
C	-9.536083	-1.686505	-0.249646
C	-11.046457	-2.506910	-1.993384
C	-9.812717	-1.902088	-1.611545
C	-6.904705	-7.830532	4.550463
C	-5.087616	-4.704928	5.572700
C	-6.224640	-6.899605	5.333592
C	-7.164852	-7.564600	3.208469
C	-4.676243	-3.528074	5.026900
C	-5.791019	-5.680548	4.788707
C	-6.749162	-6.358219	2.620658
C	-6.997600	-6.048614	1.244247
C	-4.929826	-3.216042	3.648047
C	-6.053785	-5.397619	3.412603
C	-4.512319	-2.002853	3.079831
C	-6.586223	-4.877663	0.682398
C	-5.623747	-4.163931	2.832807
C	-4.773256	-1.719623	1.748739

C	-5.880249	-3.884970	1.449759
C	-5.443332	-2.636704	0.920582
C	-6.696214	0.211194	-3.981951
C	-5.630437	-2.284864	-0.510881
C	-4.257449	0.579059	-3.845602
C	-5.490304	0.672941	-4.570918
C	-6.681282	-0.338449	-2.724071
C	-5.460514	-0.445886	-2.006714
C	-3.097778	1.618043	-5.714816
C	-4.313409	1.704431	-6.433555
C	-4.266626	-0.004240	-2.537573
C	-3.069455	1.070148	-4.451822
C	-5.482042	1.244194	-5.871893
C	-8.792803	-1.499758	-2.618264
H	-10.182645	-1.883559	1.784294
H	-16.649338	-5.115805	-2.214987
H	-14.495204	-3.892502	1.878239
H	-16.070346	-4.716491	0.162041
H	-15.061093	-4.478125	-4.009809
H	-12.337746	-2.855642	2.464726
H	-12.886466	-3.507737	-4.708122
H	-7.529808	-6.778255	0.639477
H	-10.735626	-2.494519	-4.141963
H	-8.596234	-1.226737	0.025423
H	-7.232139	-8.768489	4.989002
H	-4.889586	-4.926574	6.618125
H	-6.021630	-7.111379	6.379957
H	-7.694254	-8.292602	2.599742
H	-3.971789	-1.276822	3.679161
H	-6.776515	-4.679167	-0.362526
H	-4.431310	-0.778232	1.340519
H	-7.624964	0.283246	-4.531741
O	-5.870332	-3.030767	-1.435426
H	-4.146672	-2.794505	5.628500
H	-2.179008	1.987634	-6.160233
H	-4.321760	2.137019	-7.429685
H	-2.135683	1.020592	-3.903591

H	-6.420247	1.308774	-6.416112
O	-8.781944	-1.763571	-3.800715
O	-7.807513	-0.735560	-2.026923
O	-5.475685	-0.924273	-0.703295

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3c.

–7965.21326046 hartree

C	0.127089	-3.627785	2.519671
C	-0.065293	-2.700949	1.520925
C	1.704826	0.215893	0.015797
C	2.093014	-1.656276	2.068414
C	0.909793	-1.701142	1.256958
C	0.739802	-0.748960	0.201360
C	0.382278	-3.312483	-3.288134
C	-1.827502	-2.445466	-3.759038
C	-0.557780	-1.601286	-1.833606
C	2.265079	-2.641399	3.078632
C	1.307188	-3.605381	3.296347
C	2.840846	0.297231	0.854574
C	3.060265	-0.619941	1.858406
C	-1.743539	-1.571493	-2.641503
C	-2.801895	-0.661539	-2.317884
C	0.495697	-2.484769	-2.194305
C	-0.792046	-3.296131	-4.074056
C	-2.659678	0.157132	-1.219920
C	-1.512712	0.092715	-0.394366
C	-0.466231	-0.754945	-0.682144
C	-3.537751	2.354933	-1.158453
C	-2.077990	0.550886	1.853443
C	2.209831	1.028651	-2.155749
C	3.503470	2.566797	1.009053
C	-4.744241	3.127357	-0.772228
C	-4.702720	4.541833	-0.608631
C	-5.954218	2.432603	-0.602720
C	-5.918984	5.223010	-0.275513
C	-3.503255	5.329125	-0.727896
C	-7.127806	3.101954	-0.295188

C	-5.927134	6.640548	-0.091932
C	-7.139614	4.494310	-0.126021
C	-3.517741	6.679073	-0.545471
C	-4.720863	7.388560	-0.227939
C	-7.141737	7.320932	0.230761
C	-8.345743	5.204196	0.195507
C	-4.748560	8.780964	-0.043326
C	-7.122522	8.713768	0.405257
C	-8.348016	6.554061	0.366023
C	-5.937503	9.434818	0.269598
C	-1.724577	1.439355	2.988682
C	-2.482924	1.449775	4.194748
C	-0.577191	2.242858	2.872872
C	-2.045995	2.299504	5.263937
C	-3.673837	0.667391	4.400277
C	-0.153767	3.051652	3.915136
C	-2.774747	2.346922	6.492670
C	-0.871875	3.102447	5.119563
C	-4.363592	0.719500	5.573949
C	-3.946247	1.551824	6.662395
C	-2.335690	3.186973	7.562333
C	-0.453634	3.937504	6.210741
C	-4.647276	1.609488	7.878496
C	-3.068377	3.213260	8.759665
C	-1.152541	3.978949	7.377794
C	-4.212131	2.432093	8.914442
C	1.764341	2.033012	-3.153488
C	2.551326	2.355636	-4.295592
C	0.505989	2.632633	-2.974501
C	2.023181	3.294456	-5.241368
C	3.862210	1.815327	-4.544189
C	-0.005244	3.527906	-3.900571
C	2.778967	3.655552	-6.399555
C	0.732814	3.877393	-5.041676
C	4.579428	2.169737	-5.646902
C	4.070972	3.092701	-6.617278
C	2.248646	4.583162	-7.348614

C	0.224233	4.805744	-6.012445
C	4.798853	3.460021	-7.761342
C	3.011004	4.920103	-8.478332
C	0.947354	5.142999	-7.114928
C	4.272735	4.363768	-8.680918
C	4.616358	3.490884	0.673908
C	4.456165	4.905956	0.719703
C	5.862159	2.938472	0.328668
C	5.589749	5.729284	0.413469
C	3.214058	5.563821	1.031936
C	6.954725	3.739480	0.043473
C	5.477513	7.154066	0.441173
C	6.847114	5.137973	0.079143
C	3.114294	6.922270	1.050964
C	4.232849	7.769457	0.764510
C	6.609011	7.974759	0.144199
C	7.967895	5.986061	-0.213182
C	4.141560	9.171023	0.787052
C	6.472040	9.371604	0.179543
C	7.855263	7.341711	-0.182053
C	5.250489	9.962099	0.497741
O	-2.528826	2.777486	-1.685959
H	-0.634496	-4.377215	2.712584
H	-0.976809	-2.712657	0.934508
H	1.200328	-3.977831	-3.547190
H	-2.724078	-2.428401	-4.368721
H	3.170517	-2.627762	3.674307
H	1.457452	-4.348790	4.073356
H	1.401362	-2.492790	-1.598866
H	-0.876142	-3.954043	-4.934034
O	-3.687999	1.016015	-0.859511
O	-1.423918	0.944685	0.695058
O	1.527772	1.181551	-0.966166
O	3.785539	1.280831	0.593370
H	0.006305	2.215692	1.962621
O	-2.807783	-0.415958	1.862513
O	3.038019	0.153778	-2.307262

O	2.466693	2.834238	1.580477
H	-5.975539	1.357324	-0.729974
H	-2.579449	4.824531	-0.970786
H	-8.052292	2.542172	-0.188199
H	-2.594653	7.245427	-0.639324
H	-9.263522	4.632424	0.301266
H	-3.825673	9.345149	-0.147795
H	-8.048673	9.227310	0.649101
H	-9.268828	7.077329	0.609967
H	-5.941884	10.511812	0.408880
H	-4.009936	0.020664	3.602802
H	0.750057	3.641337	3.796529
H	-5.255159	0.110807	5.699890
H	0.438852	4.543149	6.078756
H	-5.538147	0.999585	8.001850
H	-2.730738	3.853138	9.570572
H	-0.824859	4.617237	8.194202
H	-4.765874	2.464974	9.848092
H	-0.093265	2.379036	-2.110493
H	4.271108	1.111242	-3.833843
H	-0.990764	3.952799	-3.737002
H	5.568429	1.747577	-5.805634
H	-0.757426	5.238763	-5.841109
H	5.783392	3.028746	-7.921223
H	2.603829	5.624763	-9.198470
H	0.550210	5.848585	-7.839925
H	4.848289	4.636963	-9.560341
H	5.965911	1.861580	0.299923
H	2.352247	4.952721	1.255911
H	7.908568	3.284442	-0.206659
H	2.161477	7.388761	1.287773
H	8.915159	5.515999	-0.462220
H	3.189744	9.633526	1.033940
H	7.335327	9.991911	-0.045865
H	8.712333	7.971208	-0.406131
H	5.163335	11.044279	0.519702
C	9.026519	-1.282782	2.400124

C	5.584079	0.849266	5.938220
C	3.183086	0.780110	4.489051
C	4.305430	-0.533982	2.682763
C	4.452458	1.446732	6.443749
C	3.242730	1.412701	5.710688
C	5.461094	-1.120194	2.210412
C	6.677854	-1.069125	2.941643
C	5.558757	0.185185	4.682308
C	4.331380	0.145564	3.942694
C	5.464223	-3.072741	0.854289
C	6.723071	-0.434628	4.158508
C	5.276235	-3.511395	-0.553545
C	5.575388	-4.839980	-0.971734
C	4.749641	-2.588893	-1.473726
C	5.343355	-5.190210	-2.342780
C	6.116077	-5.853019	-0.102333
C	4.506327	-2.940224	-2.792067
C	5.645455	-6.505617	-2.814142
C	4.800602	-4.231726	-3.254500
C	6.407457	-7.102710	-0.561095
C	6.186512	-7.480455	-1.925091
C	5.406627	-6.857473	-4.178799
C	4.567594	-4.613815	-4.619415
C	6.477421	-8.767672	-2.406700
C	5.712542	-8.156002	-4.616205
C	4.857531	-5.867563	-5.061991
C	6.242688	-9.099938	-3.738480
C	9.942805	-2.248899	1.734970
C	11.316447	-1.945259	1.499664
C	9.425931	-3.493700	1.331911
C	12.128993	-2.929432	0.843068
C	11.942775	-0.703725	1.874902
C	10.216082	-4.438194	0.700327
C	13.510560	-2.670740	0.581187
C	11.570690	-4.182022	0.440582
C	13.260419	-0.466249	1.622222
C	14.095027	-1.430295	0.971084

C	14.319517	-3.650586	-0.073186
C	12.405178	-5.147561	-0.216418
C	15.454421	-1.193974	0.707051
C	15.673696	-3.371475	-0.317208
C	13.719307	-4.894828	-0.462416
C	16.234160	-2.155638	0.069689
O	5.446597	-1.697090	0.946465
O	7.731889	-1.753894	2.367925
O	9.315373	-0.221008	2.910709
H	6.518303	0.876041	6.492382
H	2.255830	0.770333	3.927832
H	4.486165	1.949130	7.406010
H	2.353663	1.889720	6.112012
H	4.154988	-3.870220	-5.295661
O	5.604994	-3.772678	1.835438
H	7.649348	-0.391987	4.715682
H	4.506207	-1.586393	-1.148792
H	6.265803	-5.606891	0.939060
H	4.078157	-2.204481	-3.465732
H	6.810570	-7.846936	0.121231
H	6.888301	-9.505991	-1.723338
H	5.529188	-8.419423	-5.654428
H	4.678203	-6.141484	-6.098314
H	6.472379	-10.099603	-4.095098
H	8.385385	-3.715764	1.528014
H	11.340876	0.042205	2.372259
H	9.782647	-5.386750	0.396767
H	13.702849	0.480953	1.920139
H	11.958713	-6.091953	-0.514927
H	15.892794	-0.246194	1.007602
H	16.284669	-4.119840	-0.814702
H	14.339331	-5.635212	-0.960874
H	17.283547	-1.957687	-0.127173
C	-15.833691	-3.349564	-0.818689
C	-13.086069	-5.830096	-0.180731
C	-15.173683	-4.507511	-0.411821
C	-15.124492	-2.308735	-1.412614

C	-11.742969	-5.947949	-0.363693
C	-13.788236	-4.647755	-0.591488
C	-13.737270	-2.405824	-1.611775
C	-12.973432	-1.357900	-2.218450
C	-10.978783	-4.896811	-0.973157
C	-13.050898	-3.585386	-1.199922
C	-9.593987	-5.012468	-1.165386
C	-11.627770	-1.459046	-2.405866
C	-11.639122	-3.701693	-1.394755
C	-8.873658	-3.988332	-1.755103
C	-10.897895	-2.633744	-2.003076
C	-9.491827	-2.798371	-2.178898
C	-7.288911	-3.563433	6.805189
C	-5.038596	-5.789301	4.782998
C	-6.451179	-4.620769	6.456067
C	-7.597586	-2.574781	5.874077
C	-4.517775	-5.859448	3.527843
C	-5.904673	-4.710926	5.165767
C	-7.073068	-2.624880	4.571421
C	-7.366286	-1.627533	3.586492
C	-4.815115	-4.860862	2.540650
C	-6.216103	-3.702853	4.202091
C	-4.280261	-4.926760	1.245032
C	-6.857889	-1.687423	2.323709
C	-5.675388	-3.771616	2.880392
C	-4.583485	-3.957253	0.304778
C	-5.993198	-2.762566	1.910995
C	-5.434160	-2.878040	0.604465
C	-6.485549	-0.587128	-4.588695
C	-5.724810	-1.888116	-0.465141
C	-4.160083	0.190658	-4.309981
C	-5.391980	0.194064	-5.043222
C	-6.370795	-1.335744	-3.444517
C	-5.154434	-1.338989	-2.712223
C	-3.210446	1.734962	-5.932074
C	-4.423625	1.731448	-6.660364
C	-4.059871	-0.606225	-3.124540

C	-3.080956	0.984838	-4.784805
C	-5.489632	0.979668	-6.223034
C	-8.649827	-1.738477	-2.796646
H	-9.085276	-5.916377	-0.843098
H	-16.905742	-3.258929	-0.671656
H	-13.652111	-6.633982	0.282298
H	-15.729679	-5.317988	0.051674
H	-15.640576	-1.406407	-1.729226
H	-11.219267	-6.846376	-0.049175
H	-13.493922	-0.457422	-2.534479
H	-8.017155	-0.802749	3.865151
H	-11.079398	-0.647733	-2.860579
H	-7.806070	-4.098025	-1.890595
H	-7.702849	-3.510770	7.807704
H	-4.804270	-6.552176	5.520644
H	-6.210978	-5.389901	7.185129
H	-8.254059	-1.752697	6.146635
H	-3.622946	-5.750396	0.981156
H	-7.100108	-0.921125	1.603054
H	-4.157299	-4.025319	-0.687388
H	-7.416295	-0.583939	-5.141368
O	-6.478213	-0.937989	-0.410465
H	-3.861883	-6.678941	3.247083
H	-2.374650	2.336187	-6.277222
H	-4.512324	2.327669	-7.563729
H	-2.153106	1.006008	-4.224766
H	-6.426980	0.976853	-6.772527
O	-8.991490	-0.625331	-3.129477
O	-7.355096	-2.189573	-2.979941
O	-5.017010	-2.176229	-1.612749

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3d.

–7965.20936824 hartree

C	-0.063460	2.598969	-3.512125
C	-0.193236	1.847938	-2.366660
C	1.812745	-0.565058	-0.349090
C	2.050942	0.908706	-2.723634

C	0.855708	0.992899	-1.932221
C	0.753772	0.235684	-0.720044
C	0.068061	3.458451	2.097616
C	-1.997236	2.442012	2.843192
C	-0.651621	1.360747	1.093318
C	2.151036	1.702898	-3.898398
C	1.120695	2.530997	-4.280477
C	2.973838	-0.678570	-1.148564
C	3.112116	0.036970	-2.317546
C	-1.809186	1.358291	1.941949
C	-2.731454	0.263203	1.885195
C	0.278519	2.429973	1.208155
C	-1.083865	3.468599	2.915780
C	-2.494354	-0.759079	0.990518
C	-1.381464	-0.728289	0.113305
C	-0.455842	0.293308	0.159272
C	-4.363036	-2.018095	0.184552
C	-1.641043	-1.676738	-2.045269
C	2.332206	-0.844340	1.946554
C	3.949034	-2.816699	-0.764569
C	-5.022823	-3.341323	0.333305
C	-6.340386	-3.577878	-0.153815
C	-4.306163	-4.382575	0.946527
C	-6.894571	-4.892405	-0.005160
C	-7.163474	-2.566949	-0.765599
C	-4.843179	-5.651986	1.078026
C	-8.214612	-5.177730	-0.473144
C	-6.135158	-5.935314	0.609673
C	-8.423367	-2.845710	-1.201841
C	-8.996666	-4.152641	-1.081469
C	-8.763633	-6.489768	-0.335097
C	-6.710674	-7.244562	0.734724
C	-10.291975	-4.451376	-1.535266
C	-10.062117	-6.743703	-0.804781
C	-7.966198	-7.510774	0.282769
C	-10.817114	-5.733952	-1.398383
C	-1.221375	-2.836427	-2.871056

C	-1.980034	-3.249411	-3.999852
C	-0.010571	-3.473317	-2.559599
C	-1.467904	-4.315321	-4.807773
C	-3.254120	-2.681099	-4.354114
C	0.491193	-4.490412	-3.358422
C	-2.199886	-4.769877	-5.947597
C	-0.216887	-4.929756	-4.487634
C	-3.951857	-3.128434	-5.434847
C	-3.454823	-4.177109	-6.276237
C	-1.681943	-5.820543	-6.766086
C	0.280694	-5.981714	-5.330271
C	-4.159540	-4.638898	-7.400199
C	-2.419917	-6.247665	-7.881396
C	-0.417786	-6.406648	-6.418387
C	-3.645732	-5.662207	-8.193041
C	2.044808	-1.715796	3.114890
C	2.756777	-1.587130	4.342239
C	1.011665	-2.663237	3.001519
C	2.378080	-2.428138	5.440802
C	3.853034	-0.675471	4.542294
C	0.648845	-3.469512	4.067507
C	3.059681	-2.332557	6.693526
C	1.312357	-3.370039	5.300492
C	4.502777	-0.596495	5.737015
C	4.132875	-1.408469	6.857182
C	2.674105	-3.160675	7.792350
C	0.946553	-4.191287	6.420059
C	4.790137	-1.327341	8.095916
C	3.357928	-3.044295	9.013095
C	1.595555	-4.090162	7.612127
C	4.404778	-2.136649	9.161738
C	5.205235	-3.449641	-0.290922
C	5.231237	-4.791578	0.183430
C	6.390879	-2.697674	-0.343207
C	6.486418	-5.336989	0.608765
C	4.062654	-5.625027	0.294979
C	7.604239	-3.239359	0.047876

C	6.559661	-6.671592	1.114842
C	7.679920	-4.553436	0.532413
C	4.139682	-6.894538	0.782793
C	5.381256	-7.469327	1.207737
C	7.811689	-7.217521	1.535134
C	8.924924	-5.130116	0.956135
C	5.472679	-8.777501	1.711510
C	7.855730	-8.529838	2.031635
C	8.989139	-6.401746	1.435694
C	6.697456	-9.300179	2.118856
O	-4.685858	-1.119216	-0.560517
H	-0.875778	3.248690	-3.823559
H	-1.107166	1.894960	-1.787127
H	0.791140	4.265473	2.167711
H	-2.883078	2.456853	3.467016
H	3.062598	1.658459	-4.483208
H	1.218945	3.135453	-5.177145
H	1.167593	2.422635	0.588977
H	-1.250084	4.289783	3.606368
O	-3.272597	-1.910894	1.023201
O	-1.195829	-1.810508	-0.738530
O	1.728783	-1.332981	0.806124
O	4.035903	-1.442987	-0.684999
H	0.564976	-3.145610	-1.703918
O	-2.268520	-0.710206	-2.413629
O	2.982301	0.180274	1.931285
O	2.954572	-3.371998	-1.183209
H	-3.306468	-4.181243	1.309137
H	-6.757812	-1.572367	-0.879059
H	-4.261869	-6.441534	1.545533
H	-9.021741	-2.059790	-1.655235
H	-6.115704	-8.023910	1.202845
H	-10.883148	-3.665025	-1.996612
H	-10.475009	-7.743284	-0.698826
H	-8.388850	-8.506822	0.384556
H	-11.820141	-5.948337	-1.755019
H	-3.654107	-1.884696	-3.741477

H	1.447147	-4.939634	-3.107326
H	-4.915252	-2.686886	-5.675983
H	1.233595	-6.436298	-5.073324
H	-5.116100	-4.185515	-7.645614
H	-2.022580	-7.045695	-8.502890
H	-0.028807	-7.205118	-7.044840
H	-4.203369	-6.006425	-9.059010
H	0.485900	-2.751997	2.059632
H	4.154091	-0.046487	3.717742
H	-0.159789	-4.185594	3.953891
H	5.329837	0.098783	5.855015
H	0.135006	-4.902174	6.291400
H	5.607984	-0.621710	8.213696
H	3.060129	-3.674750	9.846515
H	1.307779	-4.718263	8.450990
H	4.922758	-2.060762	10.113042
H	6.366389	-1.681722	-0.714794
H	3.111581	-5.223092	-0.024024
H	8.502344	-2.634099	-0.023471
H	3.239485	-7.499184	0.857701
H	9.821142	-4.519913	0.887077
H	4.571150	-9.380321	1.780539
H	8.809742	-8.941552	2.349871
H	9.938647	-6.823346	1.754903
H	6.750879	-10.313302	2.506210
C	8.555264	0.947328	-2.017099
C	5.825268	-1.978372	-6.025176
C	3.401627	-1.824869	-4.620759
C	4.375345	-0.089541	-3.108110
C	4.755774	-2.757877	-6.401910
C	3.535446	-2.681896	-5.690158
C	5.471838	0.667186	-2.750179
C	6.701792	0.555250	-3.443510
C	5.723413	-1.085580	-4.925414
C	4.483389	-0.999328	-4.209977
C	5.277521	2.854787	-1.849581
C	6.825037	-0.292860	-4.510525

