Electronic Supplementary Information

Chiral exciplex dyes showing circularly polarized luminescence: extension of the excimer chirality rule

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Table of contents

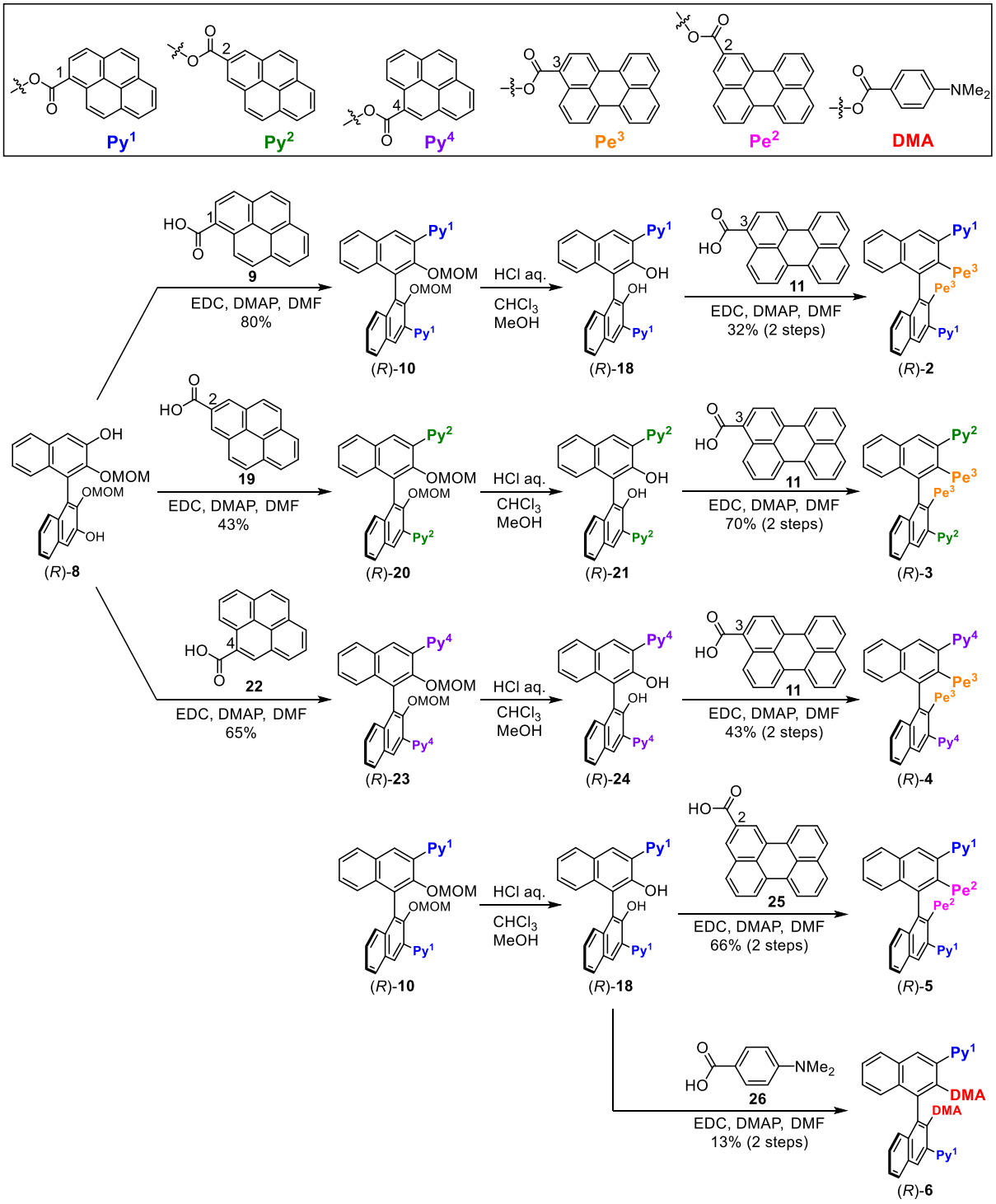
1. General information

Melting points were measured on a Yanaco melting point apparatus (uncorrected). 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 or a JEOL JEM-ECZ600R. 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, m = multiplet, br = broadened), and coupling constants (Hz). High-resolution mass spectra were performed on an Agilent G6520+G4240, a Bruker Ultraflextreme, or a JEOL JMS-700N. UV-Vis spectra were recorded on a Shimadzu UV-2600. CD spectra were recorded on a JASCO J-1500. Fluorescence spectra were recorded on a JASCO FP-750 (band width = 5 nm). Absolute fluorescence quantum yields were determined by a Hamamatsu Photonics K. K. C9920-02G. CPL spectra were measured on a JASCO CPL-200 (slit width = 3000 μm). 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). GPC was performed with Bio-Beads™ S-X1 Support (BIO-RAD, 200-400 mesh). Preparative HPLC was performed on a LC-5060 HPLC system (Japan Analytical Industry) using a JAIGEL-1HH (ø 20 mm × 600 mm) and a JAIGEL-2HH (ø 20 mm × 600 mm) (Japan Analytical Industry).

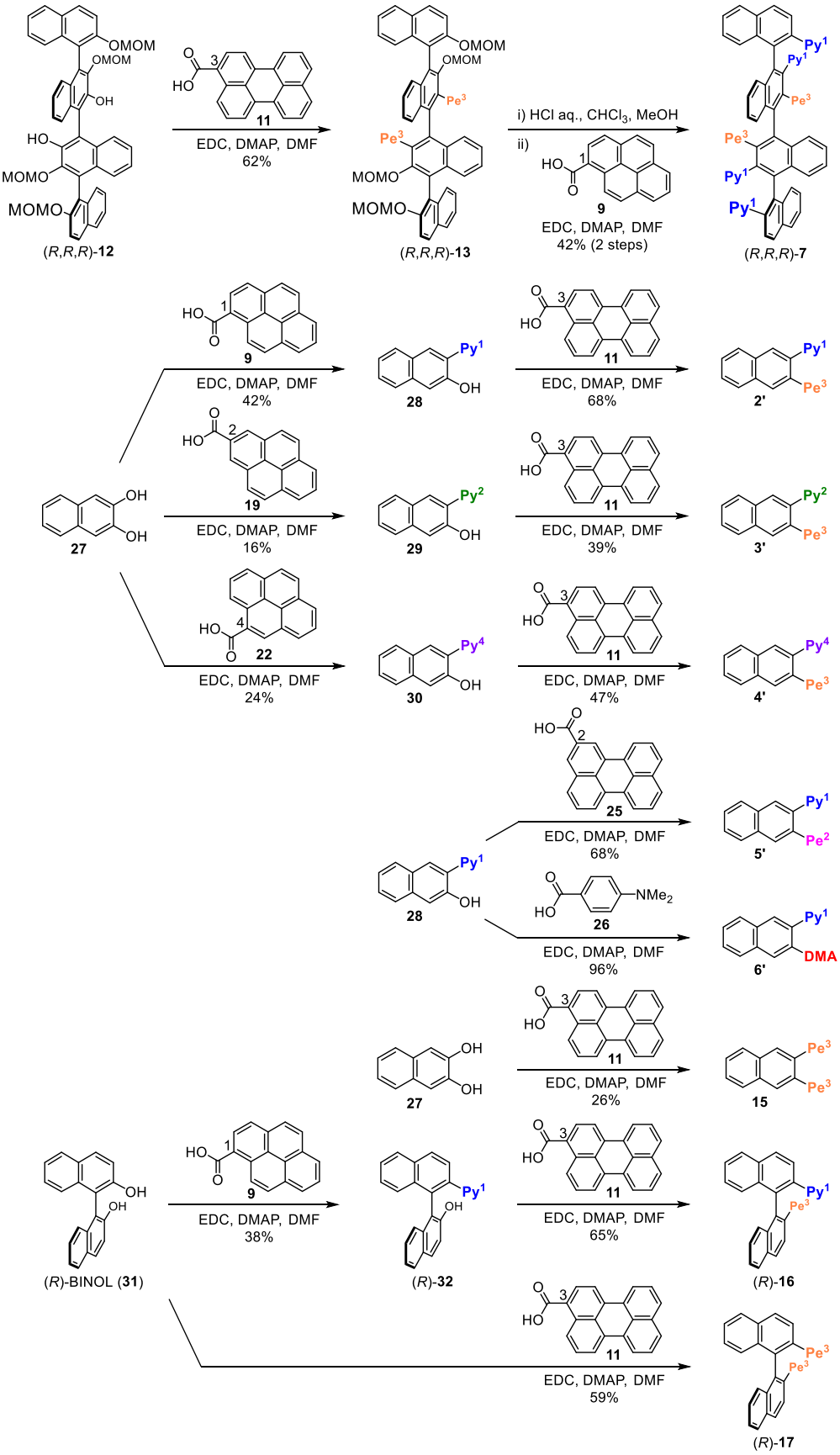
The full citation of reference 21: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, *Gaussian 16 (Revision C.01)*, Gaussian, Inc., Wallingford CT, 2019.

2. Synthetic methods and characterization

Compounds **9**, **27**, and **31** are commercially available. Compounds (*R*)-**8**[S1], **11**[S2], (*R*,*R*,*R*)-**12**[S3], **25**[S4], and (*R*)-**32**[S2] were synthesized according to the literature. (*S*)-**2** was synthesized in a similar manner to that for (*R*)-**2** with the exception that (*S*)-**8** was used as a starting material.

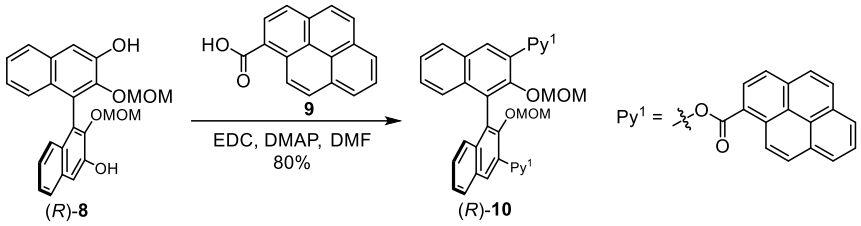


Scheme S1 Synthesis of fluorophore-tethered binaphthyls **2**–**6**.



Scheme S2 Synthesis of fluorophore-tethered quaternaphthyls, binaphthyls, and naphthalenes.

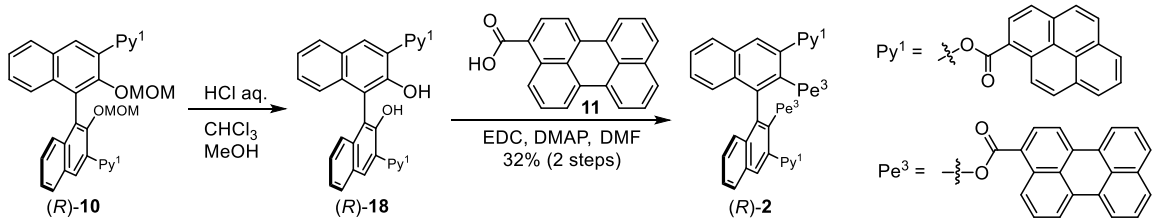
Synthesis of (*R*)-10



A solution of (*R*)-**8** (100 mg, 246 μmol), pyrene-1-carboxylic acid (**9**) (185 mg, 754 μmol), EDC·HCl (149 mg, 777 μmol), and DMAP (92.4 mg, 756 μmol) in dry DMF (14 mL) was stirred at room temperature for 21 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (twice). The organic layer was washed successively with water (three 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*)-**10** (169 mg, 196 μmol, 80%) as a yellow powder.

mp 131–136 °C; **[α]**$_D^{16}$ = –52 ($CHCl_3$, *c* 0.11); **IR** (KBr) 3042, 2826, 1730, 1506, 1431, 1360, 1246, 1225, 1163, 1078, 1009, 972, 820, 748, 709 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.68 (s, 6H), 4.94 (ABq, Δν = 45.4 Hz, *J* = 9.2 Hz, 4H), 7.35–7.45 (m, 4H), 7.50 (ddd, *J* = 1.6, 6.6, 8.2 Hz, 2H), 7.95 (d, *J* = 8.1 Hz, 2H), 8.03 (s, 2H), 8.09 (t, *J* = 7.6 Hz, 2H), 8.15 (d, *J* = 9.0 Hz, 2H), 8.25 (d, *J* = 10.2 Hz, 2H), 8.28–8.33 (m, 8H), 9.04 (d, *J* = 8.2 Hz, 2H), 9.48 (d, *J* = 9.6 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 56.7, 99.5, 122.2, 124.4, 125.2, 125.9, 126.56, 126.60, 126.69, 126.72, 127.2, 127.4, 127.8, 129.3, 130.1, 130.3, 130.6, 130.9, 131.2, 132.3, 132.4, 135.2, 143.8, 147.5, 166.0; **HR MS** (FAB$^+$; NBA) Calcd for $C_{58}H_{38}O_8$: 862.2561 [M]$^+$. Found: 862.2565.