C	4.993043	3.567955	-0.578812
C	5.153179	4.978946	-0.459563
C	4.507538	2.822727	0.509644
C	4.820458	5.597730	0.790256
C	5.649376	5.822886	-1.515406
C	4.166181	3.430497	1.707038
C	4.979614	7.007649	0.964165
C	4.317433	4.815098	1.876040
C	5.804693	7.165073	-1.339348
C	5.478834	7.810698	-0.103115
C	4.638560	7.626254	2.206578
C	3.978097	5.463769	3.111699
C	5.629713	9.194473	0.086922
C	4.805342	9.012678	2.351449
C	4.131844	6.806523	3.270786
C	5.296562	9.787261	1.302059
C	9.518557	2.010566	-1.628416
C	10.690087	1.723621	-0.872374
C	9.228356	3.335759	-1.995984
C	11.543061	2.813563	-0.498384
C	11.086663	0.395702	-0.482825
C	10.049460	4.385756	-1.619512
C	12.733589	2.573724	0.255155
C	11.212474	4.153545	-0.869876
C	12.227147	0.174395	0.228318
C	13.089766	1.245068	0.630327
C	13.577750	3.661153	0.638425
C	12.077321	5.227264	-0.469410
C	14.263675	1.028992	1.370790
C	14.740712	3.398466	1.379710
C	13.207144	4.993099	0.251756
C	15.078891	2.095634	1.741022
O	5.390015	1.491861	-1.636849
O	7.760984	1.368636	-3.061939
O	8.432334	-0.154112	-1.523108
H	6.767960	-2.036674	-6.562495
H	2.466436	-1.781712	-4.074302

H	4.847375	-3.436965	-7.244402
H	2.697855	-3.306577	-5.985357
H	3.596464	4.850764	3.923480
O	5.396069	3.330529	-2.958875
H	7.773440	-0.356543	-5.033889
H	4.375832	1.753748	0.411883
H	5.880307	5.368866	-2.468193
H	3.769543	2.824100	2.515222
H	6.179375	7.776132	-2.156686
H	6.009452	9.800783	-0.731054
H	4.544030	9.479060	3.297529
H	3.872627	7.283325	4.212384
H	5.418094	10.858436	1.432587
H	8.332162	3.533135	-2.570631
H	10.451467	-0.431452	-0.764617
H	9.790203	5.402323	-1.900330
H	12.501849	-0.840028	0.505900
H	11.806377	6.238918	-0.758241
H	14.529785	0.014103	1.653563
H	15.379172	4.228139	1.670923
H	13.852205	5.816069	0.547718
H	15.982729	1.911788	2.314086
C	-15.862698	2.303233	0.615530
C	-13.255337	4.927000	-0.040184
C	-15.264511	3.486531	0.186418
C	-15.106814	1.327120	1.259753
C	-11.926576	5.132271	0.168680
C	-13.895275	3.717699	0.393786
C	-13.733692	1.515888	1.488635
C	-12.922473	0.534949	2.144620
C	-11.115229	4.150008	0.830184
C	-13.110699	2.722825	1.055098
C	-9.744411	4.354650	1.047287
C	-11.591616	0.727118	2.363695
C	-11.714368	2.932572	1.279288
C	-8.976886	3.393007	1.681856
C	-10.927168	1.934256	1.944552

C	-9.536936	2.185260	2.135417
C	-5.648595	8.771004	-3.707547
C	-4.449413	5.448272	-4.988313
C	-5.179958	7.785387	-4.574404
C	-5.879218	8.475637	-2.366400
C	-4.218641	4.189266	-4.526158
C	-4.933470	6.481309	-4.116505
C	-5.646069	7.184550	-1.864224
C	-5.864510	6.843739	-0.490162
C	-4.450484	3.844272	-3.151116
C	-5.168829	6.167079	-2.742110
C	-4.222053	2.546380	-2.669448
C	-5.630325	5.589393	-0.011944
C	-4.927936	4.846647	-2.250152
C	-4.463390	2.229383	-1.341636
C	-5.156266	4.533771	-0.869612
C	-4.921165	3.199063	-0.431157
C	-6.275286	0.199435	4.374280
C	-5.102879	2.798008	0.988834
C	-3.915512	-0.453324	4.035373
C	-5.103177	-0.454994	4.836543
C	-6.274102	0.834785	3.156259
C	-5.093273	0.850000	2.363252
C	-2.770990	-1.738012	5.755922
C	-3.944283	-1.741320	6.546537
C	-3.935874	0.219881	2.772250
C	-2.757883	-1.111830	4.529406
C	-5.083251	-1.115276	6.094599
C	-8.648463	1.201777	2.812868
H	-9.280048	5.275636	0.706702
H	-16.923188	2.142031	0.446405
H	-13.857006	5.679367	-0.543207
H	-15.857049	4.246185	-0.316270
H	-15.574917	0.404895	1.593248
H	-11.450065	6.049832	-0.165025
H	-13.394044	-0.387485	2.473785
H	-6.218649	7.620202	0.183433

H	-11.008956	-0.029370	2.868282
H	-7.921888	3.573382	1.842215
H	-5.832949	9.774338	-4.079915
H	-4.271730	5.693555	-6.032095
H	-4.999057	8.019767	-5.620005
H	-6.241810	9.246305	-1.691433
H	-3.848379	1.777688	-3.339430
H	-5.777536	5.370064	1.035750
H	-4.287390	1.216568	-1.001459
H	-7.171754	0.180412	4.977871
O	-5.206758	3.520398	1.959633
H	-3.856809	3.412665	-5.194489
H	-1.873234	-2.229516	6.118947
H	-3.943252	-2.238688	7.512019
H	-1.854786	-1.113425	3.928853
H	-5.988760	-1.114297	6.695135
O	-8.982227	0.227278	3.453482
O	-7.329090	1.544024	2.618544
O	-5.120676	1.427043	1.104034

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3e.

–7965.20596653 hartree

C	-0.110154	-3.280246	-3.164326
C	0.117679	-2.457276	-2.084604
C	-1.630537	0.227599	-0.175899
C	-2.092771	-1.426008	-2.393189
C	-0.860837	-1.517079	-1.662982
C	-0.650917	-0.675326	-0.524896
C	-0.104143	-3.427908	2.781115
C	2.132812	-2.590918	3.175238
C	0.755025	-1.627627	1.386251
C	-2.299519	-2.302547	-3.492813
C	-1.332673	-3.207215	-3.869157
C	-2.819647	0.360164	-0.931784
C	-3.074769	-0.452680	-2.013240
C	1.983530	-1.639444	2.128573
C	3.029025	-0.716192	1.793831

C	-0.278654	-2.533720	1.750425
C	1.116469	-3.462472	3.492437
C	2.838413	0.144169	0.730236
C	1.647617	0.114681	-0.036841
C	0.606653	-0.730968	0.281967
C	4.115160	2.138307	1.031258
C	1.277237	2.200456	-1.153171
C	-2.037257	0.812542	2.091387
C	-3.498904	2.617233	-0.834167
C	5.287383	2.853385	0.462758
C	5.478035	4.247333	0.670171
C	6.240762	2.112851	-0.254912
C	6.658495	4.859786	0.136447
C	4.533776	5.087476	1.359080
C	7.387369	2.707797	-0.756172
C	6.888255	6.259031	0.313670
C	7.621460	4.079311	-0.574722
C	4.756335	6.421754	1.517265
C	5.936433	7.058793	1.012087
C	8.071172	6.868368	-0.207067
C	8.801902	4.717256	-1.085799
C	6.180469	8.432204	1.176708
C	8.274105	8.244554	-0.017268
C	9.017837	6.049207	-0.910005
C	7.337561	9.016675	0.667432
C	1.073444	2.762136	-2.514536
C	0.784156	4.142076	-2.724822
C	1.147891	1.891057	-3.615859
C	0.584185	4.599291	-4.070321
C	0.676595	5.111566	-1.665738
C	0.952286	2.338379	-4.911308
C	0.290859	5.973694	-4.332508
C	0.669415	3.688523	-5.167938
C	0.397985	6.419631	-1.924250
C	0.195369	6.904116	-3.256521
C	0.088762	6.429383	-5.671979
C	0.461874	4.172142	-6.503875

C	-0.093302	8.251468	-3.532718
C	-0.198324	7.784579	-5.901593
C	0.184153	5.482251	-6.745969
C	-0.287730	8.685294	-4.842191
C	-1.477210	1.644041	3.185967
C	-2.144089	1.782440	4.437529
C	-0.220557	2.243924	2.988185
C	-1.493510	2.525838	5.476152
C	-3.447425	1.238765	4.717262
C	0.407957	2.949245	4.002474
C	-2.121312	2.690657	6.749836
C	-0.203937	3.102854	5.255659
C	-4.044208	1.408928	5.930234
C	-3.409656	2.129854	6.992731
C	-1.464871	3.416336	7.791466
C	0.433540	3.825242	6.321131
C	-4.010614	2.301878	8.250991
C	-2.102343	3.561598	9.033798
C	-0.167693	3.974853	7.532952
C	-3.362289	3.010008	9.259515
C	-4.539991	3.513870	-0.271149
C	-4.584292	4.904217	-0.584514
C	-5.501672	2.961618	0.593333
C	-5.628190	5.699110	-0.004251
C	-3.647198	5.562309	-1.457772
C	-6.501255	3.736766	1.155422
C	-5.720908	7.095802	-0.294732
C	-6.590215	5.107864	0.871720
C	-3.744050	6.893603	-1.731144
C	-4.775627	7.710865	-1.167030
C	-6.760036	7.888339	0.283411
C	-7.622746	5.927353	1.440018
C	-4.883654	9.084215	-1.442463
C	-6.829049	9.257573	-0.019396
C	-7.705042	7.256205	1.159513
C	-5.899894	9.847947	-0.874020
O	3.463539	2.450874	2.000445

H	0.650241	-3.992502	-3.470352
H	1.052851	-2.520451	-1.538907
H	-0.905500	-4.112521	3.041857
H	3.068239	-2.627568	3.720361
H	-3.240009	-2.254368	-4.029269
H	-1.511925	-3.869572	-4.710658
H	-1.213981	-2.511763	1.203332
H	1.254950	-4.182055	4.293779
O	3.843024	0.995411	0.294023
O	1.566963	0.852596	-1.211318
O	-1.408272	1.082580	0.894252
O	-3.760637	1.291516	-0.523261
H	1.354020	0.843932	-3.438479
O	1.211218	2.784371	-0.092892
O	-2.908470	-0.030310	2.174962
O	-2.527378	2.921311	-1.491614
H	6.081640	1.050730	-0.394418
H	3.636911	4.633874	1.756175
H	8.118618	2.109398	-1.291830
H	4.024608	7.032550	2.039740
H	9.524288	4.106866	-1.620615
H	5.451855	9.037189	1.709578
H	9.175716	8.704447	-0.412819
H	9.916211	6.518080	-1.302664
H	7.511143	10.079883	0.804318
H	0.815808	4.775664	-0.649478
H	1.013886	1.640037	-5.741039
H	0.320679	7.125313	-1.101374
H	0.534137	3.462391	-7.323473
H	-0.158707	8.955706	-2.707636
H	-0.351409	8.125601	-6.921907
H	0.029645	5.834459	-7.762398
H	-0.508467	9.730191	-5.038947
H	0.278113	2.145690	2.032555
H	-3.948896	0.681424	3.939492
H	1.392360	3.370790	3.823659
H	-5.031045	0.989633	6.109278

H	1.413575	4.254718	6.132885
H	-4.993031	1.872987	8.429510
H	-1.598960	4.112923	9.823467
H	0.326314	4.525603	8.329118
H	-3.840261	3.133186	10.226810
H	-5.448690	1.905707	0.824216
H	-2.851687	4.975953	-1.892482
H	-7.228311	3.282761	1.822440
H	-3.020089	7.358390	-2.395513
H	-8.343020	5.457289	2.103835
H	-4.160615	9.545624	-2.109677
H	-7.621047	9.855996	0.422840
H	-8.492843	7.864054	1.596596
H	-5.969519	10.908386	-1.097603
C	-9.036307	-1.380042	-2.316444
C	-5.909830	1.326136	-5.751221
C	-3.429058	1.243515	-4.443457
C	-4.372161	-0.332133	-2.747397
C	-4.844768	2.047562	-6.239594
C	-3.595645	2.008504	-5.576331
C	-5.468618	-1.023733	-2.277751
C	-6.729128	-0.960295	-2.930710
C	-5.775965	0.528946	-4.582769
C	-4.506849	0.480030	-3.918505
C	-5.313821	-3.095856	-1.111621
C	-6.876137	-0.207263	-4.069791
C	-5.054404	-3.641419	0.247363
C	-5.292353	-5.008870	0.567735
C	-4.532969	-2.774252	1.222805
C	-5.013597	-5.453546	1.902292
C	-5.815715	-5.972959	-0.365616
C	-4.241054	-3.216307	2.503218
C	-5.260419	-6.810468	2.278842
C	-4.481049	-4.548402	2.872571
C	-6.051509	-7.263888	0.002369
C	-5.788142	-7.734469	1.329544
C	-4.980013	-7.254421	3.608230

C	-4.203928	-5.023090	4.199446
C	-6.025658	-9.063337	1.718582
C	-5.233981	-8.591531	3.952851
C	-4.443520	-6.315287	4.552381
C	-5.751709	-9.485203	3.017100
C	-9.840610	-2.443097	-1.653877
C	-11.189942	-2.223135	-1.249976
C	-9.240116	-3.694605	-1.427234
C	-11.893131	-3.297548	-0.609452
C	-11.890701	-0.977782	-1.430037
C	-9.926965	-4.728866	-0.815169
C	-13.244019	-3.122182	-0.175747
C	-11.253959	-4.557594	-0.393502
C	-13.177713	-0.819015	-1.012418
C	-13.905003	-1.874534	-0.374030
C	-13.944561	-4.192285	0.461992
C	-11.980984	-5.615531	0.248968
C	-15.232278	-1.720084	0.059418
C	-15.270318	-3.993186	0.878879
C	-13.266985	-5.442326	0.658113
C	-15.906310	-2.769373	0.679021
O	-5.353392	-1.719280	-1.081675
O	-7.710253	-1.749765	-2.363120
O	-9.434166	-0.326235	-2.766226
H	-6.874877	1.358778	-6.249430
H	-2.475257	1.234819	-3.928239
H	-4.963017	2.655501	-7.131770
H	-2.763606	2.593168	-5.957242
H	-3.799548	-4.318434	4.920833
O	-5.467768	-3.715605	-2.143571
H	-7.834785	-0.154575	-4.567286
H	-4.335336	-1.740924	0.972046
H	-5.997765	-5.653956	-1.381882
H	-3.820553	-2.518933	3.221247
H	-6.441782	-7.969623	-0.726713
H	-6.426570	-9.762804	0.989882
H	-5.019498	-8.925250	4.964567

H	-4.231668	-6.659739	5.561142
H	-5.940645	-10.515925	3.302066
H	-8.217966	-3.849618	-1.746828
H	-11.371536	-0.164299	-1.914865
H	-9.431476	-5.681412	-0.651035
H	-13.678458	0.133880	-1.163479
H	-11.475103	-6.564471	0.403489
H	-15.729743	-0.766418	-0.095109
H	-15.798830	-4.809929	1.363099
H	-13.804789	-6.252056	1.144115
H	-16.932170	-2.633695	1.008288
C	16.068936	-2.497316	-0.802932
C	13.444424	-5.113279	-1.419425
C	15.452959	-3.664232	-1.251280
C	15.349423	-1.562809	-0.062605
C	12.133986	-5.343658	-1.134645
C	14.102043	-3.920341	-0.967245
C	13.995947	-1.778190	0.245958
C	13.222644	-0.841171	1.003760
C	11.361033	-4.405763	-0.370906
C	13.355122	-2.968671	-0.206413
C	10.010109	-4.638179	-0.072029
C	11.911667	-1.060534	1.302927
C	11.978805	-3.205764	0.099496
C	9.281485	-3.722824	0.667696
C	11.230775	-2.253144	0.868911
C	9.860654	-2.533889	1.146694
C	6.147672	-8.432751	-4.979374
C	5.033819	-4.976146	-5.940372
C	5.738382	-7.349405	-5.754469
C	6.286815	-8.297621	-3.600321
C	4.768914	-3.778891	-5.350625
C	5.459812	-6.106162	-5.164562
C	6.019984	-7.072136	-2.967780
C	6.147383	-6.894726	-1.552173
C	4.908636	-3.599029	-3.933162
C	5.601665	-5.956290	-3.750418

C	4.645040	-2.365282	-3.319067
C	5.886020	-5.701989	-0.947071
C	5.327580	-4.700495	-3.124582
C	4.802841	-2.206430	-1.952328
C	5.470432	-4.549589	-1.705162
C	5.212005	-3.271555	-1.130622
C	6.822642	-0.890601	3.881185
C	5.353383	-3.026253	0.329933
C	4.445699	-0.215346	3.871204
C	5.707840	-0.313111	4.542195
C	6.696543	-1.347453	2.593107
C	5.443021	-1.268004	1.929225
C	3.502064	0.853399	5.842391
C	4.744250	0.742056	6.510529
C	4.327806	-0.726534	2.536165
C	3.356462	0.389077	4.554506
C	5.822738	0.176058	5.871560
C	9.017899	-1.608141	1.951306
H	9.531198	-5.545440	-0.428792
H	17.114765	-2.316332	-1.032341
H	14.017579	-5.832606	-1.998320
H	16.017140	-4.391423	-1.828984
H	15.831318	-0.653342	0.285850
H	11.643777	-6.248736	-1.482270
H	13.707613	0.069072	1.347054
H	6.453561	-7.747299	-0.951221
H	11.358425	-0.338270	1.884747
H	8.243295	-3.927180	0.894432
H	6.357566	-9.386975	-5.453153
H	4.926260	-5.097021	-7.014976
H	5.629432	-7.458831	-6.830064
H	6.603449	-9.144429	-2.997451
H	4.319246	-1.526273	-3.927014
H	5.966934	-5.606076	0.125868
H	4.599382	-1.244009	-1.500648
H	7.774901	-0.949959	4.390428
O	5.449165	-3.851646	1.213087

H	4.447182	-2.929093	-5.946154
H	2.657740	1.315264	6.345329
H	4.845875	1.111416	7.526799
H	2.408160	0.497829	4.042437
H	6.783685	0.096590	6.372388
O	9.386134	-0.652958	2.601298
O	7.692978	-1.980275	1.873694
O	5.361234	-1.674786	0.601814

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3f.

–7965.21517284 hartree

C	-0.297389	-3.771068	-2.120408
C	-0.053611	-2.714439	-1.272712
C	-1.622992	0.524693	-0.289819
C	-2.110617	-1.610319	-2.044400
C	-0.950578	-1.614245	-1.199980
C	-0.727656	-0.521622	-0.301496
C	-0.637560	-2.529318	3.546401
C	1.632548	-1.789289	3.939154
C	0.461909	-1.141998	1.876719
C	-2.335068	-2.723046	-2.899516
C	-1.452223	-3.778703	-2.934534
C	-2.738710	0.552405	-1.160024
C	-3.003174	-0.489128	-2.020719
C	1.631924	-1.082084	2.706128
C	2.761583	-0.309867	2.283580
C	-0.667878	-1.870642	2.338608
C	0.525950	-2.497972	4.347720
C	2.707651	0.336656	1.068383
C	1.575176	0.234349	0.227439
C	0.458883	-0.478276	0.607613
C	3.791436	2.416854	0.712350
C	2.231718	0.394913	-2.048671
C	-2.100600	1.633690	1.743360
C	-3.242914	2.812119	-1.667870
C	5.098470	2.995711	0.312518
C	5.213478	4.346039	-0.122866

C	6.243296	2.188387	0.415016
C	6.516148	4.845090	-0.450208
C	4.091631	5.233385	-0.284118
C	7.501900	2.683020	0.113633
C	6.680833	6.190704	-0.902884
C	7.666392	4.005321	-0.323845
C	4.255738	6.512777	-0.722201
C	5.547022	7.044245	-1.042686
C	7.980756	6.692498	-1.220104
C	8.960553	4.537338	-0.647195
C	5.729198	8.363752	-1.489234
C	8.115358	8.018174	-1.661727
C	9.111953	5.819912	-1.075213
C	7.000192	8.843710	-1.794635
C	1.983075	1.189727	-3.277632
C	2.837547	1.099894	-4.412791
C	0.840471	2.006610	-3.319531
C	2.493838	1.853313	-5.582982
C	4.045984	0.318299	-4.446235
C	0.506196	2.720966	-4.459076
C	3.323746	1.800306	-6.745374
C	1.315249	2.662528	-5.604164
C	4.835980	0.279220	-5.555322
C	4.508583	1.006822	-6.745193
C	2.975552	2.541346	-7.916730
C	0.989390	3.396091	-6.795271
C	5.311606	0.967413	-7.897171
C	3.807090	2.470678	-9.045672
C	1.781257	3.338093	-7.900506
C	4.962715	1.691709	-9.034283
C	-1.589786	2.708897	2.630968
C	-2.320684	3.149928	3.771611
C	-0.323256	3.252543	2.355392
C	-1.732493	4.155501	4.607864
C	-3.624251	2.654816	4.129887
C	0.245327	4.213675	3.175688
C	-2.427704	4.633080	5.761807

C	-0.439680	4.686205	4.305210
C	-4.280457	3.116014	5.231120
C	-3.715473	4.114817	6.088294
C	-1.839109	5.629514	6.600616
C	0.128555	5.685655	5.166330
C	-4.382307	4.594888	7.227820
C	-2.542775	6.080342	7.728708
C	-0.539620	6.137600	6.262458
C	-3.801405	5.567566	8.037529
C	-4.311138	3.834139	-1.533127
C	-4.045507	5.221442	-1.718273
C	-5.616636	3.398586	-1.246517
C	-5.138429	6.143009	-1.610967
C	-2.736258	5.760923	-1.979358
C	-6.668069	4.296131	-1.155364
C	-4.922016	7.545487	-1.783065
C	-6.458944	5.671804	-1.333393
C	-2.537032	7.099390	-2.135972
C	-3.612610	8.041540	-2.051869
C	-6.013238	8.463057	-1.685911
C	-7.536866	6.615928	-1.242503
C	-3.419292	9.422963	-2.218347
C	-5.773689	9.835337	-1.860706
C	-7.325375	7.949399	-1.411354
C	-4.489627	10.308806	-2.124012
O	2.804254	3.013415	1.088670
H	0.402115	-4.600519	-2.162064
H	0.837008	-2.708157	-0.655062
H	-1.513237	-3.074897	3.884446
H	2.525664	-1.768860	4.553149
H	-3.219311	-2.731830	-3.526894
H	-1.643279	-4.619705	-3.594425
H	-1.564952	-1.887387	1.730667
H	0.545967	-3.032089	5.292869
O	3.815250	1.040105	0.614251
O	1.563885	0.936346	-0.970078
O	-1.398523	1.605989	0.547967

O	-3.618519	1.622932	-1.079484
H	0.191127	2.067316	-2.456605
O	2.895671	-0.615896	-1.945735
O	-2.987125	0.839198	1.967922
O	-2.168530	2.936595	-2.219749
H	6.150303	1.166850	0.759331
H	3.104639	4.864690	-0.043634
H	8.365896	2.035576	0.224738
H	3.389312	7.158991	-0.837026
H	9.822718	3.884579	-0.542389
H	4.861422	9.009343	-1.594506
H	9.105621	8.396558	-1.900779
H	10.098065	6.207563	-1.317237
H	7.123611	9.866404	-2.138445
H	4.317787	-0.246640	-3.566165
H	-0.396299	3.324437	-4.460320
H	5.745070	-0.316565	-5.548922
H	0.090585	4.006641	-6.790484
H	6.213876	0.361874	-7.890379
H	3.538100	3.034556	-9.934840
H	1.522540	3.900154	-8.794041
H	5.594371	1.649962	-9.916627
H	0.236942	2.899003	1.500673
H	-4.074914	1.892942	3.510382
H	1.235925	4.591315	2.942151
H	-5.259444	2.714683	5.479500
H	1.110519	6.077926	4.916396
H	-5.362625	4.194547	7.471976
H	-2.091470	6.838032	8.363697
H	-0.097797	6.896057	6.903440
H	-4.330630	5.927855	8.914760
H	-5.807461	2.341145	-1.110945
H	-1.903987	5.076255	-2.052428
H	-7.669661	3.931431	-0.946419
H	-1.535784	7.476027	-2.328892
H	-8.533451	6.237127	-1.033122
H	-2.418665	9.794548	-2.422158

H	-6.606586	10.529470	-1.787365
H	-8.151357	8.652043	-1.339153
H	-4.323355	11.373852	-2.255506
C	-7.915500	-2.798532	-2.613984
C	-5.243284	0.540932	-6.387996
C	-2.933365	0.567788	-4.796751
C	-4.209767	-0.448817	-2.903262
C	-4.059905	1.028244	-6.893705
C	-2.896605	1.041967	-6.089106
C	-5.413149	-0.927723	-2.429306
C	-6.568644	-0.957931	-3.250275
C	-5.316542	0.042588	-5.060399
C	-4.137739	0.053312	-4.244400
C	-6.166314	-0.795984	-0.177810
C	-6.525481	-0.479430	-4.531166
C	-6.157334	-1.547601	1.102821
C	-6.618705	-0.965979	2.319416
C	-5.691616	-2.874266	1.095555
C	-6.600350	-1.768638	3.507916
C	-7.093483	0.388654	2.433749
C	-5.678084	-3.643551	2.246318
C	-7.057859	-1.232166	4.751507
C	-6.127879	-3.116644	3.466418
C	-7.526938	0.892919	3.623063
C	-7.532898	0.110213	4.822581
C	-7.045179	-2.033818	5.934382
C	-6.125111	-3.899512	4.669669
C	-7.984199	0.618674	6.052292
C	-7.503305	-1.483705	7.142288
C	-6.563240	-3.383105	5.849819
C	-7.968338	-0.171398	7.199219
C	-9.183000	-3.133322	-1.913583
C	-9.741857	-4.442918	-1.959055
C	-9.825848	-2.122644	-1.177404
C	-10.963754	-4.686413	-1.248570
C	-9.162501	-5.537438	-2.693893
C	-10.998297	-2.368735	-0.482968

C	-11.569167	-5.980996	-1.273717
C	-11.591294	-3.640269	-0.504057
C	-9.748266	-6.767235	-2.715411
C	-10.964938	-7.041167	-2.011101
C	-12.784098	-6.225432	-0.562102
C	-12.809955	-3.914048	0.203644
C	-11.574820	-8.306559	-2.024820
C	-13.358134	-7.505991	-0.603561
C	-13.380923	-5.148855	0.176312
C	-12.758748	-8.534680	-1.327989
O	-5.470932	-1.477519	-1.156454
O	-7.763979	-1.428163	-2.723344
O	-7.085422	-3.563319	-3.054881
H	-6.141797	0.527747	-6.998979
H	-2.040111	0.595335	-4.183651
H	-4.016774	1.404675	-7.911449
H	-1.965914	1.430554	-6.491315
H	-5.762525	-4.922231	4.615086
O	-6.703547	0.267840	-0.408715
H	-7.422867	-0.509373	-5.140474
H	-5.345517	-3.300640	0.163031
H	-7.103799	1.003776	1.546625
H	-5.320322	-4.668347	2.208015
H	-7.880509	1.919575	3.674902
H	-8.351032	1.640763	6.097425
H	-7.491460	-2.097383	8.038951
H	-6.555170	-3.987534	6.752926
H	-8.320161	0.236471	8.142104
H	-9.377938	-1.137551	-1.143301
H	-8.238158	-5.364566	-3.225634
H	-11.466902	-1.572324	0.087862
H	-9.286582	-7.573529	-3.279560
H	-13.269361	-3.105538	0.765446
H	-11.109097	-9.110186	-2.588778
H	-14.281645	-7.687691	-0.060488
H	-14.304165	-5.341115	0.716407
H	-13.217360	-9.518737	-1.348726

C	14.866910	-3.136993	-1.012682
C	12.774709	-5.871790	0.490296
C	14.448533	-4.403617	-0.609285
C	14.076502	-2.019901	-0.754276
C	11.590142	-6.020834	1.142999
C	13.228380	-4.578688	0.062779
C	12.847705	-2.148035	-0.085852
C	12.008267	-1.023238	0.200985
C	10.749027	-4.892989	1.428604
C	12.409291	-3.438957	0.331468
C	9.529953	-5.037263	2.108011
C	10.815176	-1.159216	0.844029
C	11.162141	-3.589257	1.013457
C	8.734177	-3.935936	2.376620
C	10.335936	-2.446846	1.274144
C	9.106927	-2.644758	1.965022
C	4.438850	-10.308446	-0.855764
C	3.628865	-7.337560	-3.008617
C	4.072528	-9.545612	-1.963290
C	4.744449	-9.689850	0.353677
C	3.570477	-5.981478	-2.911903
C	4.005797	-8.145635	-1.883311
C	4.690931	-8.291559	0.479711
C	4.993729	-7.618743	1.707159
C	3.884705	-5.306666	-1.683524
C	4.319597	-7.500525	-0.647081
C	3.829989	-3.908745	-1.578591
C	4.935307	-6.262089	1.820332
C	4.260942	-6.076303	-0.538573
C	4.146107	-3.276477	-0.387106
C	4.568806	-5.429801	0.703880
C	4.511549	-4.006580	0.757272
C	6.413118	-0.079556	4.589535
C	4.785296	-3.258484	2.010579
C	4.126814	0.741154	4.174911
C	5.345847	0.791807	4.929108
C	6.275895	-0.969954	3.559305

C	5.065529	-1.045343	2.828145
C	3.228497	2.539581	5.545520
C	4.426865	2.579926	6.296483
C	4.002831	-0.211871	3.112070
C	3.081343	1.644303	4.509747
C	5.462465	1.726829	5.991638
C	8.173366	-1.521798	2.245565
H	9.208345	-6.026148	2.421404
H	15.813967	-3.020928	-1.531076
H	13.401110	-6.734937	0.281461
H	15.067716	-5.273041	-0.813039
H	14.405143	-1.033288	-1.069494
H	11.256134	-7.003742	1.463373
H	12.344612	-0.037340	-0.109544
H	5.271456	-8.219876	2.569347
H	10.199663	-0.293003	1.038362
H	7.795501	-4.066094	2.900559
H	4.484602	-11.390403	-0.936663
H	3.390712	-7.834197	-3.945523
H	3.832790	-10.031823	-2.905103
H	5.027318	-10.286568	1.216729
H	3.531490	-3.309198	-2.432796
H	5.148282	-5.785091	2.766006
H	4.088086	-2.197763	-0.340115
H	7.345426	-0.044818	5.143693
O	4.834063	-3.692365	3.142212
H	3.287074	-5.377311	-3.769234
H	2.418341	3.221964	5.784158
H	4.528874	3.290385	7.111467
H	2.165097	1.630379	3.930759
H	6.389167	1.757404	6.558248
O	8.135334	-0.438544	1.700127
O	7.297098	-1.860755	3.253094
O	4.973680	-1.912877	1.749386

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3g.

–7965.21178170 hartree

C	0.574357	-2.317928	-3.553861
C	0.583943	-1.614253	-2.370963
C	-1.732276	0.461107	-0.311147
C	-1.742389	-0.923348	-2.754471
C	-0.567366	-0.906426	-1.931347
C	-0.585973	-0.204828	-0.681782
C	0.173443	-3.341661	2.205371
C	2.242914	-2.290157	2.888987
C	0.847939	-1.254287	1.150929
C	-1.719560	-1.668198	-3.964793
C	-0.589377	-2.350290	-4.354523
C	-2.873220	0.488551	-1.148140
C	-2.903864	-0.192493	-2.344538
C	2.027485	-1.229748	1.967504
C	2.963908	-0.153669	1.829822
C	-0.065949	-2.332345	1.300678
C	1.339300	-3.322267	3.002652
C	2.703302	0.839693	0.912824
C	1.527251	0.827685	0.122084
C	0.612396	-0.197467	0.212171
C	4.366393	2.013345	-0.316106
C	1.045710	3.098927	-0.392322
C	-2.438689	0.625845	1.944925
C	-4.036888	2.532405	-0.918198
C	5.133726	3.284435	-0.311673
C	6.279301	3.471896	-1.137220
C	4.689394	4.327582	0.519656
C	6.949820	4.738552	-1.091872
C	6.823028	2.454507	-1.998556
C	5.334615	5.552284	0.548059
C	8.109405	4.971854	-1.894270
C	6.467657	5.784939	-0.246178
C	7.932486	2.682837	-2.755348
C	8.615392	3.941707	-2.740061
C	8.773339	6.236609	-1.855389

C	7.152662	7.046396	-0.228330
C	9.756936	4.188847	-3.520530
C	9.910268	6.439694	-2.653649
C	8.254195	7.263375	-0.997105
C	10.395941	5.425400	-3.476783
C	0.991252	4.050700	-1.530244
C	0.429493	5.352724	-1.392885
C	1.538377	3.650557	-2.761823
C	0.450404	6.226258	-2.529762
C	-0.175792	5.842538	-0.181854
C	1.557549	4.500525	-3.854533
C	-0.095587	7.544298	-2.440071
C	1.021453	5.794144	-3.766522
C	-0.695335	7.099827	-0.104526
C	-0.672715	8.000067	-1.218577
C	-0.067299	8.417948	-3.570422
C	1.035642	6.691871	-4.886625
C	-1.198115	9.301373	-1.147049
C	-0.606276	9.709282	-3.454308
C	0.515709	7.945895	-4.794177
C	-1.164901	10.145373	-2.254518
C	-2.301059	1.468576	3.159850
C	-3.179812	1.325825	4.271779
C	-1.248104	2.398530	3.208966
C	-2.951625	2.142533	5.428015
C	-4.305726	0.428728	4.295326
C	-1.029813	3.176927	4.334656
C	-3.808672	2.038909	6.567263
C	-1.863592	3.068992	5.457995
C	-5.121999	0.340601	5.382356
C	-4.906902	1.129657	6.558277
C	-3.575469	2.845359	7.723733
C	-1.652811	3.866910	6.632951
C	-5.738068	1.041251	7.687304
C	-4.431006	2.722590	8.830091
C	-2.469144	3.760125	7.716329
C	-5.500653	1.829438	8.810564

C	-5.364037	3.089665	-0.555096
C	-5.562957	4.488808	-0.372976
C	-6.449229	2.204525	-0.435296
C	-6.881840	4.951460	-0.053460
C	-4.513480	5.469021	-0.477362
C	-7.722609	2.661020	-0.138663
C	-7.131212	6.345057	0.144105
C	-7.966135	4.027224	0.063627
C	-4.759928	6.795706	-0.289601
C	-6.067728	7.287496	0.025364
C	-8.446535	6.807502	0.458160
C	-9.277573	4.520003	0.378672
C	-6.332975	8.653423	0.219631
C	-8.664732	8.181590	0.645462
C	-9.508158	5.847271	0.569057
C	-7.617689	9.093894	0.527068
O	4.381285	1.144912	-1.164152
H	1.463653	-2.857509	-3.865697
H	1.477695	-1.598449	-1.757509
H	-0.538211	-4.155850	2.302865
H	3.143245	-2.285625	3.492021
H	-2.615876	-1.703096	-4.573493
H	-0.594152	-2.918826	-5.279623
H	-0.967194	-2.346188	0.699377
H	1.526158	-4.126494	3.707809
O	3.570989	1.918170	0.806436
O	1.342588	1.824078	-0.827130
O	-1.760151	1.177624	0.878119
O	-4.003715	1.161853	-0.712150
H	1.967233	2.660177	-2.844821
O	0.884011	3.347413	0.785107
O	-3.035070	-0.426672	1.843303
O	-3.073540	3.123177	-1.355312
H	3.812604	4.168013	1.134360
H	6.326047	1.496354	-2.039052
H	4.962197	6.345464	1.189712
H	8.321651	1.892925	-3.392504

H	6.768481	7.829293	0.419592
H	10.138460	3.398834	-4.161641
H	10.411575	7.403297	-2.621778
H	8.763068	8.223324	-0.972309
H	11.277460	5.600260	-4.086309
H	-0.205380	5.189644	0.677541
H	1.996764	4.168722	-4.790834
H	-1.144651	7.439669	0.825070
H	1.475492	6.343813	-5.817113
H	-1.629896	9.644757	-0.210612
H	-0.582031	10.370135	-4.316534
H	0.533778	8.614639	-5.650602
H	-1.575352	11.148158	-2.182991
H	-0.586904	2.500306	2.357457
H	-4.493442	-0.182928	3.425035
H	-0.203205	3.881792	4.348257
H	-5.966602	-0.343429	5.367653
H	-0.820528	4.565509	6.635602
H	-6.573843	0.346938	7.673522
H	-4.249018	3.336564	9.708054
H	-2.297321	4.371265	8.598462
H	-6.152412	1.748591	9.675377
H	-6.296559	1.146627	-0.601939
H	-3.516306	5.133174	-0.722414
H	-8.540612	1.950558	-0.071648
H	-3.947318	7.510927	-0.386924
H	-10.087819	3.801003	0.462554
H	-5.518433	9.366595	0.125418
H	-9.666528	8.528758	0.883956
H	-10.506264	6.205042	0.807960
H	-7.805576	10.153356	0.674406
C	-8.166261	-1.735589	-2.146048
C	-5.739206	1.604891	-6.077099
C	-3.351272	1.695617	-4.606614
C	-4.156078	-0.178432	-3.162414
C	-4.756393	2.509351	-6.407442
C	-3.555568	2.556914	-5.661179

C	-5.170149	-1.059721	-2.849018
C	-6.389796	-1.066261	-3.569220
C	-5.564441	0.704485	-4.993005
C	-4.340852	0.741249	-4.245750
C	-4.766051	-3.237365	-1.990758
C	-6.580887	-0.214024	-4.622657
C	-4.483489	-3.951793	-0.719758
C	-4.489743	-5.374556	-0.640412
C	-4.168205	-3.187452	0.416973
C	-4.186871	-5.986476	0.620559
C	-4.800295	-6.239526	-1.748841
C	-3.856295	-3.785924	1.627032
C	-4.197055	-7.409572	0.754904
C	-3.864875	-5.182768	1.758558
C	-4.811750	-7.595057	-1.611419
C	-4.513324	-8.233925	-0.364795
C	-3.889473	-8.020089	2.010067
C	-3.556763	-5.823092	3.006727
C	-4.519241	-9.630618	-0.213373
C	-3.907611	-9.419920	2.115190
C	-3.568911	-7.178407	3.128074
C	-4.219947	-10.215560	1.014331
C	-9.026489	-2.907980	-1.835273
C	-10.195272	-2.790879	-1.030693
C	-8.644246	-4.164237	-2.336678
C	-10.954567	-3.975668	-0.755727
C	-10.677279	-1.544792	-0.494450
C	-9.373919	-5.307153	-2.054553
C	-12.140986	-3.906005	0.038362
C	-10.534144	-5.241765	-1.268428
C	-11.812172	-1.485770	0.256545
C	-12.584705	-2.654095	0.556765
C	-12.893409	-5.087908	0.319434
C	-11.307458	-6.413521	-0.968116
C	-13.753309	-2.605181	1.334696
C	-14.054871	-4.991944	1.102285
C	-12.434754	-6.341111	-0.209626

C	-14.479185	-3.762813	1.603676
O	-5.026120	-1.899317	-1.754025
O	-7.363703	-1.998559	-3.236713
O	-8.127725	-0.671693	-1.565020
H	-6.668915	1.569190	-6.638452
H	-2.437575	1.750862	-4.026015
H	-4.903622	3.194826	-7.236740
H	-2.791174	3.284058	-5.917547
H	-3.316138	-5.193665	3.859009
O	-4.778048	-3.691995	-3.115168
H	-7.518229	-0.243557	-5.168531
H	-4.146909	-2.108404	0.349316
H	-5.009018	-5.787428	-2.707671
H	-3.598073	-3.160873	2.476241
H	-5.047327	-8.221688	-2.467975
H	-4.759925	-10.252948	-1.071115
H	-3.672608	-9.879764	3.071318
H	-3.335536	-7.648783	4.079607
H	-4.228336	-11.296820	1.114642
H	-7.748572	-4.233777	-2.941055
H	-10.109346	-0.648152	-0.695512
H	-9.045460	-6.267703	-2.440551
H	-12.151749	-0.529751	0.646779
H	-10.968806	-7.366760	-1.364289
H	-14.086213	-1.648006	1.726833
H	-14.623474	-5.893241	1.314761
H	-13.010242	-7.236673	0.009006
H	-15.380232	-3.707945	2.207201
C	16.074200	-2.138856	0.154898
C	13.497721	-4.844297	-0.237951
C	15.485176	-3.358077	-0.174755
C	15.321046	-1.134991	0.758365
C	12.180719	-5.057879	0.028986
C	14.128093	-3.598132	0.093512
C	13.960027	-1.331504	1.045597
C	13.152033	-0.323080	1.662597
C	11.372888	-4.047990	0.651996

C	13.346567	-2.575024	0.714064
C	10.014341	-4.261627	0.929416
C	11.833304	-0.523235	1.939979
C	11.962760	-2.793347	0.999382
C	9.250576	-3.274268	1.527750
C	11.179072	-1.767018	1.625050
C	9.801657	-2.029797	1.882416
C	6.261141	-8.864780	-3.490422
C	5.259123	-5.576898	-5.006762
C	5.901665	-7.905944	-4.435717
C	6.358146	-8.522366	-2.144135
C	5.002555	-4.299010	-4.616199
C	5.631822	-6.582487	-4.052592
C	6.097275	-7.210224	-1.715585
C	6.181725	-6.820249	-0.340065
C	5.094676	-3.907247	-3.237848
C	5.729244	-6.220321	-2.673491
C	4.835716	-2.590538	-2.828050
C	5.923376	-5.545446	0.066627
C	5.460603	-4.879561	-2.256167
C	4.940827	-2.226479	-1.495107
C	5.555002	-4.516293	-0.871764
C	5.296271	-3.162891	-0.507820
C	6.601681	-0.023582	4.175862
C	5.373736	-2.702524	0.904131
C	4.229645	0.612161	3.906793
C	5.444709	0.637743	4.664995
C	6.559250	-0.685469	2.973585
C	5.351486	-0.723189	2.223231
C	3.143107	1.937169	5.633512
C	4.343037	1.963321	6.382289
C	4.206319	-0.092716	2.660312
C	3.087700	1.280339	4.424428
C	5.467407	1.328924	5.906129
C	8.919279	-1.022167	2.531059
H	9.556694	-5.210786	0.665881
H	17.125310	-1.971241	-0.060196

H	14.097113	-5.618057	-0.710296
H	16.075519	-4.139357	-0.645885
H	15.781827	-0.184698	1.014116
H	11.711311	-6.003622	-0.227071
H	13.615982	0.627519	1.912904
H	6.452216	-7.575145	0.394000
H	11.252940	0.255236	2.412647
H	8.205842	-3.462968	1.737446
H	6.465160	-9.883754	-3.805443
H	5.186373	-5.858650	-6.053844
H	5.825553	-8.176706	-5.485351
H	6.636255	-9.271972	-1.408183
H	4.554481	-1.846213	-3.567632
H	5.971639	-5.287772	1.114546
H	4.736165	-1.202514	-1.208084
H	7.519515	0.011286	4.746311
O	5.445077	-3.385778	1.905032
H	4.723776	-3.543868	-5.346058
H	2.257328	2.436227	6.015106
H	4.374315	2.485386	7.334088
H	2.164498	1.267237	3.855482
H	6.393768	1.345887	6.473687
O	9.254383	0.001334	3.088544
O	7.600303	-1.406357	2.422423
O	5.346154	-1.327113	0.973224

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3h.