Synthesis of (*R*)-2

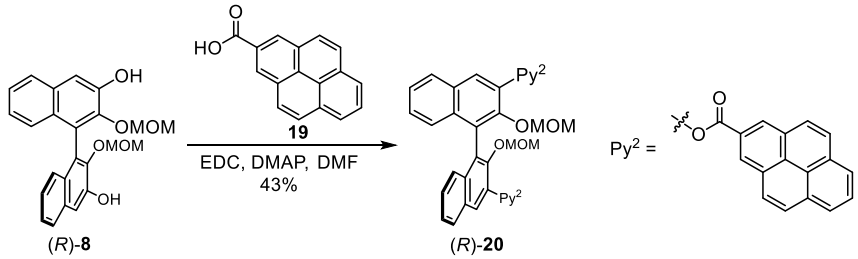


A solution of (*R*)-**10** (165 mg, 191 μmol) in a mixed solvent of 6 M HCl aq. (1.7 mL), $CHCl_3$ (1.8 mL), and MeOH (1.4 mL) was stirred and refluxed for 20 h under N_2 atmosphere. The mixture was cooled, diluted with water, and extracted with $CHCl_3$ (twice). The organic layer was washed successively with water (twice) and brine. After dried over Na_2SO_4, the solvent was evaporated to afford crude diol (*R*)-**18** (156 mg) as a yellow powder. A solution of the crude (*R*)-**18** (15.8 mg), perylene-3-carboxylic acid (**11**) (16.9 mg, 57.0 μmol), EDC·HCl (10.9 mg, 56.9 μmol), and DMAP (8.3 mg, 68 μmol) in dry DMF (1.1 mL) was stirred at room temperature for 20 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (twice). The organic layer was washed successively with water (twice) 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*)-**2** (8.5 mg, 6.2 μmol, 32%) as an orange

powder.

mp 243–244 °C; **[α]**$_D^{23}$ = +774 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3047, 2841, 1734, 1503, 1437, 1362, 1244, 1190, 1167, 1076, 1016, 968, 895, 851, 812, 770, 746, 708 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.15–7.25 (m, 2H), 7.25–7.50 (m, 8H), 7.50–8.10 (m, 26H), 8.10–8.30 (m, 6H), 8.30–8.50 (m, 2H), 8.50–8.75 (m, 4H), 8.80–9.15 (m, 2H); **HR MS** (FAB$^+$; NBA) Calcd for $C_{96}H_{51}O_8$: 1331.3578 $[M + H]^+$. Found: 1331.3579.

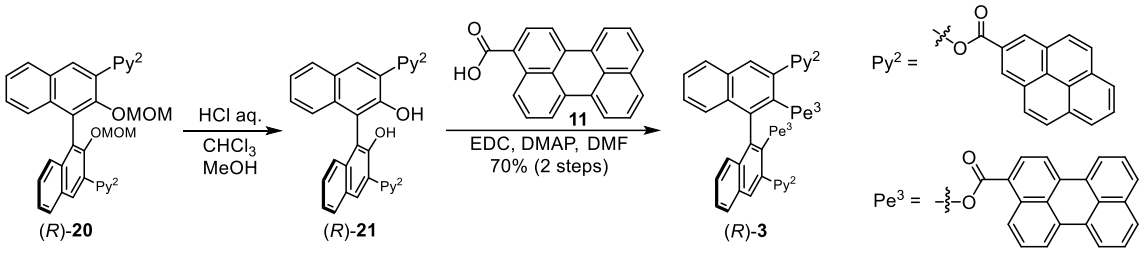
Synthesis of (*R*)-20



A solution of (*R*)-**8** (51.5 mg, 125 μmol), pyrene-2-carboxylic acid (**19**) (113 mg, 457 μmol), EDC·HCl (145 mg, 756 μmol), and DMAP (91.6 mg, 750 μmol) in dry DMF (4.0 mL) was stirred at 40 °C for 16 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (three times). The organic layer was washed successively with water (twice) and brine. After dried over Na_2SO_4, the solvent was evaporated to give a residue. The residue was purified by silica gel column chromatography ($CHCl_3$) and HPLC ($CHCl_3$) to afford (*R*)-**20** (46.1 mg, 53.4 μmol, 43%) as a yellow powder.

mp 263–267 °C; **[α]**$_D^{26}$ = –118 ($CHCl_3$, *c* 0.11); **IR** (KBr) 3055, 2953, 2893, 2824, 1742, 1501, 1433, 1360, 1294, 1244, 1203, 1186, 1157, 1107, 1074, 962, 918, 826, 748, 708 cm^{-1}; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 2.69 (s, 6H), 4.89 (d, *J* = 6.1 Hz, 2H), 5.03 (d, *J* = 6.1 Hz, 2H), 7.40 (t, *J* = 7.9 Hz, 2H), 7.46 (d, *J* = 8.3 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 2H), 7.95 (d, *J* = 8.0 Hz, 2H), 8.04 (s, 2H), 8.08 (t, *J* = 7.6 Hz, 2H), 8.13 (d, *J* = 8.9 Hz, 4H), 8.17 (d, *J* = 8.9 Hz, 4H), 8.22 (d, *J* = 7.6 Hz, 4H), 9.08 (s, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 56.2, 99.5, 122.0, 124.3, 125.7, 125.9, 126.3, 126.4, 126.6, 127.2, 127.3, 127.4, 127.8, 128.5, 130.8, 131.2, 131.9, 132.2, 143.5, 147.2, 165.6; **HR MS** (FAB$^+$; NBA) Calcd for $C_{58}H_{38}O_8$: 862.2561 $[M]^+$. Found: 862.2567.

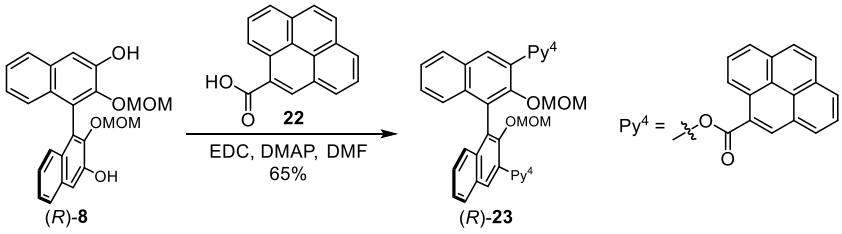
Synthesis of (*R*)-3



A solution of (*R*)-**20** (16.9 mg, 19.6 μmol) in a mixed solvent of 6 M HCl aq. (1.0 mL), $CHCl_3$ (0.5 mL), and MeOH (0.5 mL) was stirred and refluxed for 24 h under N_2 atmosphere. The mixture was cooled, diluted with water, and extracted with $CHCl_3$ (three times). The organic layer was washed successively with water (twice) and brine. After dried over Na_2SO_4, the solvent was evaporated to afford crude diol (*R*)-**21** (15.9 mg) as a yellow powder. A solution of the crude (*R*)-**21** (15.9 mg), perylene-3-carboxylic acid (**11**) (18.6 mg, 62.8 μmol), EDC·HCl (17.6 mg, 91.8 μmol), and DMAP (13.7 mg, 112 μmol) in dry DMF (2.0 mL) was stirred at 40 °C for 15 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (three times). The organic layer was washed successively with water (twice) 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*)-**3** (18.2 mg, 13.7 μmol, 70%) as an orange powder.

mp 229–232 °C; $[\alpha]_D^{26}$ = –925 ($CHCl_3$, *c* 0.10); **IR** (KBr) 2926, 2848, 1736, 1589, 1503, 1445, 1362, 1240, 1184, 1107, 1070, 930, 899, 812, 746, 708 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.95–7.25 (m, 4H), 7.25–7.60 (m, 18H), 7.60–7.80 (m, 14H), 7.80–8.25 (m, 6H), 8.25–8.70 (m, 8H); **HR MS** (FAB^+; NBA) Calcd for $C_{96}H_{51}O_8$: 1331.3578 $[M + H]^+$. Found: 1331.3583.

Synthesis of (*R*)-23

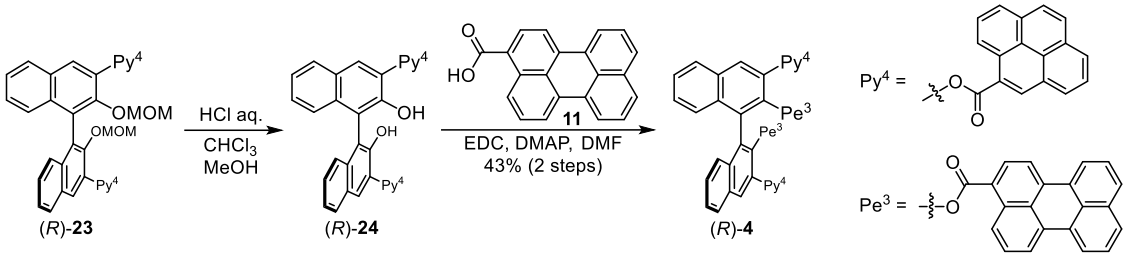


A solution of (*R*)-**8** (25.3 mg, 62.2 μmol), pyrene-4-carboxylic acid (**22**) (59.4 mg, 242 μmol), EDC·HCl (92.8 mg, 484 μmol), and DMAP (59.6 mg, 488 μmol) in dry DMF (2.0 mL) was stirred at 40 °C for 18 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (three times). The organic layer was washed successively with water (twice) 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, $CHCl_3$) and HPLC ($CHCl_3$) to afford (*R*)-**23** (35.0 mg, 40.6 μmol, 65%) as a yellow powder.

mp 131–135 °C; $[\alpha]_D^{26}$ = +24 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3045, 2951, 2891, 2824, 1732, 1501, 1431, 1360, 1269, 1246, 1221, 1192, 1167, 1105, 1091, 991, 968, 908, 829, 748, 716 cm^{-1}; **^{1}H NMR** (600 MHz,

$CDCl_3$) δ 2.75 (s, 6H), 4.93 (d, *J* = 6.1 Hz, 2H), 5.04 (d, *J* = 6.1 Hz, 2H), 7.41 (ddd, *J* = 1.3, 7.1, 8.6 Hz, 2H), 7.47 (d, *J* = 8.6 Hz, 2H), 7.53 (ddd, *J* = 1.3, 7.1, 8.5 Hz, 2H), 7.97 (d, *J* = 8.1 Hz, 2H), 8.05–8.10 (m, 6H), 8.10–8.15 (m, 4H), 8.26 (d, *J* = 7.4 Hz, 2H), 8.32 (d, *J* = 7.4 Hz, 2H), 8.36 (d, *J* = 7.4 Hz, 2H), 9.34 (s, 2H), 9.51 (d, *J* = 7.6 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 56.7, 99.5, 122.2, 124.5, 125.2, 125.4, 125.9, 126.1, 126.2, 126.4, 126.6, 126.8, 127.0, 127.2, 127.3, 127.8, 127.9, 128.3, 128.4, 129.3, 130.8, 131.2, 131.3, 132.3, 135.1, 143.5, 147.4, 165.5; **HR MS** (FAB$^+$; NBA) Calcd for $C_{58}H_{38}O_8$: 862.2561 $[M]^+$. Found: 862.2566.

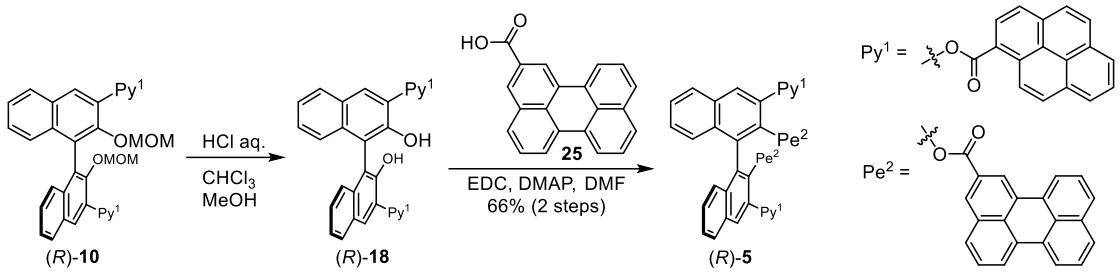
Synthesis of (*R*)-4



A solution of (*R*)-**23** (5.3 mg, 6.1 μmol) in a mixed solvent of 6 M HCl aq. (1.0 mL), $CHCl_3$ (0.5 mL), and MeOH (0.5 mL) was stirred and refluxed for 20 h under N_2 atmosphere. The mixture was cooled, diluted with water, and extracted with $CHCl_3$ (three times). The organic layer was washed successively with water (twice) and brine. After dried over Na_2SO_4, the solvent was evaporated to afford crude diol (*R*)-**24** (5.0 mg) as a yellow powder. A solution of the crude (*R*)-**24** (5.0 mg), perylene-3-carboxylic acid (**11**) (7.4 mg, 25 μmol), EDC·HCl (7.1 mg, 37 μmol), and DMAP (4.5 mg, 37 μmol) in dry DMF (1.0 mL) was stirred at 40 °C for 18 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (three times). The organic layer was washed successively with water (twice) 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, $CHCl_3$) and HPLC ($CHCl_3$) to afford (*R*)-**4** (3.5 mg, 2.6 μmol, 43%) as an orange powder.

mp 240–243 °C; **[α]**$_D^{26}$ = +39 ($CHCl_3$, *c* 0.031); **IR** (KBr) 3049, 1732, 1651, 1506, 1435, 1339, 1242, 1192, 1169, 1109, 1059, 895, 829, 812, 760, 716 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.15–7.25 (m, 2H), 7.25–7.55 (m, 8H), 7.55–8.10 (m, 28H), 8.10–8.30 (m, 4H), 8.30–8.55 (m, 2H), 8.60–8.80 (m, 2H), 8.85–8.95 (m, 2H), 9.19 (br s, 2H); **HR MS** (FAB$^+$; NBA) Calcd for $C_{96}H_{51}O_8$: 1331.3578 $[M + H]^+$. Found: 1331.3589.

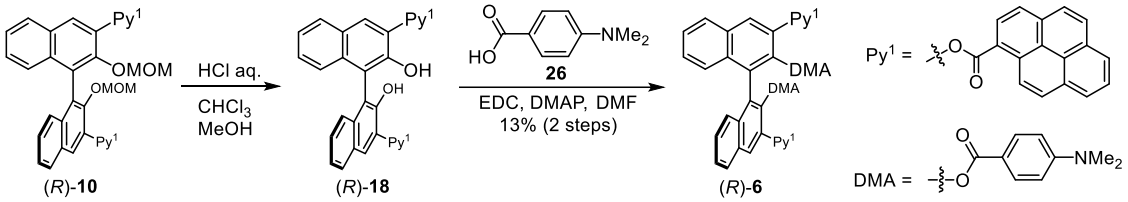
Synthesis of (*R*)-5



A solution of (*R*)-**10** (38.1 mg, 44.2 μmol) in a mixed solvent of 6 M HCl aq. (0.4 mL), $CHCl_3$ (0.6 mL), and MeOH (0.3 mL) was stirred at 65 °C for 12 h under N_2 atmosphere. The mixture was cooled, diluted with water, and extracted with $CHCl_3$ (twice). The organic layer was washed successively with water (twice) and brine. After dried over Na_2SO_4, the solvent was evaporated to afford crude diol (*R*)-**18** (37.7 mg) as a yellow powder. A solution of the crude (*R*)-**18** (10.1 mg), perylene-2-carboxylic acid (**25**) (11.6 mg, 39.1 μmol), EDC·HCl (8.0 mg, 42 μmol), and DMAP (5.0 mg, 41 μmol) in dry DMF (0.8 mL) was stirred at room temperature for 12 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (twice). The organic layer was washed successively with water (twice) 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*)-**5** (10.4 mg, 7.81 μmol, 66%) as an orange powder.

mp 248–249 °C; **[α]**$_D^{23}$ = –522 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3049, 2855, 1732, 1506, 1456, 1362, 1240, 1190, 1167, 1076, 849, 810, 768, 745, 706 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.75–7.25 (m, 6H), 7.27–7.65 (m, 16H), 7.65–7.90 (m, 12H), 7.90–8.10 (m, 6H), 8.10–8.40 (m, 6H), 8.50–9.10 (m, 4H); **HR MS** (MALDI$^+$-TOF; DCTB) Calcd for $C_{96}H_{50}O_8$: 1330.3500 $[M]^+$. Found: 1330.3530.

Synthesis of (*R*)-6

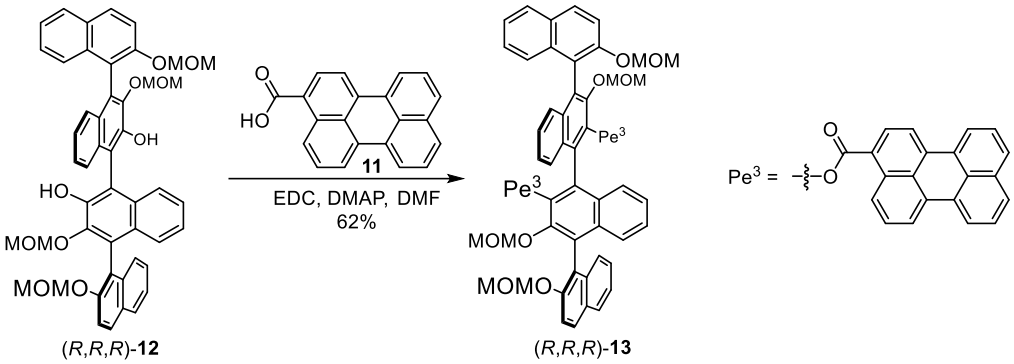


A solution of (*R*)-**10** (155 mg, 180 μmol) in a mixed solvent of 6 M HCl aq. (1.6 mL), $CHCl_3$ (1.7 mL), and MeOH (1.3 mL) was stirred and refluxed for 15 h under N_2 atmosphere. The mixture was cooled, diluted with water, and extracted with $CHCl_3$ (twice). The organic layer was washed successively with water (twice) and brine. After dried over Na_2SO_4, the solvent was evaporated to afford crude diol (*R*)-**18** (83.5 mg) as a yellow powder. A solution of the crude (*R*)-**18** (83.5 mg), 4-(dimethylanimo)benzoic acid (**26**) (54.6 mg, 331 μmol), EDC·HCl (67.1 mg, 350 μmol), and DMAP (42.8 mg, 350 μmol) in dry DMF (6.7 mL) was stirred at room temperature for 18 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (twice). The organic layer was washed successively with water (twice) 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, $CHCl_3$/EtOAc = 9/1) to afford (*R*)-**6** (24.4 mg, 22.8 μmol, 13%) as a yellow powder.

mp 196–197 °C; **[α]**$_D^{23}$ = +331 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3046, 2890, 1730, 1605, 1530, 1506, 1443, 1371, 1269, 1224, 1180, 1120, 1097, 1076, 1043, 1018, 968, 851, 822, 746, 710; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.66 (s, 12H), 6.26 (d, *J* = 8.9 Hz, 4H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.64 (d, *J* = 8.2 Hz, 2H), 7.86 (d, *J* = 8.8 Hz, 4H), 7.90–8.02 (m, 10H), 8.05–8.25 (m, 10H), 8.82 (d, *J* = 9.5 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 39.8, 110.7, 115.6, 122.0, 122.2, 124.0, 124.1, 124.4, 124.5, 125.0, 125.98, 126.03, 126.1, 126.3, 126.38, 126.44, 126.6, 126.7, 127.3, 128.0, 129.1, 129.2, 129.5, 130.4, 130.9, 131.3, 131.9, 132.1, 134.5, 141.3, 142.4, 153.3, 164.6, 165.3; **HR MS** (FAB$^+$; NBA) Calcd for $C_{72}H_{48}N_2O_8$: 1068.3405 [M]$^+$. Found: 1068.3409.

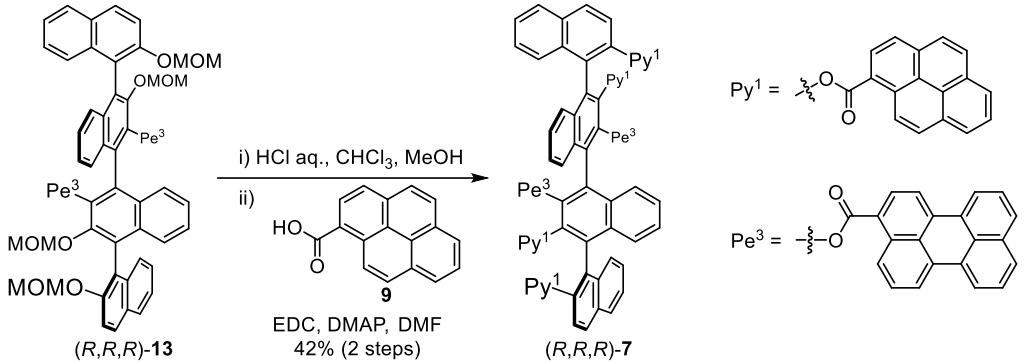
Synthesis of (*R*,*R*,*R*)-13



A solution of (*R*,*R*,*R*)-**12** (52.0 mg, 66.8 μmol), perylene-3-carboxylic acid (**11**) (77.9 mg, 263 μmol), EDC·HCl (98.6 mg, 514 μmol), and DMAP (69.7 mg, 571 μmol) in dry DMF (5.5 mL) was stirred at 40 °C for 22 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (twice). The organic layer was washed with water (three times). After dried over Na_2SO_4, the solvent was evaporated to give a residue. The residue was purified by column chromatography (SiO_2, $CHCl_3$/EtOAc = 9/1) and GPC ($CHCl_3$) to afford (*R*,*R*,*R*)-**13** (55.4 mg, 41.5 μmol, 62%) as an orange powder.

mp 174–176 °C; **[α]**$_D^{19}$ = +50 ($CHCl_3$, *c* 0.11); **IR** (KBr) 3051, 2826, 1736, 1622, 1504, 1422, 1387, 1242, 1213, 1169, 1153, 1090, 1063, 1034, 999, 964, 812, 762 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.70 (s, 6H), 3.42 (s, 6H), 4.75 (s, 2H), 4.87 (s, 2H), 5.30 (ABq, Δν = 19.4 Hz, *J* = 6.6 Hz, 4H), 6.71 (br s, 2H), 6.90 (br s, 2H), 7.07 (t, *J* = 7.1 Hz, 2H), 7.20–7.30 (m, 6H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.40–7.53 (m, 6H), 7.64 (d, *J* = 9.0 Hz, 2H), 7.65–7.75 (m, 8H), 7.97 (d, *J* = 9.0 Hz, 2H), 8.07 (t, *J* = 9.4 Hz, 4H), 8.21 (t, *J* = 7.7 Hz, 4H), 8.55 (d, *J* = 8.6 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 56.4, 56.6, 95.9, 99.2, 117.6, 117.7, 117.8, 119.6, 120.7, 120.87, 120.93, 121.0, 121.2, 122.2, 124.2, 125.1, 125.7, 125.8, 126.1, 126.4, 126.5, 126.7, 127.0, 127.1, 127.8, 128.1, 128.3, 128.4, 129.1, 129.4, 130.0, 130.2, 130.3, 130.5, 131.1, 131.3, 132.4, 133.1, 134.1, 134.5, 136.0, 142.7, 147.5, 153.4, 164.4; **HR MS** (FAB$^+$; NBA) Calcd for $C_{90}H_{62}O_{12}$: 1334.4236 [M]$^+$. Found: 1334.4289.

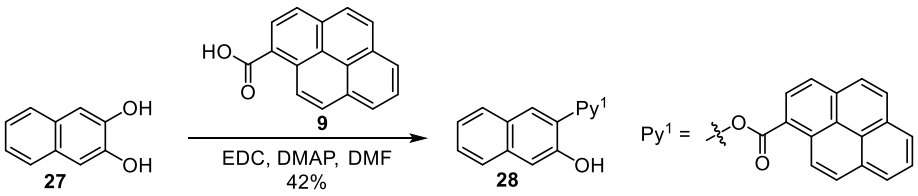
Synthesis of (*R*,*R*,*R*)-7



A solution of (*R*,*R*,*R*)-**13** (20.5 mg, 15.4 μmol) in a mixed solvent of 6 M HCl aq. (1.4 mL), $CHCl_3$ (1.4 mL), and MeOH (1.4 mL) was stirred and refluxed for 14 h under N_2 atmosphere. The mixture was cooled, diluted with water, and extracted with $CHCl_3$ (twice). The organic layer was washed with water (twice). After dried over Na_2SO_4, the solvent was evaporated to afford a crude tetraol (18.9 mg) as an orange powder. A solution of the crude tetraol (18.9 mg), pyrene-1-carboxylic acid (**9**) (30.6 mg, 124 μmol), EDC·HCl (47.3 mg, 247 μmol), and DMAP (30.9 mg, 253 μmol) in dry DMF (1.3 mL) was stirred at 40 °C for 18 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (twice). The organic layer was washed with water (three times). After dried over Na_2SO_4, the solvent was evaporated to give a residue. The residue was purified by column chromatography (SiO_2, $CHCl_3$), GPC ($CHCl_3$), and recrystallization from $CHCl_3$/hexane to afford (*R*,*R*,*R*)-**7** (13.3 mg, 6.42 μmol, 42%) as an orange powder.

mp 266–268 °C; **[α]**$_D^{20}$ = –320 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3049, 2878, 1732, 1506, 1404, 1325, 1246, 1192, 1076, 1020, 970, 849, 812, 762, 708 cm^{-1}; **^{1}H NMR** (400 MHz, THF-d_8) δ 6.70–7.20 (m, 10H), 7.20–8.10 (m, 42H), 8.10–8.60 (m, 20H), 8.60–9.50 (m, 6H); **HR MS** (FAB^+; NBA) Calcd for $C_{150}H_{79}O_{12}$: 2071.5566 $[M + H]^+$. Found: 2071.5572.