–7965.21080936 hartree

C	1.044278	-1.466183	-3.752234
C	0.958604	-0.934026	-2.485561
C	-1.613567	0.531433	-0.215719
C	-1.440486	-0.518441	-2.814877
C	-0.278564	-0.454964	-1.975621
C	-0.391319	0.066945	-0.645042
C	0.716540	-3.290881	1.854005
C	2.663014	-2.110200	2.676106
C	1.155015	-1.029425	1.066087

C	-1.318320	-1.087991	-4.111274
C	-0.105778	-1.551813	-4.568555
C	-2.746617	0.521080	-1.064209
C	-2.687857	-0.002362	-2.336265
C	2.331787	-0.976429	1.885123
C	3.153735	0.199548	1.871879
C	0.364233	-2.210293	1.077542
C	1.876924	-3.240707	2.657827
C	2.777743	1.261404	1.081153
C	1.593393	1.222965	0.303537
C	0.796282	0.102308	0.262542
C	4.298539	2.661057	-0.067001
C	0.868355	3.473241	0.095020
C	-2.360965	0.339998	2.026003
C	-4.155735	2.360906	-0.605507
C	4.995063	3.968251	0.028343
C	6.058991	4.313047	-0.853611
C	4.562510	4.887861	0.999286
C	6.654009	5.611273	-0.725819
C	6.588856	3.425114	-1.855410
C	5.138886	6.141807	1.113411
C	7.723360	6.004310	-1.589085
C	6.185022	6.530440	0.262972
C	7.610225	3.806836	-2.671825
C	8.212680	5.103149	-2.579938
C	8.311304	7.301125	-1.468137
C	6.793960	7.826742	0.362635
C	9.262435	5.508561	-3.420779
C	9.358373	7.663486	-2.330454
C	7.809555	8.196147	-0.464172
C	9.827678	6.775292	-3.296365
C	0.704575	4.558119	-0.905058
C	-0.014394	5.750888	-0.606654
C	1.305654	4.398770	-2.165770
C	-0.094917	6.767080	-1.614743
C	-0.685331	5.991851	0.644154
C	1.228471	5.387071	-3.132548

C	-0.803470	7.982566	-1.362066
C	0.535279	6.581289	-2.883911
C	-1.360784	7.152077	0.876879
C	-1.443700	8.191682	-0.105317
C	-0.876580	8.999125	-2.363581
C	0.445833	7.618922	-3.871983
C	-2.130437	9.395398	0.127106
C	-1.575692	10.185324	-2.088504
C	-0.228428	8.774601	-3.624564
C	-2.195160	10.380304	-0.855609
C	-2.367691	1.058145	3.325632
C	-3.245855	0.683003	4.382545
C	-1.456289	2.112812	3.507700
C	-3.164808	1.401014	5.621012
C	-4.234250	-0.358348	4.274114
C	-1.379476	2.794901	4.711313
C	-4.027954	1.065062	6.709737
C	-2.219371	2.460406	5.784192
C	-5.057443	-0.668511	5.314219
C	-4.986296	0.018829	6.568851
C	-3.940966	1.774211	7.947340
C	-2.153734	3.155998	7.038462
C	-5.825524	-0.297707	7.649986
C	-4.798949	1.422877	9.001609
C	-2.974823	2.828519	8.072854
C	-5.730881	0.397379	8.852986
C	-5.542997	2.703106	-0.203264
C	-5.910885	4.032850	0.152592
C	-6.513696	1.686954	-0.223218
C	-7.278462	4.289759	0.497849
C	-4.986531	5.135815	0.200589
C	-7.835288	1.946248	0.099575
C	-7.695947	5.606072	0.867080
C	-8.243888	3.235811	0.469534
C	-5.392842	6.387813	0.551951
C	-6.753114	6.675452	0.896100
C	-9.060052	5.864055	1.206541

C	-9.607812	3.524036	0.813986
C	-7.183038	7.963052	1.258153
C	-9.444206	7.166222	1.563762
C	-9.998687	4.778295	1.167710
C	-8.514085	8.203937	1.588832
O	4.321586	1.871932	-0.986182
H	2.000525	-1.824323	-4.121638
H	1.844581	-0.871297	-1.863923
H	0.097262	-4.182727	1.847568
H	3.555104	-2.081347	3.291377
H	-2.202013	-1.161417	-4.734872
H	-0.033313	-1.984816	-5.561741
H	-0.534707	-2.246842	0.473769
H	2.151796	-4.096875	3.266562
O	3.545993	2.415969	1.070349
O	1.288890	2.306592	-0.507949
O	-1.736023	1.087951	1.050411
O	-3.954128	0.989552	-0.569443
H	1.853118	3.487878	-2.372146
O	0.692186	3.542580	1.294567
O	-2.810277	-0.763235	1.791274
O	-3.271054	3.114831	-0.947080
H	3.751166	4.607441	1.658838
H	6.158725	2.439285	-1.949095
H	4.777844	6.837387	1.865430
H	7.987736	3.111343	-3.417060
H	6.421836	8.511209	1.119942
H	9.630781	4.817636	-4.174361
H	9.801802	8.651068	-2.235811
H	8.260741	9.181020	-0.376857
H	10.638464	7.072703	-3.954786
H	-0.637231	5.229618	1.407423
H	1.712856	5.242429	-4.093826
H	-1.856620	7.303571	1.832257
H	0.933450	7.458373	-4.829509
H	-2.610024	9.551254	1.089918
H	-1.628139	10.955730	-2.853028

H	-0.287634	9.551286	-4.382387
H	-2.729983	11.304990	-0.660340
H	-0.791670	2.387480	2.697910
H	-4.311509	-0.897857	3.341564
H	-0.660027	3.600615	4.827644
H	-5.796275	-1.457482	5.199586
H	-1.427622	3.957590	7.142613
H	-6.554280	-1.095603	7.535597
H	-4.728226	1.963678	9.941526
H	-2.913526	3.364387	9.016386
H	-6.386834	0.139951	9.679242
H	-6.232756	0.685416	-0.520427
H	-3.954095	4.955757	-0.061869
H	-8.561796	1.140845	0.055845
H	-4.671699	7.200901	0.567472
H	-10.325885	2.709128	0.785552
H	-6.459857	8.774009	1.276042
H	-10.482556	7.357889	1.820887
H	-11.034659	4.980730	1.426739
H	-8.829801	9.205233	1.866687
C	-7.720134	-2.197812	-2.422864
C	-5.718438	1.875097	-5.870953
C	-3.362603	2.078515	-4.360362
C	-3.930100	-0.043513	-3.168336
C	-4.855436	2.927621	-6.072121
C	-3.670967	3.030905	-5.305632
C	-4.826879	-1.075229	-2.982371
C	-6.034618	-1.144168	-3.719023
C	-5.434472	0.876823	-4.901768
C	-4.226255	0.972343	-4.134899
C	-4.154473	-3.274235	-2.387455
C	-6.328909	-0.198926	-4.663676
C	-3.789640	-4.099183	-1.207197
C	-3.610865	-5.509682	-1.302692
C	-3.584402	-3.448015	0.021423
C	-3.238944	-6.229588	-0.119580
C	-3.798162	-6.262893	-2.515542

C	-3.205797	-4.147262	1.156133
C	-3.063341	-7.647665	-0.160906
C	-3.032820	-5.539012	1.115466
C	-3.632790	-7.615023	-2.545542
C	-3.261273	-8.360150	-1.380160
C	-2.686790	-8.364813	1.016712
C	-2.652201	-6.284620	2.282620
C	-3.084847	-9.753776	-1.401263
C	-2.521663	-9.757327	0.948966
C	-2.487234	-7.634602	2.236616
C	-2.719478	-10.443360	-0.248009
C	-8.428688	-3.496820	-2.274826
C	-9.610659	-3.623733	-1.491362
C	-7.887028	-4.625692	-2.913505
C	-10.218853	-4.917440	-1.380534
C	-10.249664	-2.521491	-0.821033
C	-8.470712	-5.875561	-2.789157
C	-11.413163	-5.091631	-0.614826
C	-9.638248	-6.049898	-2.030942
C	-11.390921	-2.694602	-0.097837
C	-12.015092	-3.976659	0.038963
C	-12.015407	-6.382245	-0.498021
C	-10.262490	-7.335511	-1.894055
C	-13.189182	-4.167068	0.786264
C	-13.188380	-6.526024	0.259962
C	-11.398264	-7.495352	-1.162040
C	-13.768088	-5.429015	0.894545
O	-4.582066	-2.019040	-1.995004
O	-6.884592	-2.224240	-3.519918
O	-7.819112	-1.216667	-1.716788
H	-6.635533	1.794052	-6.448130
H	-2.463272	2.173988	-3.762851
H	-5.085516	3.686290	-6.814269
H	-3.002348	3.872402	-5.459144
H	-2.502362	-5.740483	3.211025
O	-4.103796	-3.585489	-3.558691
H	-7.254170	-0.276854	-5.225170

H	-3.702885	-2.375107	0.086429
H	-4.058453	-5.725721	-3.416097
H	-3.037208	-3.604655	2.081170
H	-3.779109	-8.155371	-3.477472
H	-3.236432	-10.290388	-2.334018
H	-2.234918	-10.298396	1.846682
H	-2.200970	-8.185683	3.128521
H	-2.586716	-11.520642	-0.281178
H	-6.983795	-4.509953	-3.499316
H	-9.795656	-1.544265	-0.897571
H	-8.020826	-6.733943	-3.279391
H	-11.851002	-1.842653	0.396196
H	-9.803308	-8.184208	-2.393250
H	-13.643104	-3.313313	1.282091
H	-13.642560	-7.509338	0.347249
H	-11.859939	-8.474653	-1.067975
H	-14.675601	-5.559355	1.476420
C	11.881684	-8.901259	2.507528
C	12.840654	-5.950365	0.389396
C	12.569645	-8.104389	1.594368
C	10.761598	-8.405040	3.169757
C	12.419422	-4.680277	0.142720
C	12.150184	-6.791867	1.325172
C	10.305854	-7.097861	2.931253
C	9.158767	-6.551591	3.592619
C	11.270803	-4.133101	0.807828
C	11.001919	-6.273235	1.999424
C	10.832690	-2.823182	0.561362
C	8.722438	-5.283607	3.352542
C	10.553627	-4.940146	1.744285
C	9.726123	-2.311264	1.218090
C	9.398362	-4.421776	2.417641
C	8.997440	-3.083586	2.139349
C	8.464342	-1.859177	-7.148630
C	5.644373	-3.870692	-5.694979
C	7.430450	-2.786679	-7.035515
C	8.801110	-1.047304	-6.068523

C	4.961344	-3.989440	-4.524122
C	6.711762	-2.921553	-5.836955
C	8.108059	-1.146827	-4.850745
C	8.423923	-0.329969	-3.717593
C	5.280429	-3.170512	-3.388585
C	7.048918	-2.092629	-4.722578
C	4.583821	-3.291656	-2.176632
C	7.743127	-0.430259	-2.541233
C	6.333587	-2.209583	-3.490221
C	4.906136	-2.492824	-1.092069
C	6.666666	-1.372927	-2.373677
C	5.929009	-1.531141	-1.164641
C	6.762639	0.304665	4.252465
C	6.187734	-0.681744	0.027351
C	4.427419	1.018458	3.926317
C	5.634037	1.039331	4.699979
C	6.706617	-0.401482	3.082433
C	5.531008	-0.393187	2.290924
C	3.364779	2.437526	5.593404
C	4.557922	2.462096	6.352353
C	4.397331	0.280311	2.696723
C	3.299683	1.734533	4.411054
C	5.667052	1.776716	5.913059
C	7.807024	-2.471748	2.786247
H	11.369767	-2.208145	-0.154861
H	12.220814	-9.914129	2.703129
H	13.712430	-6.350803	-0.121219
H	13.442856	-8.495065	1.078896
H	10.226552	-9.028373	3.881061
H	12.948851	-4.051050	-0.567338
H	8.627370	-7.178153	4.304358
H	9.236016	0.387165	-3.809558
H	7.846303	-4.903547	3.857524
H	9.398238	-1.300256	1.011720
H	9.009360	-1.769353	-8.083543
H	5.392623	-4.497837	-6.546047
H	7.169711	-3.418458	-7.880301

H	9.607696	-0.324645	-6.158785
H	3.783374	-4.020811	-2.092018
H	7.997790	0.208782	-1.708590
H	4.356310	-2.603122	-0.166652
H	7.675258	0.289775	4.839254
O	6.896880	0.298140	0.102386
H	4.157374	-4.713379	-4.424294
H	2.490806	2.976439	5.946837
H	4.595262	3.020781	7.282857
H	2.380823	1.726307	3.835595
H	6.587283	1.785951	6.490860
O	6.913768	-3.034447	3.381471
O	7.820446	-1.097725	2.635615
O	5.489497	-1.147746	1.127074

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3i.

–7965.20974651 hartree

C	0.102359	-2.507966	-3.292503
C	0.227817	-1.695232	-2.188536
C	-1.809002	0.754445	-0.248899
C	-2.057903	-0.861205	-2.531187
C	-0.841296	-0.857009	-1.771845
C	-0.739730	-0.035853	-0.602081
C	-0.138012	-2.838573	2.645169
C	2.053903	-1.922080	3.104695
C	0.679406	-0.986017	1.295370
C	-2.153759	-1.716000	-3.662474
C	-1.100213	-2.520890	-4.033889
C	-2.990907	0.789055	-1.028312
C	-3.140603	-0.007256	-2.140558
C	1.893200	-0.971616	2.060373
C	2.913312	-0.012088	1.755677
C	-0.323782	-1.939117	1.620062
C	1.063009	-2.834378	3.388559
C	2.698738	0.881828	0.730830
C	1.492837	0.879626	-0.012833
C	0.497365	-0.037715	0.236711

C	4.396452	1.754090	-0.687818
C	1.153158	3.102782	-0.784430
C	-2.370073	1.140955	2.014081
C	-3.960042	2.940523	-0.875666
C	5.257500	2.950496	-0.868069
C	6.376691	2.943665	-1.749117
C	4.930001	4.119251	-0.158604
C	7.142597	4.148283	-1.884516
C	6.803302	1.788967	-2.495658
C	5.666639	5.282480	-0.304824
C	8.280362	4.188333	-2.748721
C	6.778412	5.324978	-1.159702
C	7.892683	1.833659	-3.312362
C	8.669268	3.025846	-3.476723
C	9.039356	5.390800	-2.889949
C	7.557193	6.519957	-1.322172
C	9.791062	3.083711	-4.320268
C	10.152479	5.403265	-3.745459
C	8.637473	6.552570	-2.148843
C	10.523367	4.260841	-4.452230
C	1.118284	3.913430	-2.028429
C	0.644904	5.257022	-2.035058
C	1.592641	3.332614	-3.217467
C	0.676656	5.983857	-3.270695
C	0.117559	5.927974	-0.875607
C	1.623492	4.041687	-4.406347
C	0.216365	7.336053	-3.326986
C	1.172302	5.369038	-4.461734
C	-0.320501	7.216606	-0.937283
C	-0.284937	7.972436	-2.153654
C	0.254876	8.063206	-4.556484
C	1.198667	6.122215	-5.683632
C	-0.726563	9.304526	-2.226613
C	-0.199396	9.391561	-4.583600
C	0.760614	7.409631	-5.730178
C	-0.684040	10.004762	-3.429975
C	-2.088273	2.047210	3.156967

C	-2.807223	1.951401	4.384119
C	-1.059382	2.995715	3.017669
C	-2.456193	2.845654	5.449465
C	-3.875631	1.014892	4.619186
C	-0.724246	3.851503	4.054516
C	-3.148216	2.789823	6.699084
C	-1.407000	3.801091	5.279158
C	-4.528822	0.967076	5.813762
C	-4.195923	1.843131	6.896615
C	-2.796655	3.678256	7.761940
C	-1.075475	4.682490	6.363040
C	-4.862287	1.800676	8.132617
C	-3.490678	3.600920	8.979922
C	-1.738908	4.625137	7.549626
C	-4.512603	2.671006	9.161938
C	-5.183755	3.648159	-0.418831
C	-5.283803	5.070196	-0.450648
C	-6.271448	2.878006	0.030867
C	-6.506537	5.676137	-0.008650
C	-4.227427	5.941638	-0.896545
C	-7.448493	3.472859	0.453653
C	-6.657289	7.097739	-0.023003
C	-7.593273	4.867908	0.447590
C	-4.380567	7.295463	-0.910390
C	-5.591156	7.927214	-0.479200
C	-7.876276	7.701326	0.415634
C	-8.806307	5.500511	0.883239
C	-5.758943	9.322034	-0.489933
C	-7.998905	9.099645	0.389108
C	-8.942603	6.854136	0.869421
C	-6.950261	9.900516	-0.059616
O	4.308212	0.791090	-1.421710
H	0.930420	-3.145124	-3.588658
H	1.151396	-1.690949	-1.620522
H	-0.922715	-3.549698	2.884819
H	2.978621	-1.928638	3.669622
H	-3.076700	-1.729921	-4.231477

H	-1.195469	-3.169028	-4.899983
H	-1.253619	-1.934956	1.063754
H	1.205941	-3.552739	4.190122
O	3.646566	1.860798	0.464020
O	1.352619	1.768076	-1.070899
O	-1.720154	1.570228	0.868226
O	-4.042805	1.585415	-0.606011
H	1.954376	2.312747	-3.191574
O	1.049117	3.499417	0.358034
O	-3.049223	0.137154	2.008740
O	-2.987044	3.408767	-1.427039
H	4.071409	4.106475	0.500759
H	6.233409	0.876404	-2.400043
H	5.383519	6.175106	0.245275
H	8.192395	0.943670	-3.859616
H	7.262060	7.404086	-0.764011
H	10.083136	2.193665	-4.870932
H	10.726348	6.320037	-3.850653
H	9.218254	7.464279	-2.260894
H	11.388122	4.288877	-5.108427
H	0.080040	5.386205	0.057452
H	2.004920	3.570830	-5.307712
H	-0.714305	7.694089	-0.043847
H	1.580212	5.636237	-6.577315
H	-1.099784	9.785966	-1.326507
H	-0.167583	9.940593	-5.520788
H	0.786934	7.967478	-6.662461
H	-1.028940	11.033686	-3.469614
H	-0.507519	3.048155	2.087654
H	-4.147664	0.334932	3.825439
H	0.077658	4.571904	3.919290
H	-5.324319	0.241155	5.960574
H	-0.276900	5.403652	6.211219
H	-5.658374	1.075189	8.276765
H	-3.219499	4.278314	9.785256
H	-1.477171	5.299240	8.360997
H	-5.037883	2.624970	10.111331

H	-6.192249	1.798136	0.031716
H	-3.301273	5.497565	-1.230199
H	-8.274458	2.852803	0.790018
H	-3.565900	7.923029	-1.262597
H	-9.619490	4.867016	1.226726
H	-4.942884	9.947800	-0.841264
H	-8.927769	9.553826	0.723639
H	-9.866931	7.318919	1.202336
H	-7.063641	10.980492	-0.074112
C	-7.492753	-3.169360	-3.128097
C	-6.147342	1.687354	-5.786787
C	-3.696969	1.824750	-4.426389
C	-4.433445	-0.004792	-2.892149
C	-5.186204	2.589894	-6.180461
C	-3.953093	2.659803	-5.490920
C	-5.424820	-0.887566	-2.517508
C	-6.654210	-0.957335	-3.217957
C	-5.918696	0.812848	-4.691687
C	-4.665724	0.877407	-3.997026
C	-5.791879	-1.579545	-0.271338
C	-6.898304	-0.126746	-4.277631
C	-5.352104	-2.591056	0.725157
C	-5.830003	-2.584837	2.068249
C	-4.430288	-3.572368	0.319031
C	-5.351518	-3.595162	2.967514
C	-6.768632	-1.621982	2.583844
C	-3.970788	-4.543156	1.192549
C	-5.803978	-3.632811	4.323161
C	-4.414943	-4.578725	2.523029
C	-7.196301	-1.665608	3.876955
C	-6.737894	-2.664421	4.795277
C	-5.326643	-4.638978	5.218773
C	-3.951609	-5.578524	3.443328
C	-7.174005	-2.718497	6.129982
C	-5.788130	-4.653920	6.544800
C	-4.386317	-5.608001	4.732425
C	-6.702557	-3.703465	6.994404

C	-8.533840	-3.998368	-2.464971
C	-8.828141	-5.322175	-2.900356
C	-9.224622	-3.451448	-1.369631
C	-9.840354	-6.059457	-2.201420
C	-8.181650	-5.961252	-4.017207
C	-10.191350	-4.174419	-0.690807
C	-10.179257	-7.386973	-2.608865
C	-10.521909	-5.479066	-1.087322
C	-8.513434	-7.225482	-4.401146
C	-9.516075	-7.987710	-3.718892
C	-11.184460	-8.123823	-1.909783
C	-11.525697	-6.242764	-0.401509
C	-9.862941	-9.292984	-4.105188
C	-11.498529	-9.425855	-2.330754
C	-11.843288	-7.506335	-0.793874
C	-10.843930	-10.002875	-3.417353
O	-5.176586	-1.787233	-1.489821
O	-7.632819	-1.839042	-2.780044
O	-6.617710	-3.538268	-3.880446
H	-7.098993	1.630481	-6.308249
H	-2.758700	1.898778	-3.888720
H	-5.374168	3.254704	-7.018347
H	-3.204213	3.382959	-5.799121
H	-3.241749	-6.317815	3.082670
O	-6.583776	-0.673508	-0.112748
H	-7.847525	-0.194683	-4.799042
H	-4.074397	-3.563120	-0.702561
H	-7.130053	-0.854519	1.916225
H	-3.260449	-5.288838	0.847446
H	-7.906916	-0.924182	4.233617
H	-7.890146	-1.980083	6.480914
H	-5.421373	-5.420682	7.221765
H	-4.027009	-6.370571	5.418234
H	-7.049006	-3.731688	8.023163
H	-8.977589	-2.448163	-1.046009
H	-7.411973	-5.415707	-4.543619
H	-10.701007	-3.731501	0.159970