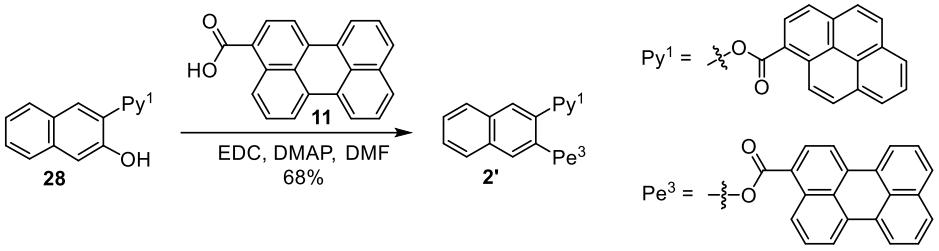
Synthesis of 28



A solution of 2,3-dihydroxynaphthalene (**27**) (100 mg, 626 μmol), pyrene-1-carboxylic acid (**9**) (153 mg, 624 μmol), EDC·HCl (370 mg, 1.93 mmol), and DMAP (238 mg, 1.24 mmol) in dry DMF (30 mL) was stirred at rt for 16 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (twice). The organic layer was washed successively with water (three 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 **28** (104 mg, 266 μmol, 42%) as a yellow powder.

mp 198–201 °C; **IR** (KBr) 3395, 3036, 1711, 1530, 1508, 1402, 1327, 1254, 1196, 1078, 1030, 970, 837, 812, 745, 708 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.54 (s, 1H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.1 Hz, 1H), 7.48 (s, 1H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.88 (s, 1H), 8.06–8.13 (m, 1H), 8.16 (d, *J* = 8.9 Hz, 1H), 8.27 (d, *J* = 8.0 Hz, 1H), 8.28–8.36 (m, 4H), 8.97 (d, *J* = 8.1 Hz, 1H), 9.40 (d, *J* = 9.4 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 112.8, 120.6, 121.5, 124.3, 124.4, 124.6, 124.7, 125.2, 126.4, 126.6, 126.7, 126.9, 127.0, 127.3, 127.7, 129.1, 129.3, 130.4, 130.5, 131.2, 132.4, 132.9, 135.5, 140.1, 146.6, 166.1; **HR MS** (FAB^+; NBA) Calcd for $C_{27}H_{16}O_3$: 388.1094 $[M]^+$. Found: 388.1086.

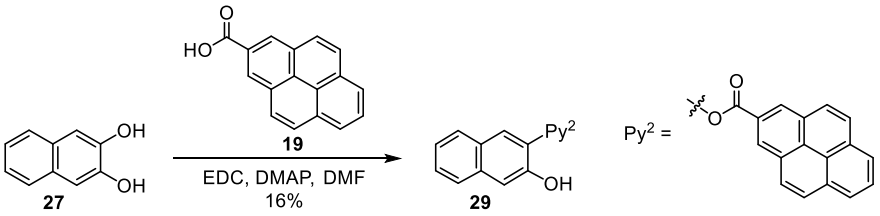
Synthesis of 2'



A solution of **28** (20.1 mg, 51.5 μmol), perylene-3-carboxylic acid (**11**) (24.9 mg, 84.0 μmol), EDC·HCl (30.4 mg, 159 μmol), and DMAP (19.8 mg, 162 μmol) in dry DMF (2.5 mL) was stirred at 40 °C for 15 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (twice). The organic layer was washed successively with water (three 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 **2'** (23.5 mg, 35.2 μmol, 68%) as an orange powder.

mp 199–202 °C; **IR** (KBr) 3047, 2924, 2852, 1730, 1570, 1506, 1468, 1325, 1246, 1230, 1190, 1093, 1015, 970, 843, 810, 745, 706 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27–7.33 (m, 2H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 3.6 Hz, 2H), 7.58 (d, *J* = 6.1 Hz, 1H), 7.59 (d, *J* = 6.1 Hz, 1H), 7.64 (d, *J* = 7.4 Hz, 1H), 7.67 (d, *J* = 8.2 Hz, 1H), 7.68 (d, *J* = 7.9 Hz, 1H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 8.9 Hz, 1H), 7.87 (d, *J* = 8.2 Hz, 1H), 7.91 (d, *J* = 8.9 Hz, 1H), 7.93–8.03 (m, 8H), 8.18 (d, *J* = 8.2 Hz, 1H), 8.70 (d, *J* = 8.8 Hz, 1H), 8.74 (d, *J* = 8.2 Hz, 1H), 9.16 (d, *J* = 9.3 Hz, 1H); **HR MS** (FAB^+; NBA) Calcd for $C_{48}H_{26}O_4$: 666.1826 $[M]^+$. Found: 666.1831.

Synthesis of 29

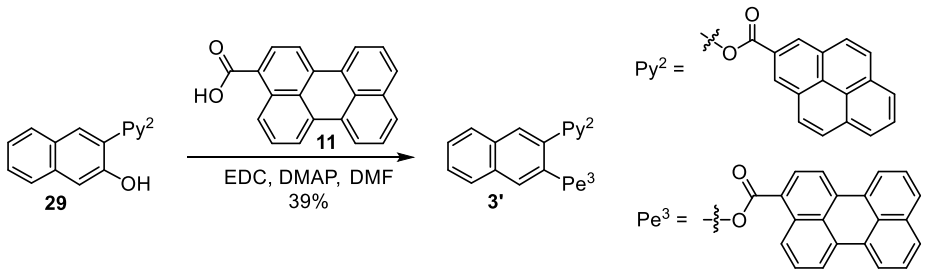


A solution of 2,3-dihydroxynaphthalene (**27**) (73.5 mg, 459 μmol), pyrene-2-carboxylic acid (**19**) (111 mg, 452 μmol), EDC·HCl (353 mg, 1.84 mmol), and DMAP (224 mg, 1.84 mmol) in dry DMF (45 mL)

was stirred at room temperature for 16 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (three times). The organic layer was washed successively with water (twice) 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, $CHCl_3$) and HPLC ($CHCl_3$) to afford **29** (28.9 mg, 74.4 μmol, 16%) as a colorless powder.

mp 222–225 °C; **IR** (KBr) 3401, 3048, 3028, 2924, 2853, 1724, 1632, 1528, 1400, 1362, 1302, 1260, 1219, 1153, 951, 905, 843, 827, 747, 710 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.72 (br s, 1H), 7.40 (ddd, *J* = 1.2, 6.9, 8.0 Hz, 1H), 7.43–7.50 (m, 2H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.84 (s, 1H), 8.12 (dd, *J* = 7.3, 8.1 Hz, 1H), 8.15–8.25 (m, 4H), 8.27 (d, *J* = 7.6 Hz, 2H), 9.06 (s, 2H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 110.7, 120.6, 123.3, 123.5, 125.8, 125.9, 126.0, 126.1, 126.3, 127.2, 127.6, 127.7, 127.8, 128.5, 130.8, 131.4, 132.6, 140.4, 148.4, 164.9; **HR MS** (FAB$^+$; NBA) Calcd for $C_{27}H_{16}O_3$: 388.1094 $[M]^+$. Found: 388.1109.

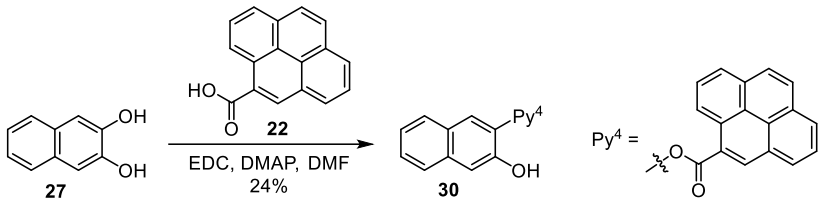
Synthesis of 3'



A solution of **29** (17.6 mg, 45.3 μmol), perylene-3-carboxylic acid (**11**) (27.1 mg, 91.5 μmol), EDC·HCl (35.3 mg, 184 μmol), and DMAP (44.5 mg, 364 μmol) in dry DMF (2.0 mL) was stirred at 40 °C for 17 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (three times). The organic layer was washed successively with water (twice) 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, $CHCl_3$) and HPLC ($CHCl_3$) to afford **3'** (11.9 mg, 17.8 μmol, 39%) as an orange powder.

mp 217–221 °C; **IR** (KBr) 3049, 2918, 1736, 1568, 1504, 1468, 1296, 1244, 1215, 1192, 1109, 1094, 996, 891, 843, 810, 745, 708 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.9 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 7.50–7.80 (m, 11H), 7.82–8.00 (m, 8H), 8.01 (d, *J* = 9.2 Hz, 1H), 8.27 (d, *J* = 9.2 Hz, 1H), 8.72 (s, 2H), 8.89 (d, *J* = 8.6 Hz, 1H); **HR MS** (FAB$^+$; NBA) Calcd for $C_{48}H_{26}O_4$: 666.1826 $[M]^+$. Found: 666.1831.

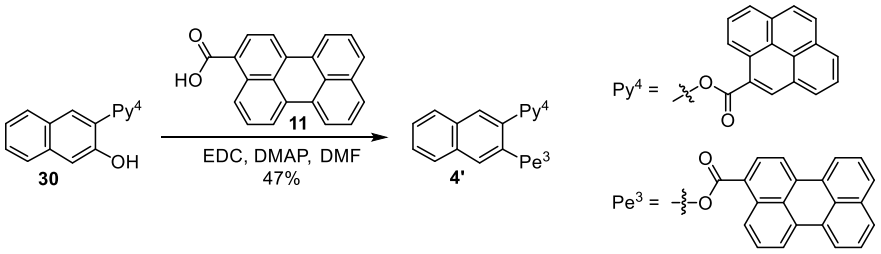
Synthesis of 30



A solution of 2,3-dihydroxynaphthalene (**27**) (33.8 mg, 211 μmol), pyrene-4-carboxylic acid (**22**) (51.5 mg, 209 μmol), EDC·HCl (159 mg, 829 μmol), and DMAP (103 mg, 843 μmol) in dry DMF (20 mL) was stirred at rt for 26 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (three times). The organic layer was washed successively with water (twice) 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 **30** (19.6 mg, 50.5 μmol, 24%) as a yellow powder.

mp 220–224 °C; **IR** (KBr) 3325, 3044, 1730, 1528, 1508, 1400, 1362, 1275, 1254, 1194, 1169, 1094, 995, 920, 841, 829, 741, 714 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.65 (s, 1H), 7.41 (ddd, *J* = 1.2, 7.0, 8.1 Hz, 1H), 7.42–7.50 (m 2H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.83 (d, *J* = 7.7 Hz, 1H), 7.88 (s, 1H), 8.08–8.18 (m, 4H), 8.30 (d, *J* = 7.2 Hz, 1H), 8.34 (d, *J* = 7.7 Hz, 1H), 8.39 (d, *J* = 7.6 Hz, 1H), 9.26 (s, 1H), 9.40 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 110.7, 120.7, 123.5, 123.6, 124.4, 124.9, 125.4, 125.9, 126.0, 126.2, 126.92, 126.95, 127.1, 127.2, 127.4, 127.5, 127.6, 128.1, 128.7, 130.6, 130.9, 132.6, 134.0, 140.3, 148.5, 165.2; **HR MS** (FAB^+; NBA) Calcd for $C_{27}H_{16}O_3$: 388.1094 $[M]^+$. Found: 388.1110.

Synthesis of 4'

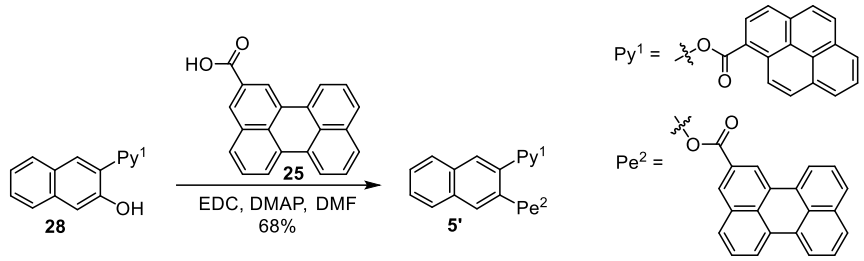


A solution of **30** (17.9 mg, 46.1 μmol), perylene-3-carboxylic acid (**11**) (27.4 mg, 92.5 μmol), EDC·HCl (35.1 mg, 183 μmol), and DMAP (45.3 mg, 371 μmol) in dry DMF (2.0 mL) was stirred at 40 °C for 18 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (three times). The organic layer was washed successively with water (twice) 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, $CHCl_3$), HPLC ($CHCl_3$), and recrystallization ($CHCl_3$/hexane) to afford **4'** (14.5 mg, 21.7 μmol, 47%) as an orange powder.

mp 194–197 °C; **IR** (KBr) 3047, 2951, 2928, 2857, 1732, 1570, 1506, 1468, 1273, 1244, 1223, 1194, 1171, 1094, 961, 841, 812, 760, 713 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38–7.46 (m, 1H), 7.50–7.61 (m, 5H), 7.62–7.80 (m, 4H), 7.82–8.04 (m, 8H), 8.07 (s, 1H), 8.08 (d, *J* = 7.1 Hz, 1H), 8.21 (d, *J* = 8.0 Hz, 1H),

8.29 (d, *J* = 8.0 Hz, 1H), 8.80 (d, *J* = 8.7 Hz, 1H), 8.81 (d, *J* = 8.6 Hz, 1H), 8.91 (s, 1H), 9.25 (d, *J* = 8.1 Hz, 1H); **HR MS** (FAB$^+$; NBA) Calcd for $C_{48}H_{26}O_4$: 666.1826 [M]$^+$. Found: 666.1831.

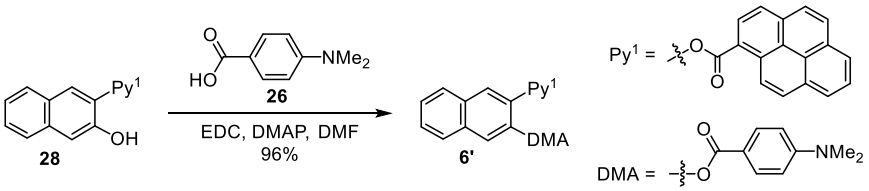
Synthesis of 5'



A solution of **28** (20.1 mg, 51.5 μmol), perylene-2-carboxylic acid (**25**) (24.9 mg, 84.0 μmol), EDC·HCl (30.4 mg, 159 μmol), and DMAP (19.8 mg, 162 μmol) in dry DMF (2.5 mL) was stirred at room temperature for 15 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (twice). The organic layer was washed successively with water (three 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 **5'** (23.5 mg, 35.2 μmol, 68%) as an orange powder.

mp 167–169 °C; **IR** (KBr) 3046, 2924, 2851, 1732, 1568, 1506, 1468, 1387, 1248, 1231, 1190, 1169, 1146, 1119, 1094, 968, 843, 810, 758, 706 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.25–7.32 (m, 1H), 7.45–7.50 (m, 1H), 7.56–7.68 (m, 5H), 7.71 (d, *J* = 9.2 Hz, 1H), 7.74–7.82 (m, 2H), 7.83–7.92 (m, 3H), 7.92–8.02 (m, 8H), 8.04 (s, 1H), 8.10 (br d, *J* = 7.6 Hz, 1H), 8.16 (d, *J* = 8.3 Hz, 1H), 8.69 (br d, *J* = 8.7 Hz, 1H), 8.71 (d, *J* = 8.2 Hz, 1H), 8.73 (d, *J* = 8.2 Hz, 1H), 9.12 (d, *J* = 9.6 Hz, 1H), 9.16 (d, *J* = 9.4 Hz, 1H); **HR MS** (FAB$^+$; NBA) Calcd for $C_{48}H_{26}O_4$: 666.1826 [M]$^+$. Found: 666.1831.

Synthesis of 6'

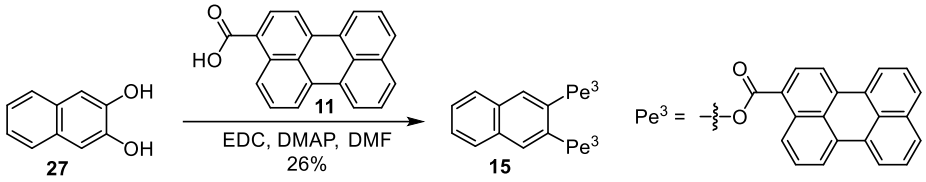


A solution of **28** (38.0 mg, 97.8 μmol), 4-(dimethylanimo)benzoic acid (**26**) (33.7 mg, 204 μmol), EDC·HCl (156 mg, 814 μmol), and DMAP (95.7 mg, 783 μmol) in dry DMF (9.0 mL) was stirred at 40 °C for 16 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (five times). The organic layer was washed successively with water (twice) 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 **6'** (50.3 mg, 93.9 μmol, 96%) as a yellow powder.

mp 152–156 °C; **IR** (KBr) 3053, 1726, 1603, 1557, 1531, 1506, 1466, 1373, 1325, 1275, 1248, 1227, 1219, 1192, 1093, 1042, 1016, 970, 945, 847, 760, 745, 710 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.71 (s, 6H), 6.24 (d, *J* = 8.8 Hz, 6H), 7.50–7.55 (m, 2H), 7.85–7.92 (m, 5H), 7.95 (s, 1H), 8.00–8.08 (m, 3H), 8.16

(t, *J* = 8.7 Hz, 2H), 8.23 (d, *J* = 7.6 Hz, 1H), 8.25 (d, *J* = 7.4 Hz, 1H), 8.79 (d, *J* = 8.2 Hz, 1H), 9.34 (d, *J* = 9.4 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 39.8, 110.5, 115.1, 121.2, 121.5, 121.7, 124.1, 124.3, 124.9, 125.0, 126.2, 126.3, 126.47, 126.52, 126.6, 127.3, 127.7, 127.7, 129.4, 129.9, 130.0, 130.5, 131.0, 131.7, 132.0, 132.08, 132.11, 135.0, 142.2, 142.3, 153.5, 165.1, 165.8; **HR MS** (FAB^+; NBA) Calcd for $C_{36}H_{25}NO_4$: 535.1778 $[M]^+$. Found: 535.1784.

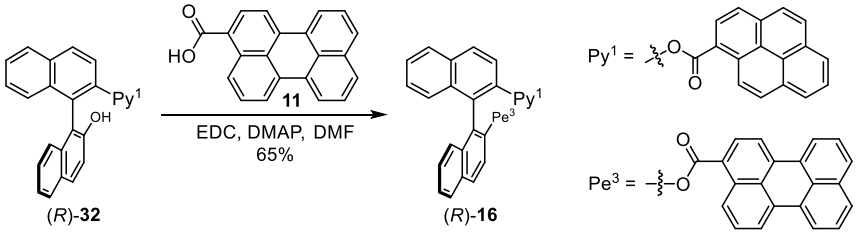
Synthesis of 15



A solution of 2,3-dihydroxynaphthalene (**27**) (5.9 mg, 0.037 mmol), pyrene-1-carboxylic acid (**11**) (43.6 mg, 147 μmol), EDC·HCl (53.5 mg, 279 μmol), and DMAP (17.7 mg, 149 μmol) in dry DMF (1.5 mL) was stirred at rt for 13 h under N_2 atmosphere. The reaction was quenched with water, and $CHCl_3$ was added. The suspension was filtered, and the organic layer of the filtrate was washed successively with water (four times). 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 **15** (7.0 mg, 9.8 μmol, 26%) as an orange powder.

mp 283–286 °C; **IR** (KBr) 2959, 2905, 1730, 1504, 1467, 1425, 1387, 1362, 1242, 1198, 1173, 1109, 1061, 991, 959, 808, 756 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 (t, *J* = 5.5 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 7.40–7.46 (m, 2H), 7.50–7.60 (m, 6H), 7.66 (d, *J* = 8.1 Hz, 2H), 7.87 (t, *J* = 6.9 Hz, 4H), 7.90–8.00 (m, 6H), 8.22 (d, *J* = 8.1 Hz, 2H), 8.81 (d, *J* = 8.2 Hz, 2H); **HR MS** (ESI^+) Calcd for $C_{52}H_{28}O_4Na$: 739.1880 $[M + Na]^+$. Found: 739.1900.

Synthesis of (*R*)-16

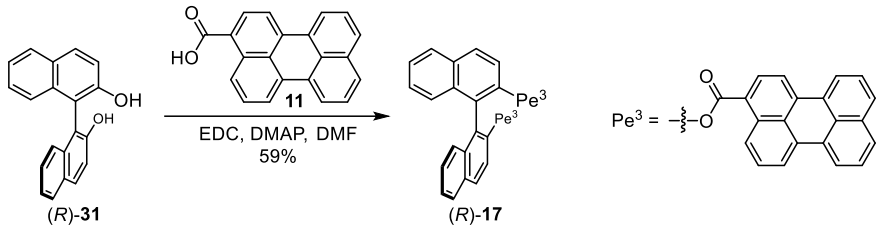


A solution of (*R*)-**32** (10.4 mg, 20.2 μmol), perylene-3-carboxylic acid (**11**) (9.1 mg, 31 μmol), EDC·HCl (11.4 mg, 59.5 μmol), and DMAP (8.0 mg, 65 μmol) in dry DMF (1.0 mL) was stirred at 40 °C for 18 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (three times). The organic layer was washed with water (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*)-**16** (10.3 mg, 13 μmol, 65%) as an orange powder.

mp 188–190 °C; **[α]**$_D^{18}$ = –263 ($CHCl_3$, *c* 0.10); **IR** (KBr) 3049, 2924, 2851, 1726, 1508, 1430, 1246,

1206, 1191, 1076, 1020, 976, 851, 804, 768, 708 cm^{-1}; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.19–7.32 (m, 4H), 7.45–7.54 (m, 6H), 7.55 (br s, 1H), 7.58 (dd, *J* = 3.5, 8.0 Hz, 1H), 7.61 (d, *J* = 8.3 Hz, 1H), 7.62 (d, *J* = 8.2 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.72–7.78 (m, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.6 Hz, 1H), 7.82 (dd, *J* = 2.3, 8.8 Hz, 1H), 7.85 (d, *J* = 7.0 Hz, 1H), 7.85–7.91 (m, 3H), 7.95 (d, *J* = 8.8 Hz, 1H), 7.96–8.02 (m, 2H), 8.03 (d, *J* = 7.9 Hz, 1H), 8.05 (d, *J* = 5.0 Hz, 1H), 8.08 (d, *J* = 9.1 Hz, 1H), 8.13 (dd, *J* = 8.1, 8.9 Hz, 1H), 8.41 (dd, *J* = 3.9, 8.5 Hz, 1H), 8.86 (d, *J* = 9.3 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 118.8, 120.3, 120.9, 121.9, 122.1, 122.5, 122.6, 123.9, 124.1, 124.2, 124.26, 124.32, 124.4, 124.5, 124.7, 125.4, 126.0, 126.1, 126.19, 126.25, 126.3, 126.4, 126.47, 126.52, 126.7, 127.0, 127.1, 127.9, 128.0, 128.2, 128.3, 128.7, 128.8, 129.2, 129.4, 129.7, 129.9, 130.2, 130.7, 130.8, 130.9, 131.5, 131.86, 131.90, 133.0, 133.8, 134.16, 134.20, 134.5, 136.0, 147.6, 147.7, 165.4, 166.0; **HR MS** (FAB^+; NBA) Calcd for $C_{58}H_{32}O_4$: 792.2295 $[M]^+$. Found: 792.2299.

Synthesis of (*R*)-17



A solution of (*R*)-BINOL (**31**) (34.9 mg, 122 μmol), perylene-3-carboxylic acid (**11**) (115 mg, 389 μmol), EDC·HCl (108 mg, 561 μmol), and DMAP (95.3 mg, 780 μmol) in dry DMF (5.0 mL) was stirred at 40 °C for 24 h under N_2 atmosphere. The reaction was quenched with water, and the product was extracted with $CHCl_3$ (three times). The organic layer was washed successively with water (twice) 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*)-**17** (60.4 mg, 71.7 μmol, 59%) as an orange powder.

mp 192–193 °C; **[α]**$_D^{26}$ = –306 ($CHCl_3$, *c* 0.031); **IR** (KBr) 3049, 1724, 1522, 1506, 1474, 1458, 1246, 1220, 1169, 1111, 1061, 1001, 916, 810, 760 cm^{-1}; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.26 (t, *J* = 8.0 Hz, 2H), 7.31 (t, *J* = 7.7 Hz, 2H), 7.36 (t, *J* = 7.8 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.53 (t, *J* = 7.5 Hz, 2H), 7.55–7.60 (m, 6H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.71 (d, *J* = 8.9 Hz, 2H), 7.85 (d, *J* = 7.6 Hz, 2H), 7.92 (d, *J* = 7.5 Hz, 2H), 7.96 (d, *J* = 7.5 Hz, 2H), 7.99 (d, *J* = 8.2 Hz, 2H), 8.10 (d, *J* = 8.8 Hz, 2H), 8.41 (d, *J* = 8.6 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 118.9, 120.5, 121.0, 122.0, 122.5, 124.4, 124.6, 125.6, 126.0, 126.6, 126.8, 127.1, 128.0, 128.2, 128.3, 128.9, 129.2, 129.8, 130.1, 131.0, 131.1, 131.6, 131.9, 133.1, 133.9, 134.4, 136.1, 147.7, 165.4; **HR MS** (FAB^+; NBA) Calcd for $C_{62}H_{34}O_4Na$: 842.2452 $[M + Na]^+$. Found: 842.2458.