H	-8.007601	-7.681074	-5.248556
H	-12.030114	-5.784088	0.444416
H	-9.353666	-9.745140	-4.951923
H	-12.263030	-9.982934	-1.795933
H	-12.605943	-8.072171	-0.265435
H	-11.100149	-11.011121	-3.728739
C	15.711579	-3.373224	-0.095839
C	12.900430	-5.864563	-0.044129
C	15.007169	-4.566576	-0.243564
C	15.074440	-2.237639	0.397804
C	11.583721	-5.923653	0.293721
C	13.648420	-4.648112	0.100577
C	13.716350	-2.273420	0.755285
C	13.025628	-1.126713	1.263705
C	10.893584	-4.774777	0.807914
C	12.985477	-3.488840	0.609679
C	9.535967	-4.828794	1.157436
C	11.708914	-1.171204	1.610577
C	11.602760	-3.544375	0.968859
C	8.886756	-3.709325	1.648937
C	10.938236	-2.381158	1.482942
C	9.556944	-2.484735	1.820242
C	5.213021	-9.563574	-2.548879
C	4.434765	-6.404245	-4.426893
C	4.897887	-8.696531	-3.593445
C	5.395652	-9.072279	-1.258739
C	4.305856	-5.070795	-4.188938
C	4.759273	-7.317694	-3.368126
C	5.266902	-7.699992	-0.987213
C	5.442499	-7.156949	0.326426
C	4.489470	-4.526357	-2.872994
C	4.945466	-6.802935	-2.047883
C	4.362331	-3.152037	-2.620711
C	5.312527	-5.824395	0.580688
C	4.811322	-5.402922	-1.790858
C	4.555039	-2.641543	-1.346883
C	4.995360	-4.886036	-0.465519

C	4.870336	-3.480853	-0.263391
C	6.645552	0.068022	3.950155
C	5.048360	-2.862579	1.077771
C	4.328713	0.881825	3.679406
C	5.572670	0.887217	4.389761
C	6.494082	-0.727745	2.841566
C	5.256944	-0.744570	2.140310
C	3.435970	2.499238	5.261766
C	4.664355	2.505257	5.963374
C	4.190915	0.036480	2.531559
C	3.272234	1.709503	4.145579
C	5.708211	1.718036	5.534295
C	8.793738	-1.328486	2.364070
H	8.988082	-5.758639	1.034921
H	16.762093	-3.329069	-0.367277
H	13.409977	-6.742439	-0.432452
H	15.507129	-5.450923	-0.629367
H	15.625109	-1.307811	0.511680
H	11.024791	-6.848207	0.179057
H	13.579188	-0.197521	1.371926
H	5.677927	-7.839647	1.139092
H	11.218591	-0.290431	1.998001
H	7.840349	-3.775185	1.916877
H	5.315511	-10.627208	-2.742202
H	4.294244	-6.801833	-5.428519
H	4.754975	-9.083248	-4.598868
H	5.639332	-9.750208	-0.445135
H	4.115183	-2.479413	-3.437179
H	5.427429	-5.448003	1.586688
H	4.451252	-1.576248	-1.181966
H	7.586411	0.086724	4.482715
O	5.103091	-3.424356	2.152575
H	4.062675	-4.386552	-4.997234
H	2.613779	3.119266	5.606367
H	4.781246	3.133035	6.841845
H	2.328144	1.713308	3.611851
H	6.655806	1.718464	6.065950

O	9.239637	-0.277354	2.772560
O	7.443675	-1.603876	2.352988
O	5.144862	-1.493007	0.976229

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3j.

–7965.21272221 hartree

C	0.061651	-3.144025	-2.903181
C	0.231830	-2.254460	-1.866910
C	-1.641824	0.500072	-0.189315
C	-1.983782	-1.290391	-2.322360
C	-0.782590	-1.314774	-1.538141
C	-0.635397	-0.405446	-0.441688
C	-0.087569	-3.139491	2.887674
C	2.098308	-2.212708	3.355430
C	0.742665	-1.308532	1.516720
C	-2.129519	-2.232801	-3.376075
C	-1.132863	-3.139508	-3.657698
C	-2.800420	0.562803	-0.999611
C	-2.996256	-0.315865	-2.040980
C	1.945088	-1.274227	2.299194
C	2.949079	-0.291241	2.015989
C	-0.264898	-2.254341	1.849033
C	1.108053	-3.125185	3.640508
C	2.746862	0.581512	0.971041
C	1.587118	0.510016	0.163586
C	0.586900	-0.400814	0.419947
C	3.508512	2.825081	0.994839
C	2.062284	1.128798	-2.067550
C	-2.137461	1.122305	2.036668
C	-3.575834	2.802637	-1.031253
C	4.675217	3.670759	0.636470
C	4.573659	5.089430	0.559221
C	5.908874	3.038853	0.402502
C	5.754349	5.839454	0.245265
C	3.346846	5.818325	0.750777
C	7.046706	3.773155	0.109527
C	5.702481	7.264865	0.151602

C	6.999221	5.172555	0.025025
C	3.304250	7.176483	0.654385
C	4.471124	7.953060	0.359399
C	6.881487	8.013266	-0.151991
C	8.168152	5.949607	-0.277653
C	4.439810	9.354307	0.264189
C	6.803599	9.412465	-0.236186
C	8.113392	7.306508	-0.361851
C	5.594696	10.074639	-0.030003
C	1.645920	2.079026	-3.131026
C	2.355113	2.181966	-4.362198
C	0.490653	2.851362	-2.919504
C	1.862832	3.090997	-5.355923
C	3.548460	1.435699	-4.665063
C	0.012801	3.717798	-3.889357
C	2.541907	3.232424	-6.605762
C	0.682331	3.860805	-5.114134
C	4.189864	1.576667	-5.858748
C	3.718029	2.471490	-6.872778
C	2.048347	4.133138	-7.599714
C	0.208457	4.757920	-6.131034
C	4.370180	2.622306	-8.107983
C	2.733457	4.252132	-8.819333
C	0.860668	4.889208	-7.318329
C	3.882420	3.503905	-9.069248
C	-1.740015	2.082959	3.097420
C	-2.460923	2.188602	4.321671
C	-0.589690	2.863551	2.890083
C	-1.985944	3.110598	5.312045
C	-3.649161	1.432647	4.621034
C	-0.129295	3.743136	3.856738
C	-2.676418	3.254886	6.555256
C	-0.811393	3.890435	5.073960
C	-4.301021	1.575473	5.808783
C	-3.846257	2.483237	6.819153
C	-2.200228	4.168462	7.545959
C	-0.355494	4.801004	6.087067

C	-4.509156	2.636194	8.048284
C	-2.895762	4.289260	8.759482
C	-1.018639	4.935074	7.267881
C	-4.038276	3.530276	9.006497
C	-4.743000	3.645526	-0.666996
C	-4.644237	5.064546	-0.587865
C	-5.974829	3.010797	-0.430785
C	-5.825770	5.811691	-0.269781
C	-3.419624	5.796810	-0.781586
C	-7.113254	3.742496	-0.133923
C	-5.776893	7.237096	-0.174132
C	-7.068616	5.141799	-0.047389
C	-3.379869	7.154913	-0.683117
C	-4.547643	7.928400	-0.383881
C	-6.956836	7.982394	0.133393
C	-8.238635	5.915721	0.258925
C	-4.519172	9.329541	-0.286495
C	-6.881865	9.381628	0.219579
C	-8.186686	7.272589	0.345019
C	-5.674940	10.046829	0.011577
O	2.484808	3.175226	1.545313
H	0.850499	-3.850677	-3.142455
H	1.153533	-2.250845	-1.296437
H	-0.872601	-3.849049	3.130905
H	3.012793	-2.201972	3.937806
H	-3.043183	-2.229147	-3.959776
H	-1.263333	-3.850317	-4.468200
H	-1.188277	-2.257337	1.281445
H	1.244269	-3.832750	4.452914
O	3.727453	1.508741	0.646442
O	1.434101	1.423063	-0.868204
O	-1.499494	1.415888	0.841815
O	-3.787143	1.485567	-0.680092
H	-0.056494	2.754284	-1.992225
O	2.821111	0.189387	-2.163056
O	-2.888838	0.176581	2.130414
O	-2.551691	3.158485	-1.577651

H	5.975317	1.959775	0.467432
H	2.449655	5.261690	0.979031
H	7.990012	3.260175	-0.054243
H	2.361862	7.697711	0.802159
H	9.104967	5.423662	-0.439769
H	3.498028	9.872604	0.423231
H	7.702865	9.977714	-0.465860
H	9.006656	7.881189	-0.592112
H	5.553523	11.157564	-0.099788
H	3.925480	0.744362	-3.925251
H	-0.896056	4.279779	-3.697338
H	5.083676	0.991984	-6.059847
H	-0.687596	5.337147	-5.925242
H	5.264896	2.038182	-8.305971
H	2.354639	4.938194	-9.572194
H	0.491667	5.574167	-8.077260
H	4.398867	3.608610	-10.018849
H	-0.033120	2.762610	1.968376
H	-4.014069	0.732219	3.883905
H	0.775341	4.313140	3.668476
H	-5.189089	0.981259	6.008078
H	0.536332	5.387642	5.884004
H	-5.398719	2.043452	8.243855
H	-2.530019	4.984956	9.509971
H	-0.662642	5.629562	8.024362
H	-4.562870	3.636332	9.951485
H	-6.040093	1.931955	-0.499292
H	-2.521557	5.242701	-1.012087
H	-8.055475	3.227575	0.030340
H	-2.439002	7.678525	-0.832198
H	-9.173974	5.387487	0.422189
H	-3.578924	9.850187	-0.446969
H	-7.781837	9.944502	0.452270
H	-9.080742	7.844905	0.578059
H	-5.635982	11.129725	0.082976
C	-7.628899	-3.072328	-2.900302
C	-5.616632	1.258577	-6.017852

C	-3.230943	1.274896	-4.541677
C	-4.252701	-0.255286	-2.849644
C	-4.534852	1.986405	-6.457845
C	-3.333430	1.994785	-5.711190
C	-5.358017	-0.969465	-2.436946
C	-6.552047	-0.985895	-3.200579
C	-5.545331	0.503555	-4.817398
C	-4.326681	0.507069	-4.061683
C	-5.963626	-1.386269	-0.175284
C	-6.647242	-0.264329	-4.359078
C	-5.759691	-2.357495	0.929665
C	-6.208623	-2.093027	2.256356
C	-5.113509	-3.572252	0.640651
C	-5.989896	-3.092643	3.261447
C	-6.859855	-0.872717	2.657038
C	-4.907510	-4.533278	1.615378
C	-6.424469	-2.875624	4.605996
C	-5.336312	-4.320524	2.934135
C	-7.270212	-0.672913	3.940917
C	-7.076394	-1.658566	4.961897
C	-6.211176	-3.873740	5.606123
C	-5.134286	-5.305868	3.958218
C	-7.501246	-1.464682	6.287394
C	-6.650425	-3.636615	6.918559
C	-5.552083	-5.093698	5.235604
C	-7.289006	-2.444518	7.254361
C	-8.802775	-3.698646	-2.236790
C	-9.208813	-5.031240	-2.533820
C	-9.509439	-2.947513	-1.281389
C	-10.347017	-5.565719	-1.844242
C	-8.555020	-5.871429	-3.503545
C	-10.599234	-3.475257	-0.609253
C	-10.800084	-6.893608	-2.117445
C	-11.042158	-4.780134	-0.873540
C	-8.995710	-7.134619	-3.760408
C	-10.125876	-7.696833	-3.083433
C	-11.931409	-7.428266	-1.427280

C	-12.174040	-5.343145	-0.193121
C	-10.586003	-8.999211	-3.339210
C	-12.356046	-8.735243	-1.714789
C	-12.599962	-6.608182	-0.457196
C	-11.689472	-9.511177	-2.661248
O	-5.265380	-1.765973	-1.303459
O	-7.646437	-1.700394	-2.732607
O	-6.744335	-3.622570	-3.519076
H	-6.543686	1.248335	-6.584697
H	-2.311128	1.299697	-3.969060
H	-4.601657	2.557823	-7.378943
H	-2.483955	2.573847	-6.060565
H	-4.636014	-6.232467	3.687000
O	-6.650962	-0.385544	-0.163793
H	-7.571848	-0.289622	-4.926519
H	-4.778452	-3.756794	-0.371663
H	-7.021662	-0.110204	1.910293
H	-4.411726	-5.465394	1.360239
H	-7.758679	0.260096	4.210200
H	-8.004302	-0.537499	6.549416
H	-6.485708	-4.398824	7.675269
H	-5.391906	-5.848627	6.000719
H	-7.623265	-2.279695	8.274301
H	-9.177238	-1.941170	-1.059621
H	-7.691954	-5.479199	-4.021626
H	-11.119184	-2.876793	0.133194
H	-8.481265	-7.744636	-4.498481
H	-12.686914	-4.730185	0.542829
H	-10.067765	-9.606206	-4.076603
H	-13.216380	-9.138197	-1.187264
H	-13.459000	-7.020725	0.065221
H	-12.032383	-10.519994	-2.870669
C	11.832504	-9.313126	2.703579
C	12.713850	-6.381032	0.526391
C	12.496573	-8.518657	1.770836
C	10.708063	-8.828089	3.366715
C	12.264815	-5.124253	0.261183

C	12.048336	-7.219769	1.482503
C	10.223911	-7.534747	3.109442
C	9.071679	-7.000081	3.771333
C	11.110782	-4.588884	0.926484
C	10.895332	-6.712719	2.157462
C	10.643742	-3.292795	0.660554
C	8.607690	-5.745554	3.512980
C	10.417923	-5.393656	1.882974
C	9.532441	-2.791759	1.317570
C	9.257838	-4.886971	2.556956
C	8.827322	-3.562226	2.258643
C	7.528786	-2.457435	-7.184873
C	5.996504	-5.196306	-5.120226
C	6.993874	-3.693040	-6.825745
C	7.629373	-1.435175	-6.244412
C	5.573402	-5.409831	-3.844747
C	6.549399	-3.932027	-5.515505
C	7.194634	-1.629018	-4.922416
C	7.273597	-0.600280	-3.928866
C	5.663450	-4.381528	-2.847161
C	6.649054	-2.890297	-4.542538
C	5.229882	-4.595329	-1.530011
C	6.856578	-0.800778	-2.647241
C	6.208050	-3.108409	-3.200368
C	5.328106	-3.592192	-0.581028
C	6.314916	-2.065298	-2.222197
C	5.867550	-2.332681	-0.896171
C	6.581441	-0.175144	4.361818
C	5.976085	-1.319509	0.184380
C	4.250100	0.554252	4.045487
C	5.462380	0.572899	4.811225
C	6.508066	-0.898561	3.202822
C	5.319530	-0.904701	2.430222
C	3.217786	2.023721	5.687702
C	4.413432	2.038050	6.443243
C	4.198786	-0.210744	2.833124
C	3.137111	1.301895	4.517707

C	5.511331	1.329666	6.011660
C	7.629669	-2.964125	2.905378
H	11.161893	-2.679995	-0.071359
H	12.193853	-10.315290	2.913917
H	13.589446	-6.772593	0.015459
H	13.373346	-8.900575	1.254864
H	10.191840	-9.449444	4.093486
H	12.775460	-4.497049	-0.464234
H	8.559409	-7.624343	4.498942
H	7.679039	0.366126	-4.217536
H	7.728659	-5.374455	4.019630
H	9.181874	-1.791986	1.094269
H	7.868730	-2.291435	-8.202755
H	5.921949	-5.984212	-5.864978
H	6.915995	-4.488374	-7.562052
H	8.049903	-0.473221	-6.525417
H	4.817370	-5.561739	-1.255165
H	6.932127	-0.005671	-1.920626
H	4.994460	-3.778461	0.431562
H	7.502259	-0.183252	4.935807
O	6.612923	-0.286287	0.166806
H	5.156242	-6.370223	-3.554846
H	2.355250	2.587093	6.030371
H	4.462919	2.611116	7.364428
H	2.221047	1.310189	3.938859
H	6.434427	1.336733	6.584937
O	6.747531	-3.536474	3.507755
O	7.620214	-1.591387	2.742583
O	5.253645	-1.701285	1.295743

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3k.

–7965.20830520 hartree

C	0.296205	1.867310	3.457966
C	0.376045	1.182848	2.265986
C	-1.774059	-0.976010	0.112969
C	-1.941496	0.416210	2.545159
C	-0.731720	0.440573	1.774352

C	-0.662351	-0.285156	0.539832
C	-0.155769	2.183031	-2.986182
C	2.065170	1.297664	-3.354844
C	0.734402	0.530459	-1.436643
C	-1.988281	1.136280	3.769657
C	-0.896064	1.845966	4.214903
C	-2.978107	-0.975278	0.859826
C	-3.075297	-0.316508	2.064376
C	1.949498	0.479287	-2.198536
C	3.018837	-0.377170	-1.775642
C	-0.303499	1.403096	-1.861554
C	1.038129	2.129722	-3.738919
C	2.848218	-1.138104	-0.641557
C	1.632519	-1.121589	0.084406
C	0.588231	-0.300733	-0.278946
C	4.586651	-1.662504	0.881976
C	1.349763	-3.269728	1.047648
C	-1.701508	-3.025819	-1.074761
C	-4.794574	-1.228629	-0.646837
C	5.506217	-2.764264	1.264480
C	6.602148	-2.555706	2.150328
C	5.259162	-4.046990	0.744478
C	7.428105	-3.678766	2.486405
C	6.947511	-1.276257	2.712731
C	6.053711	-5.128989	1.083769
C	8.545321	-3.518060	3.363370
C	7.145331	-4.973463	1.951330
C	8.017619	-1.130381	3.542974
C	8.853503	-2.235655	3.904710
C	9.364399	-4.638295	3.704269
C	7.983225	-6.081866	2.312254
C	9.956264	-2.096566	4.763732
C	10.455787	-4.453071	4.567770
C	9.043599	-5.922920	3.149952
C	10.747590	-3.194749	5.090925
C	1.100473	-3.946462	2.347160
C	1.024275	-5.365697	2.454006

C	0.913666	-3.149982	3.490697
C	0.761709	-5.939372	3.742521
C	1.203316	-6.266403	1.344335
C	0.651083	-3.709943	4.729676
C	0.685029	-7.358036	3.902446
C	0.570679	-5.102105	4.884928
C	1.131949	-7.617570	1.506490
C	0.872754	-8.217700	2.780656
C	0.420509	-7.929095	5.185622
C	0.303475	-5.701849	6.161887
C	0.796905	-9.609259	2.957228
C	0.352486	-9.325472	5.315394
C	0.231750	-7.052978	6.306742
C	0.539626	-10.155764	4.211974
C	-1.643726	-3.586677	-2.448756
C	-1.509203	-4.986590	-2.683336
C	-1.729470	-2.701623	-3.538230
C	-1.479628	-5.449838	-4.040747
C	-1.390268	-5.969204	-1.637390
C	-1.697165	-3.155972	-4.845443
C	-1.352665	-6.844804	-4.327484
C	-1.576507	-4.525214	-5.126196
C	-1.267451	-7.296447	-1.919848
C	-1.248381	-7.788982	-3.264303
C	-1.328481	-7.306895	-5.679660
C	-1.547795	-5.016256	-6.474869
C	-1.126685	-9.155839	-3.565179
C	-1.205522	-8.682302	-5.933524
C	-1.430398	-6.345513	-6.740660
C	-1.106227	-9.596209	-4.886118
C	-5.807666	-2.219290	-1.090211
C	-6.955227	-1.830978	-1.837133
C	-5.593278	-3.573906	-0.783988
C	-7.860899	-2.853200	-2.271912
C	-7.277842	-0.465152	-2.155852
C	-6.468174	-4.557329	-1.215588
C	-9.028230	-2.512226	-3.022784

C	-7.608538	-4.225317	-1.962469
C	-8.394505	-0.147047	-2.867868
C	-9.306157	-1.148889	-3.334908
C	-9.926790	-3.531307	-3.465508
C	-8.527462	-5.228865	-2.420840
C	-10.457542	-0.833226	-4.076414
C	-11.065274	-3.169783	-4.203476
C	-9.634719	-4.898681	-3.139474
C	-11.326237	-1.834457	-4.505129
O	4.445428	-0.591054	1.434426
H	1.153338	2.431672	3.812806
H	1.293387	1.204337	1.688675
H	-0.959746	2.846129	-3.291272
H	2.987710	1.275171	-3.922680
H	-2.909479	1.138160	4.340537
H	-0.954887	2.397259	5.148490
H	-1.221466	1.447966	-1.286388
H	1.150509	2.752674	-4.621097
O	3.851691	-2.004546	-0.234069
O	1.512796	-1.906418	1.222758
O	-1.735566	-1.642247	-1.103146
O	-4.047176	-1.729537	0.400014
H	0.972389	-2.074009	3.393421
O	1.417858	-3.772092	-0.053452
O	-1.726108	-3.628817	-0.023090
O	-4.589258	-0.126438	-1.109496
H	4.418240	-4.186097	0.076963
H	6.330767	-0.424610	2.466189
H	5.832546	-6.111422	0.676996
H	8.255032	-0.150253	3.948456
H	7.749496	-7.057910	1.896240
H	10.186459	-1.116056	5.171586
H	11.075457	-5.307868	4.825083
H	9.669797	-6.771180	3.413447
H	11.596582	-3.070300	5.756448
H	1.387974	-5.844419	0.367711
H	0.506079	-3.067915	5.593608