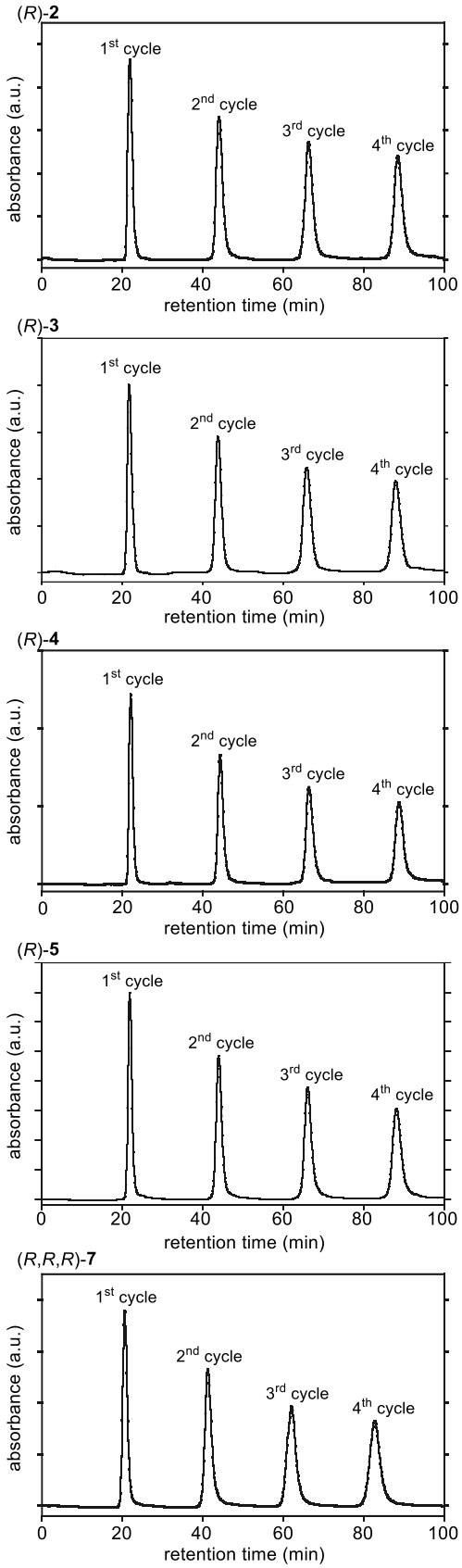


Fig. S1 Recycle HPLC charts of (*R*)-**2**–**5** and (*R*,*R*,*R*)-**7**. Conditions: JAIGEL-1HH (20 × 600 mm) and JAIGEL-2HH (20 × 600 mm) (Japan Analytical Industry), $CHCl_3$, 7.5 mL/min, UV-detection at 254 nm.

3. CD, FL, CPL, and excitation spectra and FL quantum yields

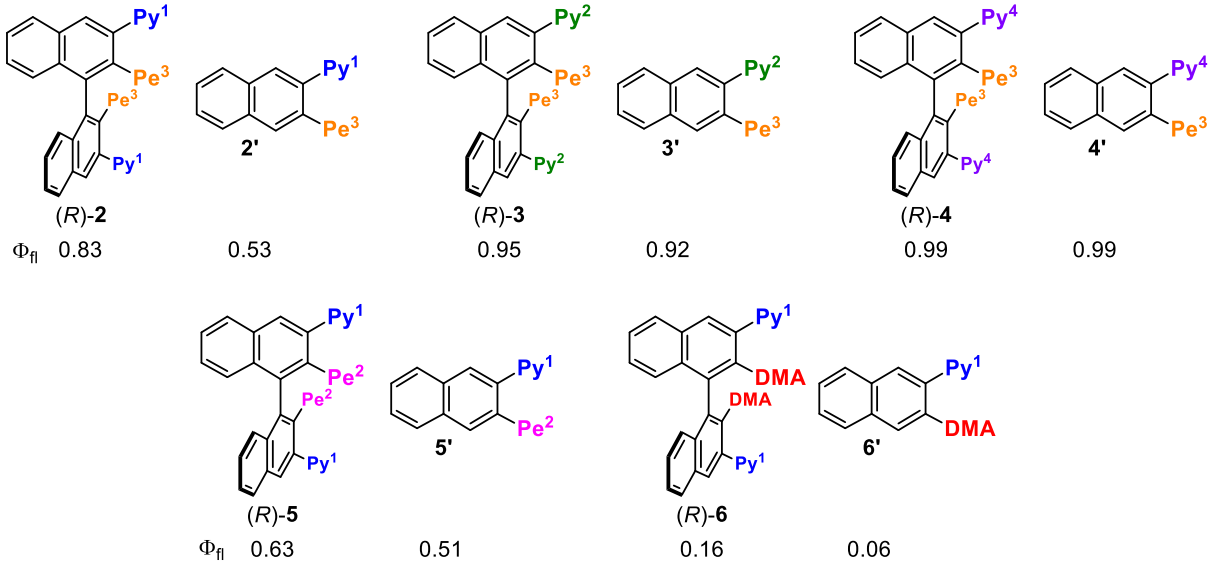


Fig. S2 FL quantum yields (Φ_{fl}) of (*R*)-**2**–**6** and their half model compounds **2'**–**6'**. Conditions: CH_2Cl_2, 1.0×10^{-5} M for **2**–**6** and 2.0×10^{-5} M for **2'**–**6'**, 20 °C, l = 1 cm.

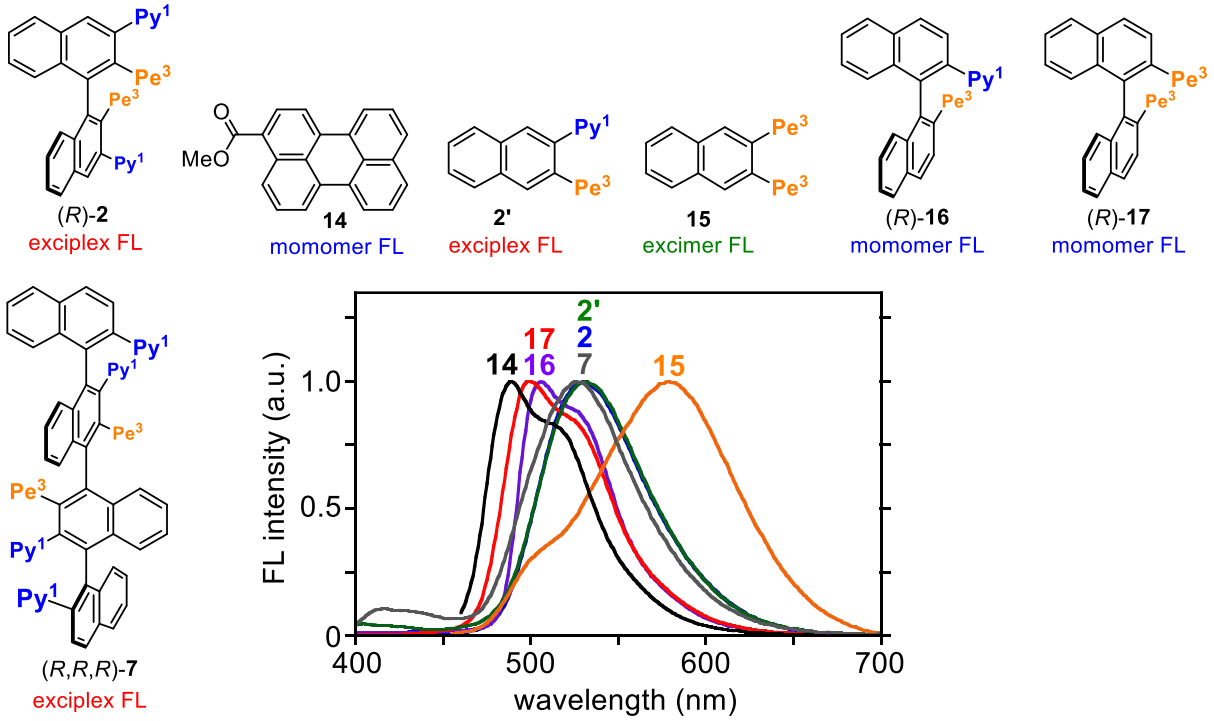


Fig. S3 FL spectra of **2** and its reference compounds **2'** and **14**–**17**. Conditions: CH_2Cl_2, 1.0×10^{-5} M for **2**, 4.0×10^{-5} M for **14**, and 2.0×10^{-5} M for **2'** and **15**–**17**, 20 °C, l = 1 cm, λ_{ex} = 355 nm for **2**, **2'**, **16**, and **17** and 445 nm for **14** and **15**.

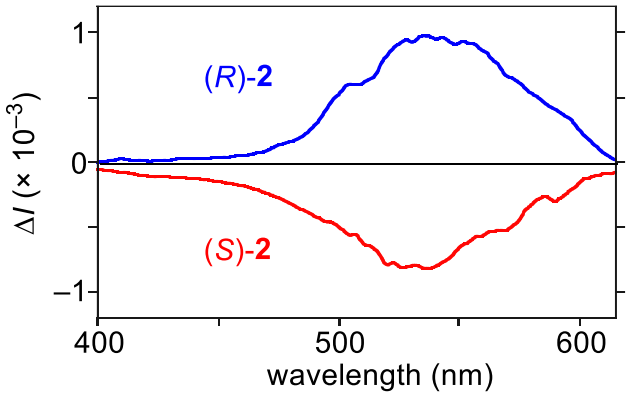


Fig. S4 CPL spectra of (*R*)-**2** (blue) and (*S*)-**2** (red). Conditions: CH_2Cl_2, 1.0×10^{-5} M, 20 °C, light path length = 1 cm, λ_{ex} = 355 nm, baseline-corrected.

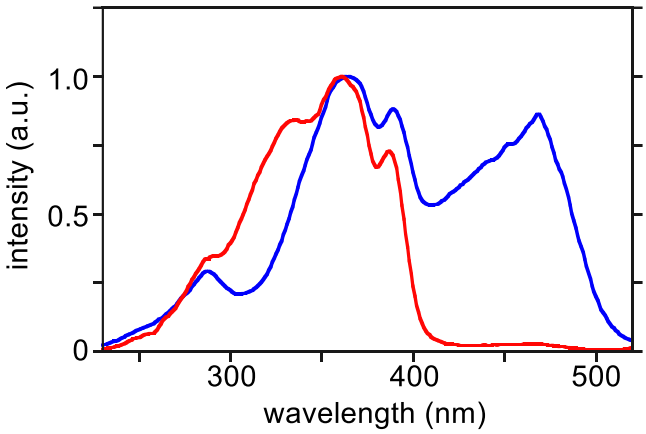


Fig. S5 Excitation spectra of (*R*)-**2** (blue) and (*R*)-**6** (red). Conditions: CH_2Cl_2, 1.0×10^{-5} M, 20 °C, light path length = 1 cm, λ_{em} = 530 nm.

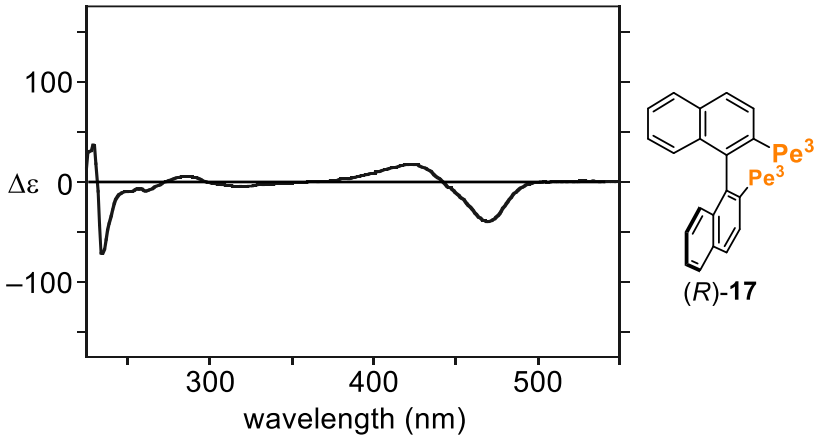


Fig. S6 CD spectra of (*R*)-**17**. Conditions: CH_2Cl_2, 1.0×10^{-5} M, 20 °C, light path length = 1 cm.