H	1.274316	-8.269430	0.648163
H	0.162459	-5.046248	7.016736
H	0.942303	-10.258464	2.097939
H	0.151148	-9.754795	6.293123
H	0.030932	-7.493246	7.279825
H	0.484151	-11.233634	4.331563
H	-1.825583	-1.641621	-3.343500
H	-1.395099	-5.629606	-0.612672
H	-1.767681	-2.448179	-5.666209
H	-1.176743	-8.010768	-1.105487
H	-1.623744	-4.295706	-7.284447
H	-1.048443	-9.870007	-2.749819
H	-1.188715	-9.028887	-6.963306
H	-1.411583	-6.703035	-7.766770
H	-1.011930	-10.656364	-5.101606
H	-4.714252	-3.848750	-0.214295
H	-6.612356	0.313633	-1.814510
H	-6.271221	-5.598736	-0.978287
H	-8.616603	0.894243	-3.084676
H	-8.316476	-6.266534	-2.177502
H	-10.660403	0.207174	-4.316123
H	-11.745131	-3.948083	-4.539498
H	-10.321439	-5.669543	-3.479071
H	-12.210562	-1.573798	-5.079171
C	-8.244474	1.393373	1.982008
C	-6.006010	-2.566962	5.443131
C	-3.594184	-2.479116	4.015572
C	-4.345596	-0.399882	2.848681
C	-5.043473	-3.528307	5.651086
C	-3.828162	-3.483210	4.928766
C	-5.330427	0.547371	2.668225
C	-6.563186	0.469250	3.364580
C	-5.797315	-1.517807	4.509360
C	-4.564118	-1.467313	3.780723
C	-4.902808	2.830890	2.183564
C	-6.789496	-0.531548	4.269176
C	-4.686051	3.761949	1.045976

C	-4.633669	5.174274	1.231356
C	-4.518442	3.215423	-0.239306
C	-4.422874	6.004395	0.080827
C	-4.793823	5.824983	2.506153
C	-4.305138	4.025495	-1.342618
C	-4.374586	7.427023	0.213010
C	-4.256941	5.421544	-1.213553
C	-4.747396	7.181576	2.623201
C	-4.537405	8.034751	1.492393
C	-4.163244	8.253816	-0.933347
C	-4.045005	6.275754	-2.347778
C	-4.487128	9.434307	1.603099
C	-4.120458	9.648236	-0.775871
C	-4.000313	7.629124	-2.215415
C	-4.280951	10.231077	0.479838
C	-9.138134	2.573967	1.850910
C	-10.199223	2.608988	0.900666
C	-8.910476	3.680853	2.686907
C	-11.018683	3.784548	0.838973
C	-10.510514	1.525010	0.004965
C	-9.696333	4.818542	2.611207
C	-12.104985	3.861039	-0.087084
C	-10.760324	4.895716	1.699856
C	-11.549743	1.604920	-0.872850
C	-12.385043	2.765599	-0.955896
C	-12.920243	5.033020	-0.150789
C	-11.592745	6.062094	1.612103
C	-13.458803	2.858030	-1.857052
C	-13.982298	5.081587	-1.067811
C	-12.625440	6.128577	0.728642
C	-14.247988	4.004216	-1.910922
O	-5.151128	1.550027	1.728100
O	-7.521715	1.451899	3.161313
O	-8.117412	0.468626	1.210513
H	-6.944686	-2.597623	5.989804
H	-2.662663	-2.457769	3.460869
H	-5.216463	-4.326091	6.367403

H	-3.073853	-4.247016	5.092432
H	-3.921121	5.811980	-3.322506
O	-4.878402	3.082509	3.370239
H	-7.737658	-0.568090	4.795629
H	-4.545882	2.140410	-0.367236
H	-4.941806	5.207158	3.379680
H	-4.177233	3.575359	-2.323055
H	-4.869379	7.642179	3.600352
H	-4.611039	9.890523	2.581598
H	-3.958895	10.272679	-1.650430
H	-3.839478	8.263116	-3.083337
H	-4.244309	11.311548	0.582368
H	-8.090538	3.640032	3.392653
H	-9.889948	0.641378	0.032587
H	-9.490393	5.663532	3.261811
H	-11.755945	0.769236	-1.536732
H	-11.377351	6.896648	2.273578
H	-13.668202	2.018702	-2.514722
H	-14.599438	5.974870	-1.113054
H	-13.247837	7.017818	0.674212
H	-15.074482	4.059292	-2.613168
C	15.632079	3.961708	-0.837817
C	12.678260	6.250082	-1.225555
C	14.861130	5.122174	-0.871049
C	15.054509	2.726125	-1.118686
C	11.354634	6.178998	-1.532651
C	13.494110	5.069795	-1.186894
C	13.690598	2.626521	-1.440165
C	13.059925	1.374573	-1.732266
C	10.724659	4.924002	-1.830510
C	12.891908	3.806882	-1.478484
C	9.360385	4.843876	-2.147540
C	11.737000	1.287595	-2.045920
C	11.502254	3.725075	-1.804329
C	8.770054	3.623909	-2.429284
C	10.898620	2.457373	-2.100164
C	9.507977	2.426712	-2.412941

C	5.177683	9.874935	0.869511
C	4.655493	7.042511	3.281702
C	4.970957	9.180681	2.060083
C	5.286789	9.185958	-0.335700
C	4.560835	5.685320	3.270203
C	4.869371	7.780424	2.069136
C	5.191717	7.784910	-0.373795
C	5.294216	7.040833	-1.593297
C	4.672013	4.939687	2.048380
C	4.980912	7.063528	0.837848
C	4.579818	3.540015	2.029337
C	5.198632	5.681567	-1.620471
C	4.882654	5.637319	0.818914
C	4.702746	2.834588	0.843363
C	4.993373	4.917235	-0.416526
C	4.910685	3.494940	-0.380877
C	6.719998	-0.603039	-4.014244
C	5.034780	2.671729	-1.612962
C	4.467801	-1.501147	-3.542267
C	5.696213	-1.550378	-4.277377
C	6.537962	0.356079	-3.049189
C	5.313500	0.418700	-2.327303
C	3.666192	-3.432649	-4.785569
C	4.876835	-3.477311	-5.515947
C	4.291526	-0.477628	-2.554859
C	3.465975	-2.469374	-3.821900
C	5.868710	-2.557445	-5.264524
C	8.805249	1.155596	-2.736972
H	8.760240	5.748998	-2.165461
H	16.687956	4.021696	-0.591363
H	13.141808	7.207282	-1.001949
H	15.314684	6.084839	-0.650926
H	15.656965	1.822190	-1.091488
H	10.744087	7.077296	-1.557538
H	13.665305	0.472355	-1.699626
H	5.443628	7.588662	-2.520402
H	11.292895	0.328637	-2.268291

H	7.717249	3.586656	-2.676613
H	5.252678	10.958193	0.882058
H	4.570023	7.593449	4.214553
H	4.884853	9.721364	2.998753
H	5.445714	9.729118	-1.263423
H	4.415791	3.003409	2.959613
H	5.256568	5.150060	-2.559092
H	4.627709	1.754195	0.857469
H	7.650607	-0.654523	-4.562390
O	5.014499	3.051334	-2.766064
H	4.399361	5.135379	4.193252
H	2.889240	-4.164792	-4.983946
H	5.022404	-4.242005	-6.273272
H	2.538687	-2.447973	-3.260104
H	6.804042	-2.587893	-5.816689
O	9.305313	0.077052	-2.976001
O	7.441206	1.353889	-2.738123
O	5.182221	1.339633	-1.297365

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3l.

–7965.20734539 hartree

C	0.542890	-0.646576	-3.718832
C	0.544190	-0.145975	-2.435937
C	-1.845897	1.397774	-0.020856
C	-1.860869	0.322901	-2.611369
C	-0.646724	0.359677	-1.846652
C	-0.659430	0.912733	-0.521584
C	-0.111318	-1.655441	2.933282
C	2.095527	-0.748669	3.323601
C	0.747036	0.062729	1.435724
C	-1.823665	-0.200230	-3.932261
C	-0.649966	-0.672735	-4.474122
C	-3.052851	1.307107	-0.754261
C	-3.083940	0.791312	-2.028984
C	1.966107	0.101474	2.191603
C	3.033356	0.968594	1.779532
C	-0.273100	-0.843758	1.833212

C	1.081516	-1.605805	3.687490
C	2.834404	1.781749	0.688070
C	1.600733	1.804361	-0.005098
C	0.576901	0.943333	0.314615
C	4.509056	2.253074	-0.897639
C	1.281790	4.009441	-0.782981
C	-1.987015	3.306246	1.361702
C	-4.832339	1.014487	0.776663
C	5.515467	3.270712	-1.289816
C	6.531316	2.984847	-2.246140
C	5.430663	4.551236	-0.717190
C	7.436590	4.035354	-2.610250
C	6.718829	1.693020	-2.853949
C	6.306184	5.562166	-1.076839
C	8.470592	3.798545	-3.568341
C	7.316303	5.332899	-2.023324
C	7.709632	1.475307	-3.762938
C	8.615896	2.510334	-4.162174
C	9.366882	4.847735	-3.939659
C	8.230681	6.368449	-2.414230
C	9.636277	2.297690	-5.103919
C	10.371579	4.589773	-4.885860
C	9.210123	6.138016	-3.330252
C	10.503299	3.327362	-5.461218
C	1.130676	4.816195	-2.021504
C	0.929336	6.227225	-1.980182
C	1.189687	4.155904	-3.261551
C	0.798276	6.933297	-3.222153
C	0.849170	6.993761	-0.763147
C	1.060229	4.843994	-4.455803
C	0.599260	8.349184	-3.233800
C	0.865043	6.232990	-4.466192
C	0.660329	8.343191	-0.783878
C	0.529069	9.074132	-2.008181
C	0.469627	9.052195	-4.471372
C	0.730902	6.963678	-5.694613
C	0.334957	10.465134	-2.039015

C	0.276221	10.442706	-4.454567
C	0.541978	8.311028	-5.698491
C	0.209978	11.140753	-3.250197
C	-2.025913	3.738076	2.782287
C	-1.967758	5.114398	3.148964
C	-2.134861	2.753302	3.779675
C	-2.035713	5.451181	4.541605
C	-1.830956	6.192870	2.204206
C	-2.201297	3.086244	5.121836
C	-1.984415	6.817468	4.959602
C	-2.156682	4.427253	5.531269
C	-1.780636	7.492002	2.611748
C	-1.859000	7.858855	3.993829
C	-2.057780	7.153363	6.346767
C	-2.227619	4.792661	6.917762
C	-1.812432	9.195627	4.423229
C	-2.007464	8.503060	6.730239
C	-2.181058	6.095050	7.308675
C	-1.886365	9.512654	5.777225
C	-5.987701	1.725884	1.380157
C	-7.019661	1.026460	2.066921
C	-6.026789	3.127762	1.292573
C	-8.071074	1.789343	2.672720
C	-7.087439	-0.407966	2.161539
C	-7.042159	3.859091	1.886782
C	-9.128978	1.131590	3.373428
C	-8.074749	3.215754	2.585803
C	-8.101276	-1.028170	2.826860
C	-9.152060	-0.291319	3.463872
C	-10.171979	1.891401	3.987170
C	-9.134673	3.954341	3.212437
C	-10.198536	-0.919870	4.159902
C	-11.198104	1.220894	4.672026
C	-10.136407	3.322861	3.882801
C	-11.209459	-0.170061	4.756910
O	4.238989	1.219350	-1.469093
H	1.465431	-1.025147	-4.148246

H	1.467768	-0.126025	-1.869112
H	-0.907237	-2.335144	3.223315
H	3.013866	-0.723487	3.898924
H	-2.742069	-0.237406	-4.506532
H	-0.643717	-1.072152	-5.483792
H	-1.193155	-0.886169	1.262089
H	1.202546	-2.246110	4.556142
O	3.846136	2.628025	0.260268
O	1.460361	2.669490	-1.080162
O	-1.885374	1.928922	1.260802
O	-4.214122	1.800640	-0.175884
H	1.338762	3.084258	-3.276887
O	1.269392	4.397956	0.365699
O	-2.044583	4.001908	0.370668
O	-4.424713	-0.094394	1.051906
H	4.654414	4.746593	0.011755
H	6.054567	0.889843	-2.571719
H	6.211482	6.546251	-0.627022
H	7.825826	0.488055	-4.202832
H	8.121254	7.348272	-1.957625
H	9.742020	1.313870	-5.553195
H	11.050046	5.390912	-5.166538
H	9.894821	6.932024	-3.616478
H	11.286453	3.145893	-6.191353
H	0.940775	6.471455	0.177456
H	1.110303	4.305988	-5.397944
H	0.608577	8.892100	0.153184
H	0.784850	6.410689	-6.628233
H	0.283333	11.011168	-1.100850
H	0.178383	10.972630	-5.398212
H	0.442585	8.851261	-6.636225
H	0.060261	12.216287	-3.256866
H	-2.169543	1.712695	3.484656
H	-1.767607	5.949797	1.154118
H	-2.290137	2.303800	5.869821
H	-1.676881	8.281610	1.871777
H	-2.319667	3.998245	7.653143

H	-1.717645	9.984409	3.681745
H	-2.064465	8.753564	7.786110
H	-2.235867	6.356768	8.362044
H	-1.849210	10.551167	6.092483
H	-5.235454	3.640802	0.760343
H	-6.315019	-0.992142	1.684426
H	-7.040995	4.942946	1.816725
H	-8.131142	-2.113464	2.871368
H	-9.118375	5.038128	3.137421
H	-10.206785	-2.004362	4.230828
H	-11.988438	1.802521	5.138880
H	-10.932069	3.895708	4.351752
H	-12.010243	-0.671391	5.292522
C	-7.671306	-2.102046	-2.093112
C	-6.714965	2.812686	-4.836332
C	-4.246311	3.078380	-3.531364
C	-4.388604	0.707441	-2.755031
C	-6.028202	4.003880	-4.890285
C	-4.784274	4.136283	-4.229807
C	-5.103913	-0.471792	-2.725111
C	-6.371363	-0.581651	-3.348437
C	-6.190038	1.701685	-4.124627
C	-4.926631	1.832921	-3.459974
C	-4.072884	-2.611168	-2.688353
C	-6.898640	0.474710	-4.040069
C	-3.384081	-3.548855	-1.762550
C	-2.731010	-4.725865	-2.233202
C	-3.346347	-3.226307	-0.393693
C	-2.033998	-5.544031	-1.283183
C	-2.719261	-5.144255	-3.611388
C	-2.683443	-4.031319	0.517773
C	-1.342366	-6.720647	-1.709359
C	-2.011813	-5.189867	0.100970
C	-2.063668	-6.270683	-4.008111
C	-1.348649	-7.098444	-3.084137
C	-0.633694	-7.526629	-0.764697
C	-1.295931	-6.019302	1.029075

C	-0.658966	-8.254887	-3.485746
C	0.044028	-8.673105	-1.210983
C	-0.635125	-7.135297	0.617001
C	0.030309	-9.032337	-2.558146
C	-8.253350	-3.469005	-2.140682
C	-9.231914	-3.897835	-1.198990
C	-7.803695	-4.352190	-3.136990
C	-9.740543	-5.234102	-1.307591
C	-9.758916	-3.060090	-0.152559
C	-8.287844	-5.646953	-3.225837
C	-10.735019	-5.705308	-0.395261
C	-9.259427	-6.112823	-2.327024
C	-10.710361	-3.515580	0.709942
C	-11.234391	-4.846432	0.627721
C	-11.238951	-7.038410	-0.500201
C	-9.780661	-7.448219	-2.407064
C	-12.213835	-5.326667	1.512811
C	-12.216782	-7.475994	0.407311
C	-10.726541	-7.891300	-1.535039
C	-12.698603	-6.627572	1.402368
O	-4.603083	-1.540487	-1.996678
O	-7.056918	-1.787146	-3.291112
O	-7.698156	-1.318312	-1.170101
H	-7.673715	2.704400	-5.336251
H	-3.295813	3.189895	-3.021111
H	-6.441062	4.846397	-5.437204
H	-4.250075	5.080664	-4.271896
H	-1.291568	-5.730840	2.076467
O	-4.180272	-2.696759	-3.893955
H	-7.868188	0.367732	-4.515521
H	-3.830822	-2.320923	-0.049833
H	-3.241261	-4.534418	-4.333649
H	-2.672852	-3.758547	1.569037
H	-2.072611	-6.557418	-5.056616
H	-0.670213	-8.537341	-4.535029
H	0.581406	-9.282464	-0.489422
H	-0.095841	-7.752288	1.330781

H	0.557026	-9.924343	-2.884050
H	-7.050024	-4.009306	-3.834935
H	-9.373142	-2.055786	-0.054238
H	-7.914145	-6.313314	-3.997932
H	-11.088847	-2.856634	1.487400
H	-9.399900	-8.101433	-3.187312
H	-12.591943	-4.666711	2.288923
H	-12.596855	-8.490644	0.324437
H	-11.112546	-8.904534	-1.608785
H	-13.455899	-6.983022	2.094750
C	9.242058	-9.255489	5.884982
C	10.584370	-7.737524	2.721318
C	9.968804	-9.096065	4.706581
C	8.379446	-8.252590	6.320307
C	10.454293	-6.596601	1.991437
C	9.847398	-7.927076	3.938565
C	8.226056	-7.066446	5.583519
C	7.349658	-6.012115	5.998490
C	9.577260	-5.539599	2.409582
C	8.964819	-6.891993	4.376553
C	9.441212	-4.358526	1.664627
C	7.205157	-4.866673	5.275432
C	8.822828	-5.691408	3.613911
C	8.594810	-3.347482	2.088418
C	7.933105	-4.655202	4.051032
C	7.835006	-3.472048	3.264412
C	6.508231	-5.832769	-5.671126
C	3.587082	-6.394235	-3.375459
C	5.346807	-6.378371	-5.127208
C	7.129598	-4.748480	-5.056935
C	3.055990	-5.870156	-2.237824
C	4.782323	-5.850091	-3.955236
C	6.599689	-4.186859	-3.883313
C	7.208511	-3.071997	-3.222012
C	3.670178	-4.754068	-1.575805
C	5.412379	-4.736971	-3.317131
C	3.129379	-4.210808	-0.401009

C	6.685729	-2.531174	-2.085583
C	4.859316	-4.179348	-2.122358
C	3.734893	-3.134185	0.224527
C	5.487705	-3.058827	-1.484138
C	4.901820	-2.542602	-0.291427
C	6.799515	0.941682	3.905075
C	5.479967	-1.374988	0.423510
C	4.702303	2.106380	3.340886
C	5.956257	2.075655	4.035197
C	6.427075	-0.106684	3.109857
C	5.206202	-0.069815	2.391570
C	4.247650	4.290076	4.315169
C	5.486626	4.259100	4.996489
C	4.338369	0.997419	2.505160
C	3.863519	3.241715	3.508776
C	6.321070	3.174153	4.857820
C	6.928449	-2.354905	3.639526
H	10.006445	-4.241193	0.744632
H	9.349130	-10.166451	6.466271
H	11.252898	-8.528804	2.392652
H	10.640553	-9.880958	4.369607
H	7.813747	-8.379258	7.239410
H	11.016566	-6.462464	1.071521
H	6.786990	-6.142320	6.919380
H	8.116929	-2.653550	-3.648638
H	6.526630	-4.094215	5.607254
H	8.497611	-2.444866	1.498346
H	6.929909	-6.255192	-6.578378
H	3.107966	-7.237629	-3.865345
H	4.863894	-7.224028	-5.609492
H	8.034903	-4.324024	-5.482722
H	2.222959	-4.640221	0.015774
H	7.163641	-1.684285	-1.615407
H	3.299200	-2.730376	1.128898
H	7.741821	0.894607	4.441076
O	6.389644	-0.657149	0.068051
H	2.150929	-6.289762	-1.808357

H	3.592192	5.148378	4.428035
H	5.776457	5.092797	5.629245
H	2.914748	3.283019	2.985718
H	7.274086	3.139200	5.378773
O	6.005612	-2.380439	4.424868
O	7.267440	-1.201123	2.959392
O	4.836873	-1.169790	1.631979

Coordinates of (*R*,*R*,*R*)-**4** in Figure S3m.