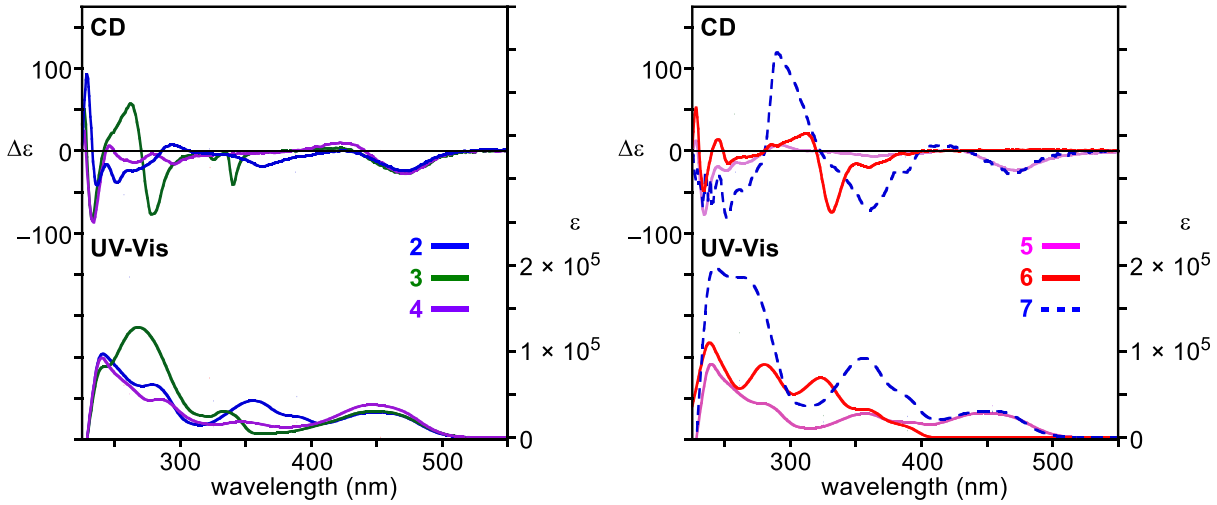


Fig. S7 CD and UV-Vis spectra of (*R*)-**2**–**6** and (*R*,*R*,*R*)-**7**. Conditions: CH_2Cl_2, 1.0×10^{-5} M for **2**–**6** and 6.7×10^{-6} M for **7**, 20 °C, l = 1 cm.

4. DFT calculation

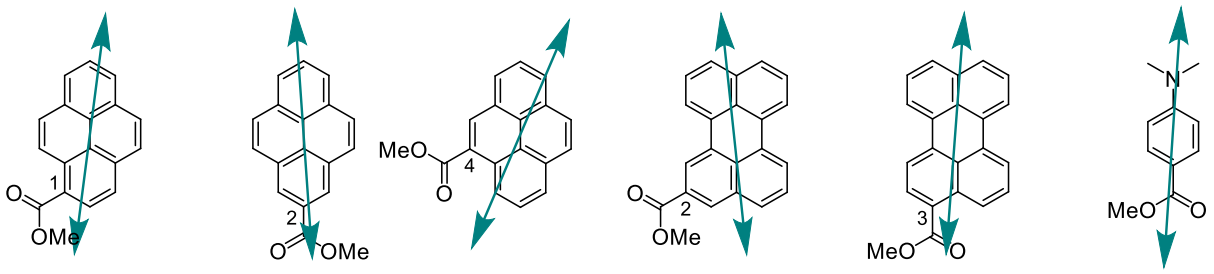


Fig. S8 Orientations of the transition dipole moments of the lowest energy transition of methyl esters calculated at the CAM-B3LYP/6-31G(d,p) level.

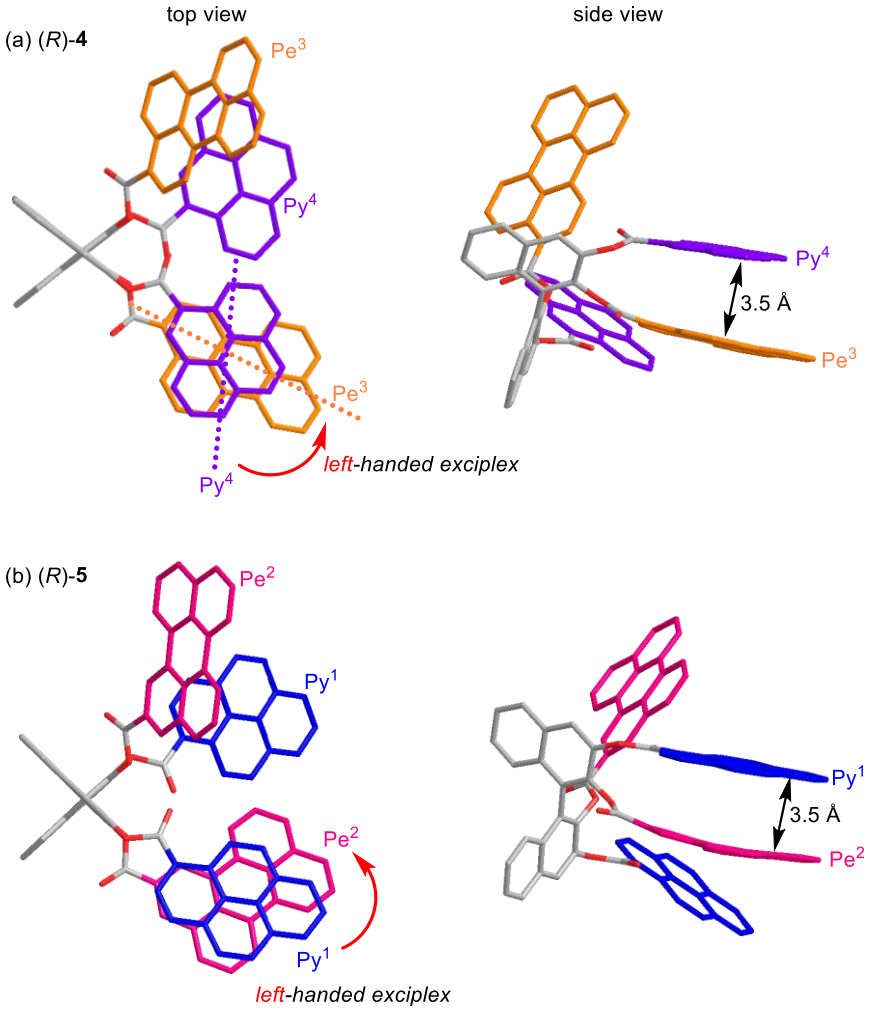


Fig. S9 TD DFT-optimized excited-state structures of (a) (*R*)-**4** and (b) (*R*)-**5** at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

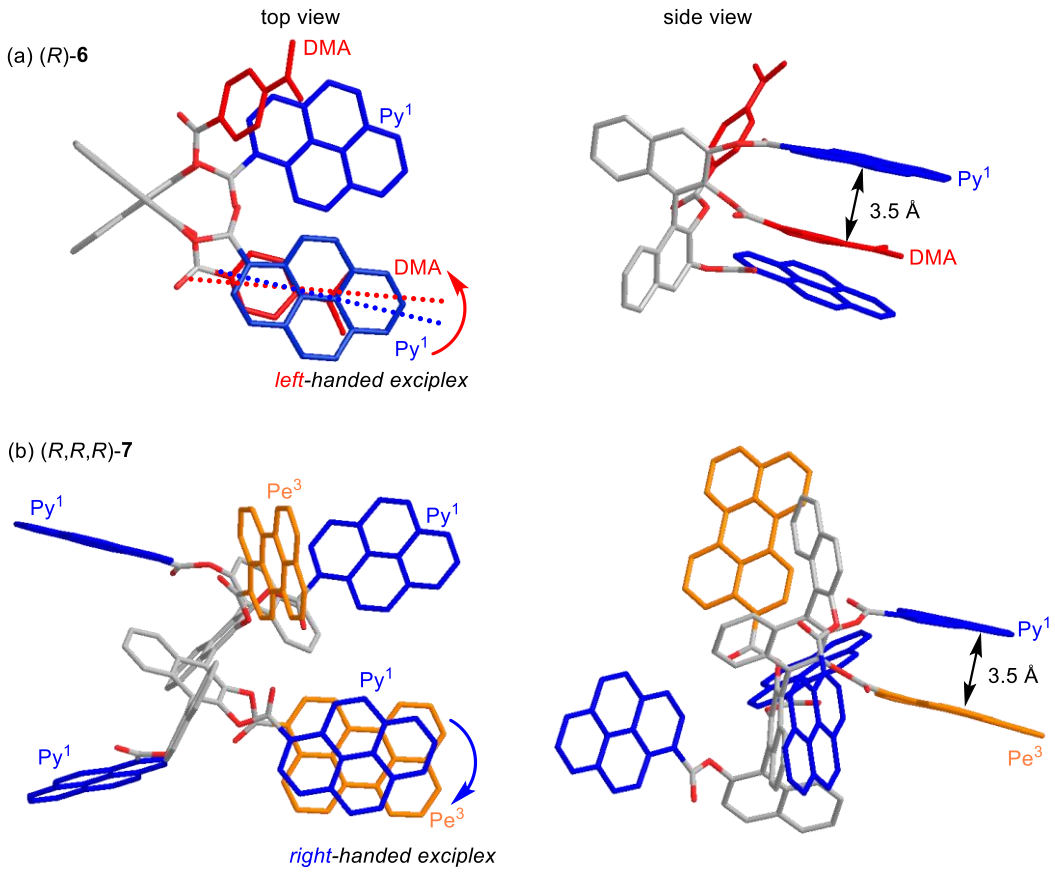


Fig. S10 TD DFT-optimized excited-state structures of (a) (*R*)-**6** and (b) (*R*,*R*,*R*)-**7** at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

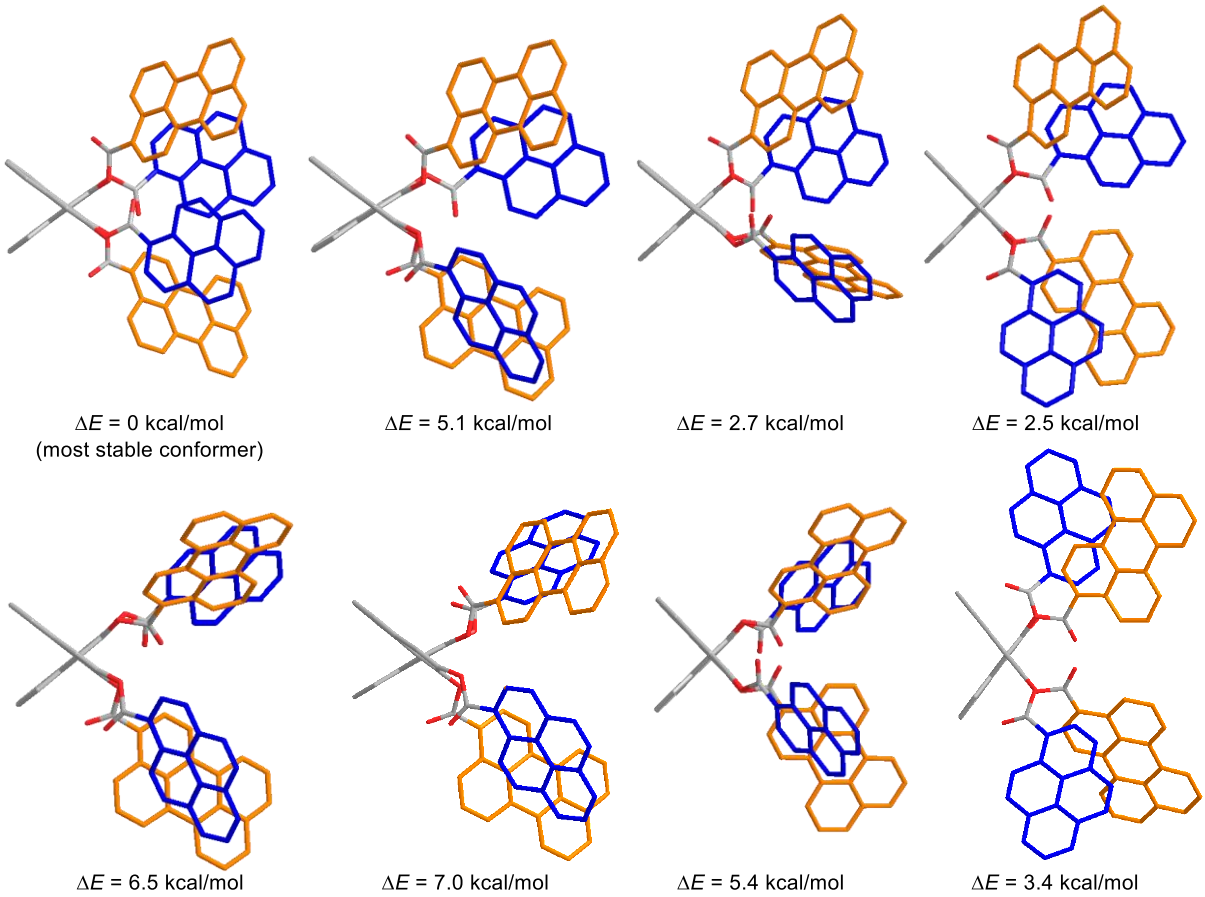


Fig. S11 DFT-optimized most stable and metastable structures of (*R*)-**2** at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