–7965.20850274 hartree

C	0.598329	-1.764771	-3.567539
C	0.620629	-1.102539	-2.360708
C	-1.710987	0.772375	-0.133449
C	-1.760961	-0.550871	-2.609196
C	-0.550274	-0.485369	-1.843268
C	-0.551147	0.176954	-0.572097
C	0.388764	-2.924556	2.300382
C	2.474127	-1.838346	2.875090
C	0.982899	-0.836060	1.199953
C	-1.749577	-1.250373	-3.846139
C	-0.598679	-1.844124	-4.313749
C	-2.891269	0.755545	-0.916193
C	-2.943952	0.095290	-2.122148
C	2.200087	-0.787301	1.958077
C	3.112920	0.302928	1.766705
C	0.093006	-1.926339	1.400041
C	1.591612	-2.882560	3.039590
C	2.786948	1.289388	0.864067
C	1.569636	1.256589	0.139611
C	0.681969	0.214162	0.271795
C	4.353723	2.420671	-0.498857
C	0.984340	3.509627	-0.320541
C	-2.324229	0.806818	2.148782
C	-4.123772	2.732393	-0.521292
C	5.142235	3.675128	-0.589807
C	6.182432	3.835391	-1.549490
C	4.822145	4.731202	0.280685

C	6.870203	5.092346	-1.602982
C	6.600517	2.799995	-2.458327
C	5.487724	5.944040	0.219897
C	7.919910	5.302151	-2.550277
C	6.514505	6.152703	-0.713248
C	7.603954	3.007534	-3.355817
C	8.297118	4.257885	-3.445007
C	8.600153	6.557443	-2.610063
C	7.214596	7.403454	-0.794928
C	9.329222	4.483989	-4.370756
C	9.625583	6.738595	-3.551832
C	8.210866	7.598073	-1.701044
C	9.984932	5.711563	-4.422579
C	0.851254	4.475428	-1.440861
C	0.204645	5.733300	-1.273625
C	1.405584	4.132375	-2.686213
C	0.144789	6.622385	-2.396775
C	-0.414506	6.160093	-0.046029
C	1.350744	4.999461	-3.764561
C	-0.495231	7.895090	-2.278707
C	0.726369	6.250491	-3.648072
C	-1.024649	7.373729	0.058438
C	-1.086452	8.288635	-1.042266
C	-0.548744	8.784546	-3.395816
C	0.658592	7.163604	-4.753889
C	-1.706726	9.545750	-0.943698
C	-1.181052	10.030037	-3.252491
C	0.049620	8.374558	-4.634619
C	-1.753136	10.405563	-2.038617
C	-2.195472	1.613188	3.389671
C	-2.921218	1.288434	4.572541
C	-1.310282	2.705798	3.385891
C	-2.728521	2.106808	5.734706
C	-3.848501	0.191021	4.671045
C	-1.126728	3.486618	4.515396
C	-3.435530	1.823934	6.944518
C	-1.824463	3.213175	5.701350

C	-4.516631	-0.072854	5.828518
C	-4.340281	0.723622	7.005569
C	-3.241864	2.637433	8.103481
C	-1.649719	4.014258	6.879900
C	-5.023577	0.459119	8.204174
C	-3.947042	2.336542	9.279612
C	-2.326695	3.740766	8.028011
C	-4.828311	1.258002	9.327963
C	-5.420647	3.224572	0.009919
C	-5.687971	4.616844	0.162261
C	-6.407885	2.279491	0.341688
C	-6.972974	5.011776	0.662420
C	-4.741951	5.657020	-0.150007
C	-7.646510	2.671443	0.821686
C	-7.290787	6.395418	0.830878
C	-7.955640	4.028604	0.994371
C	-5.053800	6.973575	0.010783
C	-6.330598	7.396832	0.502110
C	-8.572274	6.789007	1.326350
C	-9.234542	4.451920	1.491026
C	-6.662438	8.751617	0.670092
C	-8.859721	8.154629	1.479624
C	-9.530231	5.770294	1.650873
C	-7.913648	9.124864	1.154079
O	4.279296	1.529017	-1.316081
H	1.505699	-2.226991	-3.944810
H	1.542518	-1.041431	-1.793272
H	-0.311467	-3.741333	2.447147
H	3.396311	-1.814060	3.444529
H	-2.666696	-1.311666	-4.421395
H	-0.611247	-2.372573	-5.262397
H	-0.840569	-1.950448	0.850643
H	1.820990	-3.674243	3.746551
O	3.639532	2.369054	0.686678
O	1.316955	2.256075	-0.789538
O	-1.725042	1.447390	1.077094
O	-4.032397	1.355704	-0.408470

H	1.898108	3.174152	-2.792584
O	0.852071	3.731740	0.865622
O	-2.851762	-0.276227	2.015169
O	-3.222780	3.379724	-1.009941
H	4.027534	4.590158	1.002232
H	6.100037	1.844326	-2.415200
H	5.212742	6.747208	0.897411
H	7.896007	2.203758	-4.026816
H	6.927919	8.197159	-0.110577
H	9.611889	3.684569	-5.050446
H	10.139421	7.695173	-3.594680
H	8.731907	8.550531	-1.751141
H	10.780554	5.869599	-5.144635
H	-0.380541	5.494736	0.803615
H	1.798044	4.713323	-4.711996
H	-1.484307	7.665692	0.999081
H	1.108572	6.862273	-5.695761
H	-2.148228	9.842648	0.004056
H	-1.218886	10.703261	-4.104624
H	0.005882	9.055230	-5.480687
H	-2.236138	11.373752	-1.946021
H	-0.749523	2.930995	2.487430
H	-3.999895	-0.434188	3.803475
H	-0.433579	4.322679	4.484725
H	-5.202282	-0.915131	5.870951
H	-0.958818	4.851607	6.832540
H	-5.710166	-0.382247	8.244139
H	-3.796159	2.957752	10.158420
H	-2.184261	4.356395	8.912290
H	-5.364542	1.039721	10.246774
H	-6.200633	1.225605	0.204105
H	-3.770217	5.372386	-0.525549
H	-8.392601	1.919976	1.063539
H	-4.318955	7.733070	-0.243876
H	-9.966601	3.687873	1.737814
H	-5.926439	9.509429	0.415153
H	-9.835597	8.448920	1.856516

H	-10.502766	6.075686	2.027912
H	-8.154189	10.176615	1.278113
C	-6.871009	-3.440334	-3.540550
C	-6.151741	1.829938	-5.573982
C	-3.733249	2.106839	-4.178031
C	-4.230197	0.028855	-2.882307
C	-5.312190	2.885741	-5.845564
C	-4.095256	3.025166	-5.138135
C	-5.102423	-1.009005	-2.628043
C	-6.315179	-1.147200	-3.347294
C	-5.811886	0.865578	-4.588757
C	-4.574679	1.001733	-3.876340
C	-5.384962	-2.013837	-0.490621
C	-6.664624	-0.232036	-4.302536
C	-4.828953	-3.082702	0.380360
C	-5.306212	-3.300466	1.705926
C	-3.798240	-3.891969	-0.129874
C	-4.714708	-4.353820	2.479899
C	-6.351599	-2.524958	2.322155
C	-3.229903	-4.905001	0.623361
C	-5.162870	-4.614567	3.812226
C	-3.668836	-5.158661	1.931709
C	-6.774489	-2.781130	3.592032
C	-6.204985	-3.828481	4.385634
C	-4.573276	-5.663760	4.582881
C	-3.093693	-6.206057	2.727571
C	-6.635330	-4.101245	5.695109
C	-5.033308	-5.899712	5.888334
C	-3.524821	-6.448075	3.995319
C	-6.054044	-5.126240	6.437417
C	-7.794609	-4.468942	-2.992924
C	-7.929782	-5.752249	-3.595676
C	-8.532962	-4.155926	-1.838431
C	-8.834185	-6.692319	-2.999976
C	-7.225199	-6.157916	-4.784256
C	-9.394089	-5.073886	-1.260510
C	-9.012882	-7.988331	-3.575802

C	-9.566765	-6.348015	-1.822109
C	-7.404581	-7.393624	-5.328868
C	-8.296365	-8.355135	-4.752648
C	-9.910109	-8.927302	-2.979641
C	-10.459391	-7.311588	-1.242508
C	-8.485596	-9.632883	-5.304773
C	-10.067530	-10.193413	-3.565581
C	-10.624408	-8.544088	-1.794910
C	-9.362203	-10.540925	-4.716197
O	-4.740932	-1.986920	-1.711188
O	-7.173509	-2.191693	-3.031385
O	-5.961535	-3.601745	-4.324618
H	-7.090427	1.717915	-6.109814
H	-2.809784	2.232039	-3.624516
H	-5.584346	3.617700	-6.600230
H	-3.443505	3.867424	-5.349157
H	-2.301532	-6.806944	2.289418
O	-6.283661	-1.238965	-0.235438
H	-7.599028	-0.355046	-4.840359
H	-3.445154	-3.713827	-1.136857
H	-6.798472	-1.726106	1.749891
H	-2.437446	-5.515004	0.199460
H	-7.567874	-2.177983	4.026408
H	-7.433707	-3.500970	6.123489
H	-4.581027	-6.698216	6.470186
H	-3.080329	-7.244323	4.586396
H	-6.397459	-5.324171	7.448372
H	-8.406899	-3.179390	-1.388006
H	-6.535779	-5.458358	-5.234260
H	-9.942956	-4.809822	-0.361197
H	-6.858681	-7.670624	-6.227094
H	-11.004807	-7.030908	-0.345766
H	-7.936557	-9.906223	-6.201776
H	-10.750266	-10.904693	-3.108650
H	-11.304320	-9.262914	-1.345387
H	-9.496944	-11.524787	-5.155549
C	11.240944	-9.275504	3.094967

C	12.283516	-6.651364	0.616871
C	11.932918	-8.634811	2.068887
C	10.190139	-8.631513	3.743406
C	11.934402	-5.389700	0.245774
C	11.587093	-7.333756	1.670410
C	9.809236	-7.329863	3.377447
C	8.734715	-6.634423	4.020479
C	10.858516	-4.692893	0.892386
C	10.510180	-6.664277	2.329341
C	10.495275	-3.390478	0.517861
C	8.370366	-5.373299	3.656337
C	10.137635	-5.339277	1.943634
C	9.458251	-2.732718	1.158122
C	9.053403	-4.669849	2.601667
C	8.727012	-3.345849	2.190307
C	7.915516	-3.105943	-7.136456
C	5.008913	-4.722313	-5.389938
C	6.820396	-3.932384	-6.892189
C	8.351004	-2.210634	-6.162821
C	4.362323	-4.659836	-4.194330
C	6.138102	-3.880328	-5.666214
C	7.697624	-2.123515	-4.922382
C	8.114420	-1.215593	-3.896179
C	4.783000	-3.750614	-3.165682
C	6.576573	-2.964563	-4.660369
C	4.124763	-3.685333	-1.928349
C	7.471863	-1.134930	-2.697026
C	5.900354	-2.891538	-3.402792
C	4.546017	-2.802521	-0.947797
C	6.335740	-1.967881	-2.395361
C	5.634415	-1.937453	-1.155239
C	6.815420	0.398960	3.998793
C	6.000863	-0.988448	-0.071124
C	4.523207	1.241330	3.674428
C	5.759000	1.257110	4.400675
C	6.663346	-0.422193	2.915567
C	5.459408	-0.413542	2.167890

C	3.628651	2.903469	5.210071
C	4.850725	2.922581	5.921705
C	4.392463	0.379975	2.534969
C	3.467523	2.084793	4.114531
C	5.891764	2.115760	5.523807
C	7.610901	-2.585025	2.811586
H	11.035214	-2.897386	-0.285272
H	11.522679	-10.281904	3.389868
H	13.100768	-7.166123	0.118682
H	12.751976	-9.140513	1.564650
H	9.651896	-9.133175	4.543036
H	12.467848	-4.881484	-0.552702
H	8.200080	-7.139372	4.820943
H	8.973149	-0.577495	-4.090156
H	7.547231	-4.878983	4.151512
H	9.187195	-1.730003	0.852595
H	8.431054	-3.160490	-8.090614
H	4.680066	-5.416177	-6.158983
H	6.482599	-4.629578	-7.654167
H	9.205163	-1.566966	-6.355334
H	3.275558	-4.336073	-1.741243
H	7.802874	-0.430422	-1.948293
H	4.024455	-2.768821	-0.000312
H	7.748281	0.381010	4.552757
O	6.779292	-0.061310	-0.127296
H	3.510692	-5.303658	-3.992570
H	2.808263	3.538204	5.531243
H	4.963991	3.573291	6.783756
H	2.527245	2.081478	3.574624
H	6.833215	2.120218	6.066430
O	6.710707	-3.016406	3.498846
O	7.708347	-1.240017	2.509496
O	5.317937	-1.282742	1.094932

Coordinates of (*R*,*R*,*R*)-**3** in Figure S4.

–6358.92050643 hartree

C	-1.193143	3.726973	-2.893238

C	-1.007535	2.889633	-1.816993
C	1.475369	0.389561	-0.596438
C	1.085755	2.064170	-2.810896
C	0.133636	2.046055	-1.736772
C	0.356774	1.192737	-0.608518
C	0.467062	4.046262	2.661268
C	-1.413982	2.966854	3.734967
C	-0.528899	2.084693	1.619558
C	0.865168	2.949225	-3.901084
C	-0.244608	3.762550	-3.939978
C	2.389900	0.375126	-1.675984
C	2.225427	1.195280	-2.769604
C	-1.467987	1.993072	2.701076
C	-2.427550	0.927903	2.724426
C	0.438246	3.126101	1.638090
C	-0.472000	3.970243	3.714358
C	-2.438555	0.027416	1.682946
C	-1.546702	0.147772	0.591222
C	-0.593643	1.140267	0.544713
C	-2.998269	-2.261961	1.944708
C	-2.540535	-0.640942	-1.409266
C	2.594607	-0.148735	1.431964
C	3.388138	-1.776030	-1.780323
C	-4.145326	-3.203335	1.884714
C	-3.954825	-4.612292	1.799995
C	-5.446185	-2.673848	1.939976
C	-5.114603	-5.455519	1.782996
C	-2.664307	-5.242961	1.699974
C	-6.561148	-3.494755	1.934773
C	-4.975204	-6.875031	1.690795
C	-6.424661	-4.889248	1.858709
C	-2.540455	-6.596232	1.605292
C	-3.679870	-7.464161	1.602771
C	-6.130256	-7.716234	1.683122
C	-7.567600	-5.757859	1.851599
C	-3.562560	-8.860967	1.511372
C	-5.965512	-9.107513	1.591801

C	-7.428009	-7.108828	1.768480
C	-4.694382	-9.672387	1.506631
C	-2.337952	-1.617191	-2.508578
C	-3.370439	-1.914597	-3.443479
C	-1.070759	-2.208988	-2.648342
C	-3.075142	-2.815495	-4.518733
C	-4.705851	-1.383692	-3.358924
C	-0.788899	-3.068292	-3.698158
C	-4.079127	-3.146283	-5.480612
C	-1.771693	-3.388639	-4.646848
C	-5.659694	-1.709945	-4.275186
C	-5.388294	-2.592120	-5.370643
C	-3.781381	-4.033555	-6.560697
C	-1.500259	-4.276957	-5.742313
C	-6.361467	-2.927873	-6.326431
C	-4.784775	-4.339900	-7.493554
C	-2.459368	-4.585018	-6.657281
C	-6.060920	-3.792056	-7.376251
C	2.519105	-1.082762	2.582813
C	3.560122	-1.169623	3.551895
C	1.355283	-1.856917	2.731901
C	3.381678	-2.057999	4.663030
C	4.794791	-0.433735	3.472424
C	1.183848	-2.703518	3.814904
C	4.398789	-2.183016	5.659621
C	2.181596	-2.824453	4.793983
C	5.762161	-0.562936	4.423229
C	5.605966	-1.431912	5.550960
C	4.216182	-3.059225	6.773793
C	2.024732	-3.696814	5.924047
C	6.593773	-1.566860	6.540883
C	5.229888	-3.161759	7.739586
C	2.995806	-3.809123	6.870869
C	6.405985	-2.423087	7.622792
C	4.651759	-2.488563	-1.455855
C	4.844759	-3.867444	-1.761878
C	5.672891	-1.768626	-0.809714

C	6.090208	-4.479017	-1.396827
C	3.866367	-4.688315	-2.426329
C	6.869792	-2.366831	-0.455675
C	6.331976	-5.858267	-1.684818
C	7.106274	-3.720492	-0.737650
C	4.105818	-6.001272	-2.699862
C	5.337139	-6.638942	-2.342899
C	7.570502	-6.468610	-1.316302
C	8.340847	-4.358454	-0.378171
C	5.591934	-7.992913	-2.617342
C	7.781912	-7.825129	-1.609899
C	8.563907	-5.671950	-0.654144
C	6.802012	-8.578267	-2.253853
O	-1.846446	-2.522027	2.226048
H	-2.071788	4.363577	-2.934585
H	-1.740687	2.860681	-1.019244
H	1.213592	4.834721	2.654903
H	-2.135152	2.910646	4.542261
H	1.591849	2.978273	-4.705006
H	-0.392245	4.433624	-4.780777
H	1.161722	3.185826	0.833308
H	-0.450419	4.706410	4.512240
O	-3.397824	-0.977221	1.645955
O	-1.593834	-0.805106	-0.418907
O	1.672579	-0.487332	0.462895
O	3.521419	-0.420278	-1.565055
H	-0.288059	-1.975113	-1.939016
O	-3.388602	0.224842	-1.339362
O	3.329562	0.809886	1.303137
O	2.346207	-2.252719	-2.181572
H	-5.569909	-1.600200	2.000464
H	-1.784536	-4.616271	1.702543
H	-7.554705	-3.059572	1.991086
H	-1.552328	-7.042110	1.526403
H	-8.554440	-5.307560	1.912852
H	-2.572489	-9.303559	1.443414
H	-6.846494	-9.743647	1.587485

H	-8.302631	-7.753843	1.763241
H	-4.586343	-10.750563	1.435817
H	-4.940761	-0.709802	-2.547860
H	0.208335	-3.487162	-3.789016
H	-6.660282	-1.295509	-4.182606
H	-0.503895	-4.703103	-5.821392
H	-7.357453	-2.502746	-6.236660
H	-4.553877	-5.013616	-8.314323
H	-2.239346	-5.259739	-7.480376
H	-6.824447	-4.040848	-8.107221
H	0.561234	-1.779100	2.001972
H	4.938505	0.238631	2.639160
H	0.260909	-3.267862	3.904629
H	6.683913	0.006581	4.335413
H	1.106272	-4.271909	6.002522
H	7.511287	-0.991331	6.452346
H	5.086304	-3.828063	8.585911
H	2.863552	-4.474263	7.720147
H	7.179073	-2.515471	8.379758
H	5.507029	-0.724951	-0.577143
H	2.924009	-4.237758	-2.699264
H	7.636510	-1.786241	0.048974
H	3.345793	-6.593897	-3.202690
H	9.098429	-3.763056	0.123709
H	4.828937	-8.581828	-3.119173
H	8.725177	-8.284649	-1.327297
H	9.503517	-6.141912	-0.376134
H	6.983334	-9.626239	-2.472944
C	3.881646	-0.298004	-7.263640
C	1.931534	-0.421853	-5.251996
C	3.242812	1.193648	-3.865619
C	2.766255	-1.086246	-7.430280
C	1.785042	-1.148290	-6.412571
C	4.380655	1.967515	-3.740394
C	4.064447	0.467470	-6.081371
C	3.066852	0.411029	-5.052715
C	4.676400	4.016071	-2.534187

C	5.210724	1.283973	-5.890752
C	4.724345	4.537771	-1.141684
C	5.070871	5.890998	-0.857213
C	4.386589	3.667796	-0.089937
C	5.064054	6.322775	0.511035
C	5.444701	6.853244	-1.861422
C	4.371380	4.093801	1.228206
C	5.411830	7.668040	0.847380
C	4.706188	5.416024	1.557016
C	5.780112	8.131817	-1.531608
C	5.776426	8.592133	-0.175520
C	5.397946	8.100687	2.209609
C	4.698552	5.878043	2.916815
C	6.116251	9.909674	0.173930
C	5.743982	9.427187	2.512449
C	5.028489	7.160617	3.229698
C	6.099725	10.321117	1.504167
O	4.563520	2.641975	-2.536594
H	4.643031	-0.247577	-8.037721
H	1.181883	-0.487896	-4.471960
H	2.637387	-1.664287	-8.340662
H	0.908483	-1.775527	-6.545758
H	4.423660	5.171978	3.695581
O	4.714285	4.653717	-3.565837
H	5.965021	1.319673	-6.671911
H	4.119491	2.642626	-0.306193
H	5.444469	6.539702	-2.895049
H	4.093163	3.391715	2.008205
H	6.058103	8.834096	-2.313405
H	6.392804	10.608454	-0.610978
H	5.730866	9.751608	3.549505
H	5.019043	7.495903	4.263483
H	6.364469	11.343396	1.757374
C	-7.803998	9.034035	-1.935125
C	-6.318130	5.971620	-3.525158
C	-7.350439	8.143112	-2.906122
C	-7.710124	8.708984	-0.584377

C	-5.781254	4.777144	-3.155259
C	-6.793143	6.906258	-2.544535
C	-7.159467	7.482579	-0.176529
C	-7.045968	7.112198	1.202158
C	-5.669873	4.405383	-1.772576
C	-6.692657	6.562633	-1.160799
C	-5.119838	3.174234	-1.384745
C	-6.507553	5.921703	1.588163
C	-6.129531	5.309576	-0.764968
C	-5.027839	2.832042	-0.045497
C	-6.024027	4.967457	0.624190
C	-5.464260	3.702497	0.968817
C	-5.357600	0.676057	5.890433
C	-5.295361	3.278823	2.384203
C	-3.107603	0.125835	5.055556
C	-4.090820	0.068507	6.098261
C	-4.675465	1.371728	3.692031
C	-1.574377	-1.134954	6.464102
C	-2.542897	-1.185768	7.494357
C	-3.422489	0.806758	3.834713
C	-1.848313	-0.497455	5.274628
C	-3.773595	-0.598306	7.311395
H	-7.401834	7.811414	1.954582
H	-8.231869	9.986395	-2.233770
H	-6.397191	6.238989	-4.575621
H	-7.423906	8.400439	-3.959360
H	-8.063573	9.405447	0.171190
H	-4.755447	2.478904	-2.134588
H	-6.424595	5.675839	2.636727
H	-4.596414	1.876012	0.217209
H	-6.098661	0.629162	6.683576
O	-5.389873	3.964132	3.380971
H	-5.426498	4.074421	-3.904169
H	-0.605618	-1.603247	6.610855
H	-2.312485	-1.691075	8.427640
H	-1.103016	-0.475706	4.487731
H	-4.525416	-0.635127	8.095500

O	-4.988438	1.935631	2.458328
C	-5.652514	1.313299	4.710957
H	-6.615990	1.779658	4.545315
C	5.374169	2.019612	-4.743424
H	6.244835	2.645634	-4.592765

Coordinates of (*R*,*R*,*R*)-**5** in Figure S4.

–7372.88702746 hartree

C	-0.182515	-3.114881	-2.893677
C	0.075174	-2.231798	-1.869318
C	-1.638434	0.512411	0.004786
C	-2.179849	-1.280914	-2.098732
C	-0.904738	-1.294342	-1.439693
C	-0.652710	-0.382143	-0.364696
C	0.182582	-3.114368	2.894470
C	2.412979	-2.212849	3.147795
C	0.904761	-1.294085	1.440148
C	-2.412893	-2.213387	-3.147245
C	-1.440742	-3.107177	-3.536211
C	-2.894567	0.543051	-0.667154
C	-3.177843	-0.334564	-1.696082
C	2.179897	-1.280550	2.099135
C	3.177882	-0.334267	1.696287
C	-0.075144	-2.231458	1.869972
C	1.440836	-3.106565	3.536951
C	2.894557	0.543186	0.667240
C	1.638409	0.512429	-0.004659
C	0.652705	-0.382079	0.364998
C	4.843495	3.622802	0.185753
C	4.805745	5.030436	0.326453
C	5.986835	3.009822	-0.331112
C	5.941581	5.802955	-0.070160
C	3.666684	5.730117	0.860884
C	7.092488	3.759847	-0.722817
C	5.929049	7.224714	0.065332
C	7.097804	5.155631	-0.604036
C	3.656238	7.085942	0.990869

C	4.781887	7.885111	0.600324
C	7.065448	7.995140	-0.332775
C	8.224750	5.956481	-0.996793
C	4.790655	9.284171	0.725990
C	7.027811	9.390882	-0.188528
C	8.210648	7.310757	-0.868066
C	5.902539	10.025933	0.334856
C	1.412457	1.993395	-3.347855
C	1.994489	2.025144	-4.637153
C	0.202910	2.653146	-3.120853
C	1.326165	2.724915	-5.689802
C	3.241387	1.374033	-4.944832
C	-0.447072	3.343182	-4.140969
C	1.888214	2.760425	-7.002378
C	0.088773	3.391949	-5.434926
C	3.777603	1.410056	-6.196648
C	3.124661	2.099323	-7.272242
C	1.216702	3.457956	-8.053962
C	-0.562015	4.088422	-6.511003
C	3.660341	2.146998	-8.569839
C	1.790256	3.477223	-9.335040
C	-0.025701	4.118962	-7.761334
C	2.998200	2.828976	-9.587720
C	-1.412334	1.993700	3.347815
C	-1.994239	2.025484	4.637170
C	-0.202840	2.653493	3.120663
C	-1.325841	2.725336	5.689718
C	-3.241068	1.374316	4.945010
C	0.447207	3.343620	4.140677
C	-1.887748	2.760864	7.002356
C	-0.088512	3.392426	5.434685
C	-3.777147	1.410354	6.196884
C	-3.124127	2.099700	7.272381
C	-1.216159	3.458470	8.053840
C	0.562348	4.088987	6.510661
C	-3.659663	2.147388	8.570036
C	-1.789570	3.477747	9.334982

C	0.026170	4.119544	7.761050
C	-2.997447	2.829438	9.587820
C	-4.843504	3.622733	-0.186085
C	-4.805697	5.030363	-0.326806
C	-5.986868	3.009806	0.330791
C	-5.941505	5.802932	0.069800
C	-3.666613	5.729995	-0.861252
C	-7.092490	3.759878	0.722489
C	-5.928918	7.224689	-0.065712
C	-7.097751	5.155661	0.603687
C	-3.656117	7.085818	-0.991256
C	-4.781734	7.885035	-0.600718
C	-7.065288	7.995164	0.332386
C	-8.224667	5.956559	0.996433
C	-4.790449	9.284094	-0.726403
C	-7.027598	9.390903	0.188120
C	-8.210513	7.310832	0.867687
C	-5.902303	10.025903	-0.335275
H	0.583547	-3.817386	-3.207227
H	1.039719	-2.246627	-1.374002
H	-0.583472	-3.816814	3.208174
H	3.374464	-2.202655	3.648955
H	-3.374356	-2.203274	-3.648447
H	-1.640503	-3.806834	-4.342449
H	-1.039709	-2.246361	1.374697
H	1.640622	-3.806087	4.343301
O	3.859617	1.424657	0.233849
O	1.383909	1.426037	-1.003505
O	-1.383975	1.426190	1.003489
O	-3.859644	1.424580	-0.233936
H	-0.225834	2.619796	-2.126862
H	6.003196	1.930437	-0.422656
H	2.792504	5.165623	1.168050
H	7.968848	3.258326	-1.124867
H	2.782117	7.588258	1.396874
H	9.097096	5.450970	-1.402665
H	3.915916	9.783819	1.133590

H	7.891966	9.976110	-0.491521
H	9.071082	7.902284	-1.169506
H	5.893325	11.107067	0.438174
H	3.774983	0.849718	-4.159029
H	-1.387050	3.849612	-3.937565
H	4.723155	0.914074	-6.399447
H	-1.499104	4.597430	-6.300813
H	4.602202	1.644024	-8.771855
H	1.279440	4.008091	-10.133945
H	-0.529455	4.650373	-8.564382
H	3.426001	2.856479	-10.585584
H	0.225810	2.620113	2.126632
H	-3.774717	0.849934	4.159289
H	1.387139	3.850085	3.937151
H	-4.722649	0.914328	6.399806
H	1.499379	4.598052	6.300345
H	-4.601474	1.644368	8.772175
H	-1.278693	4.008671	10.133812
H	0.529979	4.651017	8.564022
H	-3.425137	2.856948	10.585731
H	-6.003267	1.930423	0.422361
H	-2.792456	5.165465	-1.168415
H	-7.968870	3.258399	1.124549
H	-2.781978	7.588095	-1.397270
H	-9.097033	5.451086	1.402310
H	-3.915692	9.783703	-1.134011
H	-7.891730	9.976167	0.491106
H	-9.070925	7.902396	1.169118
H	-5.893048	11.107036	-0.438606
C	-6.199532	0.938549	-5.488482
C	-3.642021	0.938543	-4.350043
C	-4.521414	-0.292054	-2.353068
C	-5.145362	1.520019	-6.157160
C	-3.854656	1.520806	-5.581537
C	-5.602590	-0.850783	-1.701164
C	-6.909135	-0.836550	-2.285645
C	-6.014905	0.331270	-4.218530

C	-4.707422	0.327715	-3.635015
C	-7.102660	-0.262417	-3.521380
C	-4.901438	-3.213639	1.013124
C	-4.820551	-4.584487	1.354245
C	-4.519109	-2.246507	1.945577
C	-4.340742	-4.956096	2.649030
C	-5.195656	-5.636165	0.445583
C	-4.055105	-2.603873	3.209318
C	-4.242360	-6.333725	3.013115
C	-3.952175	-3.949865	3.586036
C	-5.104027	-6.949384	0.794881
C	-4.625314	-7.350202	2.086613
C	-3.757287	-6.703375	4.305892
C	-3.467664	-4.351328	4.878710
C	-4.520776	-8.698948	2.464714
C	-3.669867	-8.064317	4.638504
C	-3.373632	-5.664709	5.222604
C	-4.048305	-9.048938	3.727186
C	-10.122972	-2.033572	-0.964546
C	-11.480249	-2.277789	-1.280666
C	-9.638720	-2.351782	0.305954
C	-12.331939	-2.863185	-0.292318
C	-12.053968	-1.957889	-2.561771
C	-10.465515	-2.922676	1.269561
C	-13.705147	-3.122680	-0.587093
C	-11.813086	-3.192096	0.997371
C	-13.364476	-2.203288	-2.840544
C	-14.239337	-2.794564	-1.869593
C	-14.553463	-3.711697	0.401087
C	-12.689840	-3.783832	1.970500
C	-15.592617	-3.057740	-2.138686
C	-15.899181	-3.957014	0.086003
C	-13.996880	-4.032758	1.686905
C	-16.410761	-3.633058	-1.169668
O	-5.451132	-1.375694	-0.439271
O	-7.875218	-1.419297	-1.520802
H	-7.194935	0.938939	-5.925309

H	-2.647490	0.940843	-3.917407
H	-5.304564	1.980138	-7.128029
H	-3.024798	1.978748	-6.111315
H	-3.175583	-3.575378	5.581380
H	-8.082584	-0.243867	-3.983691
H	-4.590292	-1.202924	1.663871
H	-5.560289	-5.378155	-0.543041
H	-3.764899	-1.832790	3.918585
H	-5.395015	-7.723047	0.089247
H	-4.812868	-9.470420	1.757353
H	-3.300963	-8.344627	5.621525
H	-3.005485	-5.952170	6.203891
H	-3.973258	-10.096503	4.003719
H	-8.600781	-2.144629	0.536660
H	-11.430924	-1.505343	-3.326116
H	-10.062521	-3.164845	2.249161
H	-13.771251	-1.950625	-3.816206
H	-12.281258	-4.030194	2.946903
H	-15.996225	-2.806566	-3.115862
H	-16.543781	-4.405327	0.837297
H	-14.647236	-4.481005	2.433250
H	-17.454978	-3.830632	-1.393260
C	16.410591	-3.633264	1.168435
C	13.996017	-4.034056	-1.687398
C	15.898703	-3.957707	-0.086985
C	15.592687	-3.057560	2.137427
C	12.688912	-3.785222	-1.970775
C	14.552912	-3.712499	-0.401839
C	14.239345	-2.794476	1.868560
C	13.364721	-2.202818	2.839494
C	11.812402	-3.193093	-0.997665
C	13.704842	-3.123085	0.586317
C	10.464773	-2.923756	-1.269642
C	12.054148	-1.957512	2.560942
C	12.331567	-2.863686	0.291772
C	9.638219	-2.352472	-0.306060
C	11.480122	-2.277894	1.280096

C	10.122774	-2.033776	0.964203
C	4.047518	-9.049608	-3.725530
C	3.373475	-5.665611	-5.221754
C	3.669295	-8.065133	-4.637094
C	4.519962	-8.699410	-2.463106
C	3.467686	-4.352167	-4.878147
C	3.756907	-6.704130	-4.304783
C	4.624686	-7.350595	-2.085300
C	5.103377	-6.949563	-0.793626
C	3.952163	-3.950491	-3.585526
C	4.241948	-6.334267	-3.012054
C	4.055259	-2.604430	-3.209095
C	5.195165	-5.636280	-0.444609
C	4.340509	-4.956572	-2.648269
C	4.519198	-2.246853	-1.945391
C	4.820265	-4.584748	-1.353525
C	4.901302	-3.213840	-1.012691
C	7.102908	-0.261876	3.521122
C	4.707673	0.328245	3.634984
C	6.015237	0.331900	4.218327
C	6.909215	-0.836223	2.285512
C	5.602598	-0.850545	1.701201
C	3.855137	1.521565	5.581463
C	5.145922	1.520892	6.156911
C	4.521509	-0.291701	2.353153
C	3.642351	0.939142	4.350072
C	6.200019	0.939362	5.488171
H	10.061541	-3.166297	-2.249052
H	17.454861	-3.830760	1.391852
H	14.646187	-4.482601	-2.433725
H	16.543116	-4.406319	-0.838261
H	15.996536	-2.806011	3.114408
H	12.280092	-4.031956	-2.946984
H	13.771732	-1.949791	3.814963
H	5.394223	-7.723110	-0.087808
H	11.431288	-1.504674	3.325266
H	8.600234	-2.145381	-0.536608

H	3.972324	-10.097224	-4.001832
H	3.005348	-5.953236	-6.202999
H	3.300408	-8.345606	-5.620076
H	4.811888	-9.470768	-1.755552
H	3.765224	-1.833463	-3.918559
H	5.559782	-5.378097	0.543975
H	4.590492	-1.203219	-1.663904
H	8.082900	-0.243225	3.983286
H	3.175771	-3.576329	-5.581010
H	3.025335	1.979539	6.111301
H	5.305242	1.981149	7.127696
H	2.647762	0.941353	3.917571
H	7.195478	0.939838	5.924868
O	7.875185	-1.419100	1.520626
O	5.450970	-1.375658	0.439415
C	9.212522	-1.413183	2.002012
H	9.264128	-1.972270	2.947840
H	9.521105	-0.378943	2.218722
C	5.373177	-2.804395	0.365508
H	4.669032	-3.167707	1.127754
H	6.358840	-3.233385	0.587255
C	3.655650	2.792931	0.618172
H	3.532966	2.839992	1.710229
H	2.730689	3.161496	0.158137
C	2.089438	1.220450	-2.237919
H	2.090881	0.146879	-2.473304
H	3.132002	1.535374	-2.113515
C	-2.089404	1.220692	2.237979
H	-2.090846	0.147134	2.473417
H	-3.131974	1.535625	2.113651
C	-3.655727	2.792784	-0.618541
H	-3.533235	2.839643	-1.710629
H	-2.730688	3.161421	-0.158727
C	-5.373424	-2.804424	-0.365103
H	-4.669395	-3.167927	-1.127364
H	-6.359142	-3.233392	-0.586656
C	-9.212488	-1.413360	-2.002373

H	-9.264012	-1.972681	-2.948067
H	-9.520926	-0.379142	-2.219396

Coordinates of (*R*)-**6** in Figure S4.

–2376.91005168 hartree

C	-2.537254	6.118309	-1.960248
C	-1.524923	4.976714	-0.075286
C	-1.248975	4.090020	-2.345532
C	0.625581	2.452606	3.773831
C	-0.733313	2.039128	1.833614
C	2.707959	3.777518	3.538257
C	1.290851	3.336989	1.574346
C	-0.986559	3.984373	-0.939649
C	-0.196838	2.891519	-0.450871
C	-2.031233	5.174231	-2.824138
C	-2.279899	6.015609	-0.572991
C	0.277363	1.964969	-1.357348
C	0.113541	2.747315	1.005166
C	1.543915	3.187820	2.978163
C	2.228277	4.063913	0.790359
C	3.349634	4.618632	1.365903
C	3.592685	4.479509	2.752482
H	-3.133241	6.943066	-2.339550
H	-1.330999	4.905413	0.989380
H	0.821444	2.342655	4.836787
H	2.888918	3.659452	4.603467
H	-2.223075	5.244197	-3.891703
H	-2.680797	6.763622	0.104744
H	2.059052	4.161925	-0.275987
H	4.056888	5.164248	0.748484
H	4.480966	4.923165	3.192256
O	-1.917267	1.538108	1.289816
O	0.952301	0.850352	-0.866670
C	-2.101511	0.176752	1.238897
C	2.289652	0.703564	-1.167714
O	-1.267184	-0.596373	1.666492
O	2.874759	1.517925	-1.851658

C	-3.409363	-0.161016	0.614573
C	-3.929279	-1.488643	0.621833
C	-4.139884	0.869754	-0.003117
C	-5.198893	-1.727053	-0.003243
C	-3.263103	-2.610288	1.232033
C	-5.359691	0.630736	-0.612186
H	-3.727823	1.870230	-0.006217
C	-5.766170	-3.039270	-0.013715
C	-5.914670	-0.657783	-0.625048
C	-3.812034	-3.857077	1.219044
H	-2.304420	-2.441742	1.699557
H	-5.896685	1.446600	-1.087356
C	-5.075432	-4.124560	0.600494
C	-7.029583	-3.277068	-0.638016
C	-7.180792	-0.924683	-1.246575
H	-3.283123	-4.682635	1.688423
C	-5.648208	-5.407040	0.581080
C	-7.564390	-4.575212	-0.633624
C	-7.714804	-2.176145	-1.253072
H	-7.707014	-0.097315	-1.714501
C	-6.879860	-5.628277	-0.029910
H	-5.115737	-6.229450	1.051016
H	-8.525071	-4.751161	-1.109990
H	-8.674743	-2.363262	-1.726890
H	-7.308991	-6.625705	-0.036606
C	2.839730	-0.532631	-0.550986
C	4.133217	-1.028175	-0.889095
C	2.052435	-1.215607	0.393485
C	4.589413	-2.230624	-0.253729
C	5.010455	-0.402236	-1.844725
C	2.505911	-2.370293	1.009304
H	1.076322	-0.826323	0.654314
C	5.874227	-2.773635	-0.567530
C	3.766927	-2.902488	0.702708
C	6.232846	-0.926987	-2.138855
H	4.678688	0.507321	-2.323309
H	1.877942	-2.871650	1.740052

C	6.714799	-2.124283	-1.518536
C	6.328873	-3.971086	0.066493
C	4.249375	-4.102629	1.325938
H	6.871434	-0.429751	-2.864583
C	7.973909	-2.672493	-1.814751
C	7.594514	-4.483354	-0.260267
C	5.472934	-4.614505	1.022535
H	3.608347	-4.596430	2.051037
C	8.407519	-3.839762	-1.191461
H	8.609173	-2.171858	-2.540478
H	7.935732	-5.393864	0.224976
H	5.824522	-5.524303	1.501973
H	9.383547	-4.250715	-1.431721
C	-0.723256	3.105542	-3.224504
H	-0.923654	3.189952	-4.288932
C	0.024432	2.060571	-2.744459
H	0.426431	1.301485	-3.405240
C	-0.492350	1.884481	3.216942
H	-1.197161	1.318727	3.814973

Coordinates of (*R*)-**7** in Figure S4.

–3983.20595488 hartree

C	1.629031	-2.469306	6.272698
C	1.214368	-1.473210	5.417314
C	-1.296291	-0.989800	2.687444
C	-0.437261	-3.004372	4.440140
C	0.168452	-1.705159	4.483415
C	-0.295853	-0.687491	3.587391
C	-1.629143	2.467461	6.273174
C	-0.168520	1.703715	4.483759
C	0.012823	-4.006856	5.339576
C	1.021242	-3.746235	6.238629
C	-1.867856	-2.284510	2.629117
C	0.437124	3.002963	4.440720
C	-1.214423	1.471540	5.417613
C	-1.021427	3.744430	6.239332
C	1.867800	2.283502	2.629605

C	1.296275	0.988763	2.687680
C	0.295835	0.686229	3.587537
C	2.569860	2.770815	0.416690
C	2.902035	-0.608536	1.979241
C	-2.901991	0.607742	1.979437
C	-2.569882	-2.770967	0.415999
C	3.795085	2.876340	-0.418752
C	3.779082	3.494086	-1.701556
C	4.990468	2.331699	0.081601
C	5.002459	3.546520	-2.447737
C	2.609330	4.095078	-2.287208
C	6.164814	2.371271	-0.651533
C	5.038859	4.169519	-3.733663
C	6.200525	2.975825	-1.917244
C	2.653066	4.690177	-3.511664
C	3.858395	4.750259	-4.283200
C	6.256854	4.218214	-4.479455
C	7.409409	3.035825	-2.689437
C	3.913669	5.358921	-5.547933
C	6.265610	4.836737	-5.739817
C	7.437430	3.629553	-3.913443
C	5.105480	5.400854	-6.267086
C	3.105500	-1.695926	0.989249
C	4.379269	-2.306276	0.797252
C	1.995175	-2.144048	0.252685
C	4.490542	-3.356938	-0.172068
C	5.570715	-1.921144	1.508350
C	2.107709	-3.170734	-0.669535
C	5.749396	-3.990716	-0.411273
C	3.343525	-3.789196	-0.907825
C	6.767228	-2.529213	1.273305
C	6.908031	-3.581315	0.311882
C	5.859477	-5.040737	-1.374664
C	3.482796	-4.847942	-1.867755
C	8.136423	-4.216624	0.064126
C	7.107350	-5.646639	-1.590091
C	4.684042	-5.445742	-2.092711

C	8.233302	-5.237772	-0.877541
C	-3.105353	1.695497	0.989838
C	-4.379124	2.305855	0.797894
C	-1.994932	2.144002	0.253659
C	-4.490301	3.356917	-0.171000
C	-5.570661	1.920332	1.508623
C	-2.107371	3.171084	-0.668136
C	-5.749159	3.990710	-0.410146
C	-3.343187	3.789568	-0.906374
C	-6.767177	2.528416	1.273636
C	-6.907888	3.580923	0.312641
C	-5.859146	5.041132	-1.373110
C	-3.482366	4.848713	-1.865876
C	-8.136278	4.216261	0.064955
C	-7.107024	5.647045	-1.588483
C	-4.683617	5.446523	-2.090784
C	-8.233066	5.237803	-0.876295
C	-3.795116	-2.876108	-0.419475
C	-3.779201	-3.493521	-1.702441
C	-4.990405	-2.331403	0.081022
C	-5.002579	-3.545537	-2.448651
C	-2.609556	-4.094594	-2.288223
C	-6.164743	-2.370549	-0.652149
C	-5.039081	-4.168206	-3.734735
C	-6.200541	-2.974748	-1.918028
C	-2.653392	-4.689383	-3.512826
C	-3.858722	-4.749040	-4.284395
C	-6.257073	-4.216476	-4.480559
C	-7.409422	-3.034309	-2.690262
C	-3.914096	-5.357387	-5.549276
C	-6.265931	-4.834689	-5.741072
C	-7.437540	-3.627721	-3.914420
C	-5.105904	-5.398908	-6.268458
O	1.416513	2.880291	0.057418
H	2.432803	-2.274840	6.976260
H	1.694569	-0.501474	5.436801
H	-2.432901	2.272822	6.976705

H	-0.452740	-4.987907	5.300552
H	1.357763	-4.522202	6.919679
H	-1.694570	0.499774	5.436921
H	-1.357992	4.520258	6.920519
O	2.900294	2.526649	1.733591
O	1.694057	0.032417	1.765221
O	-1.694055	-0.033245	1.765206
O	-2.900339	-2.527506	1.733046
H	1.025220	-1.696213	0.421493
O	3.640140	-0.271306	2.880724
O	-3.640144	0.270252	2.880784
O	-1.416536	-2.880204	0.056675
H	4.980049	1.858714	1.055564
H	1.683471	4.057317	-1.732142
H	7.070542	1.929004	-0.247053
H	1.752913	5.135713	-3.927370
H	8.308597	2.593504	-2.269729
H	3.010293	5.799282	-5.961153
H	7.193675	4.870522	-6.304023
H	8.360261	3.668116	-4.486062
H	5.131327	5.875047	-7.243602
H	5.492915	-1.143155	2.253890
H	1.224651	-3.500818	-1.207469
H	7.648045	-2.218117	1.829410
H	2.598335	-5.161919	-2.415015
H	9.015090	-3.900644	0.620050
H	7.186205	-6.444900	-2.323212
H	4.773981	-6.245297	-2.823333
H	9.190131	-5.718892	-1.057220
H	-1.024976	1.696160	0.422444
H	-5.492933	1.142026	2.253839
H	-1.224232	3.501462	-1.205757
H	-7.648067	2.217017	1.829454
H	-2.597833	5.162984	-2.412851
H	-9.015016	3.899988	0.620602
H	-7.185809	6.445613	-2.321279
H	-4.773490	6.246379	-2.821085

H	-9.189895	5.718942	-1.055923
H	-4.979911	-1.858705	1.055124
H	-1.683696	-4.057147	-1.733138
H	-7.070393	-1.928207	-0.247577
H	-1.753321	-5.134989	-3.928636
H	-8.308530	-2.591914	-2.270463
H	-3.010802	-5.797827	-5.962590
H	-7.193992	-4.868150	-6.305303
H	-8.360370	-3.665955	-4.487063
H	-5.131829	-5.872864	-7.245087
C	-1.457676	-3.266489	3.489414
H	-1.916590	-4.248255	3.434567
C	1.457551	3.265306	3.490062
H	1.916414	4.247108	3.435421
C	-0.013020	4.005265	5.340328
H	0.452488	4.986350	5.301477