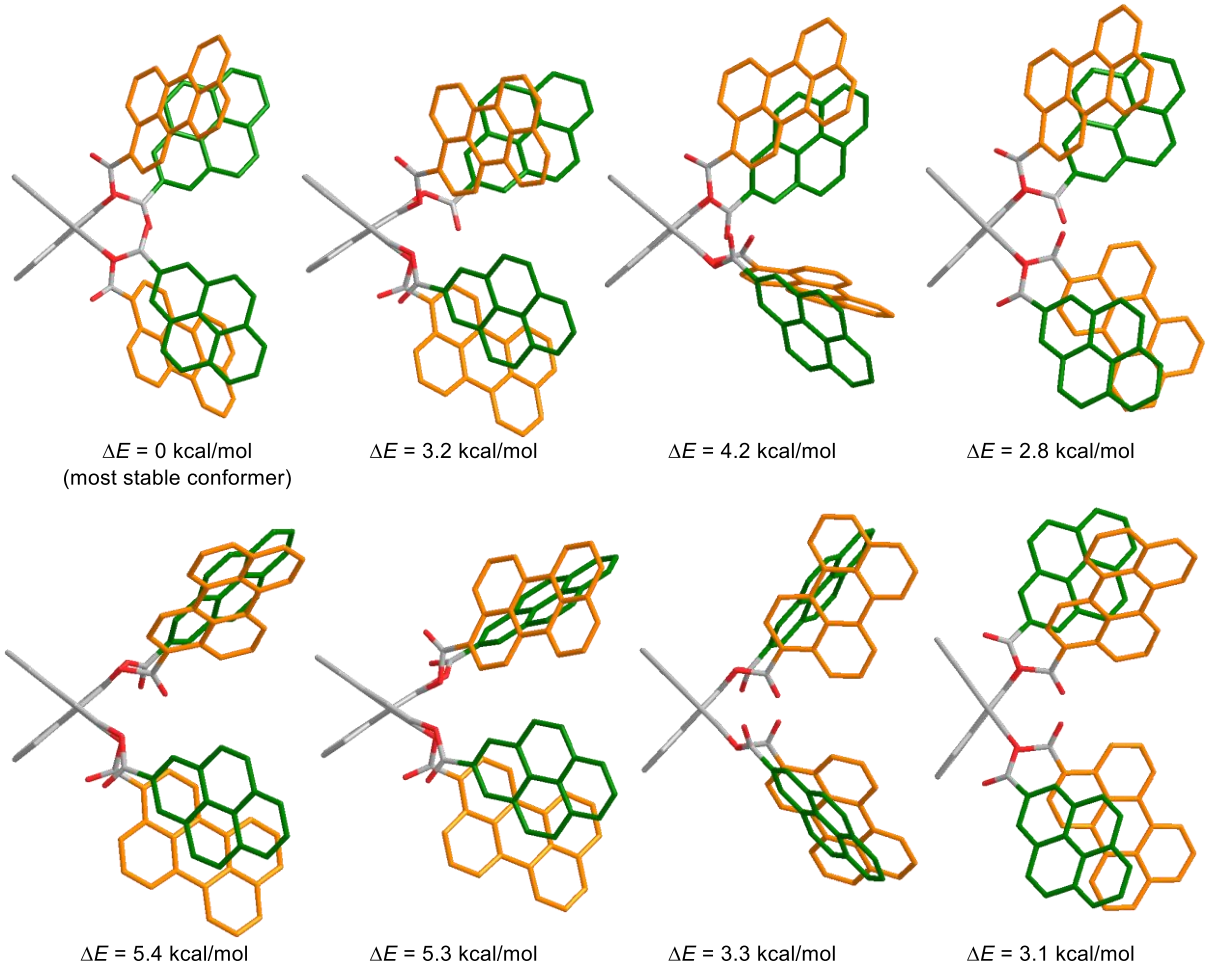


Fig. S12 DFT-optimized most stable and metastable structures of (*R*)-**3** at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

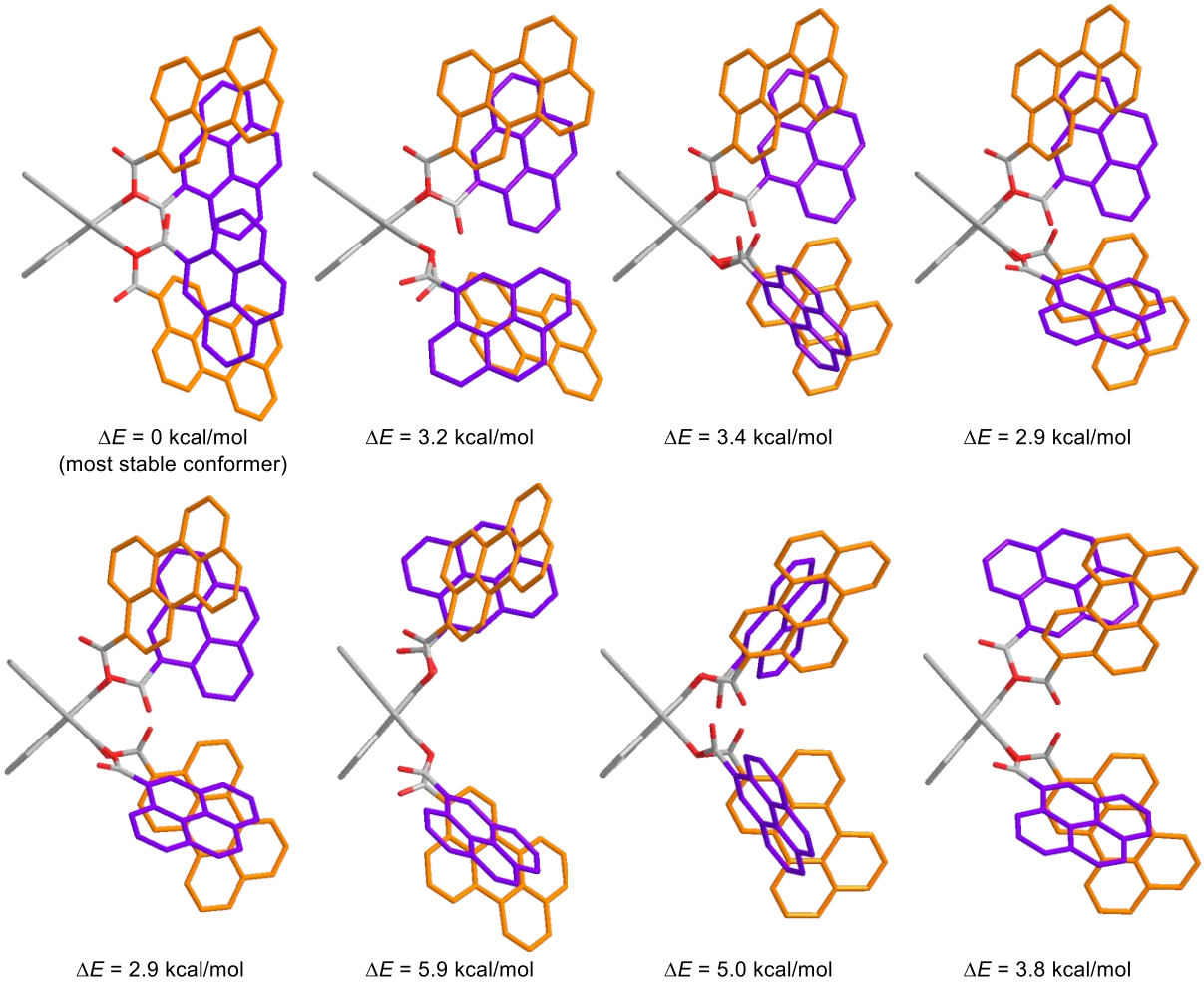


Fig. S13 DFT-optimized most stable and metastable structures of (*R*)-**4** at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

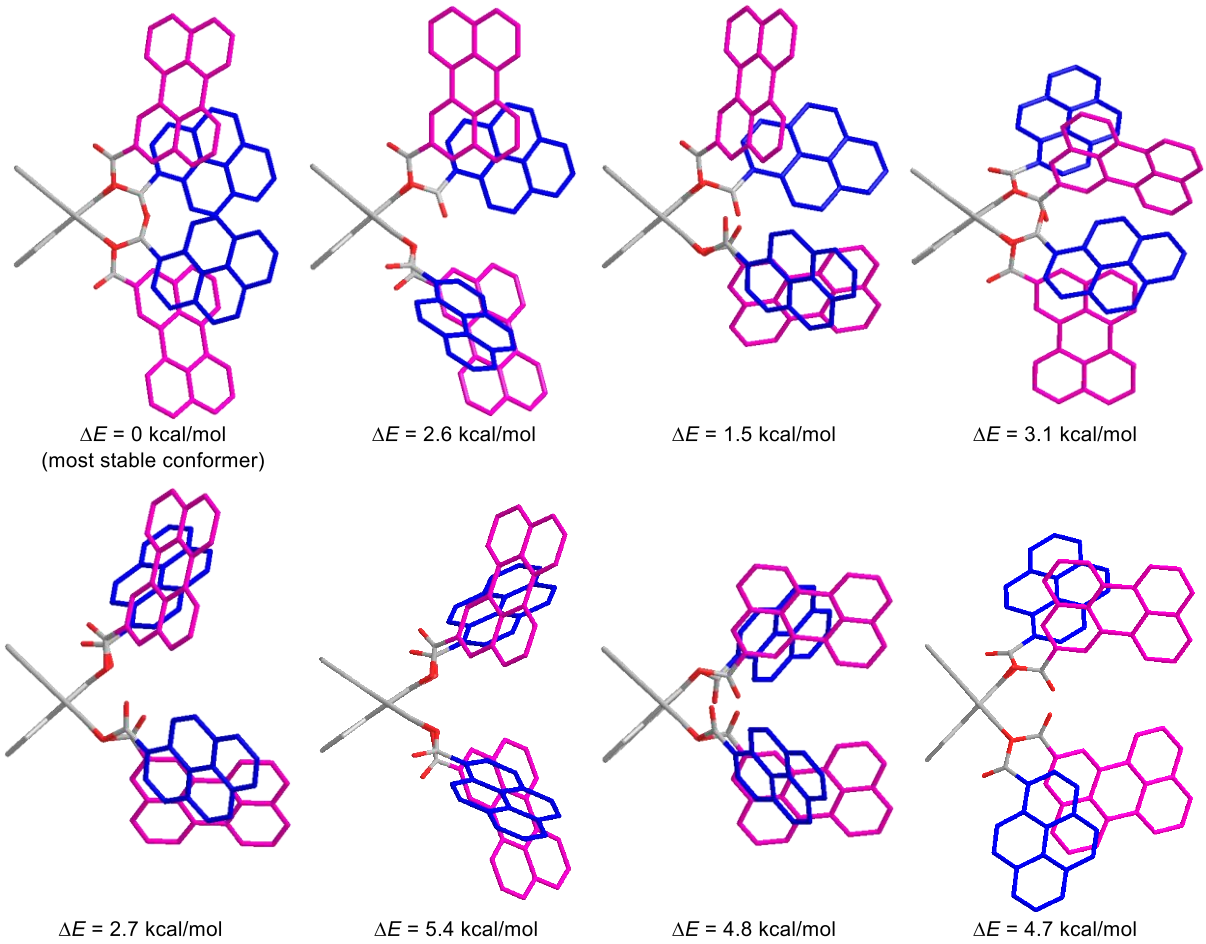


Fig. S14 DFT-optimized most stable and metastable structures of (*R*)-**5** at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

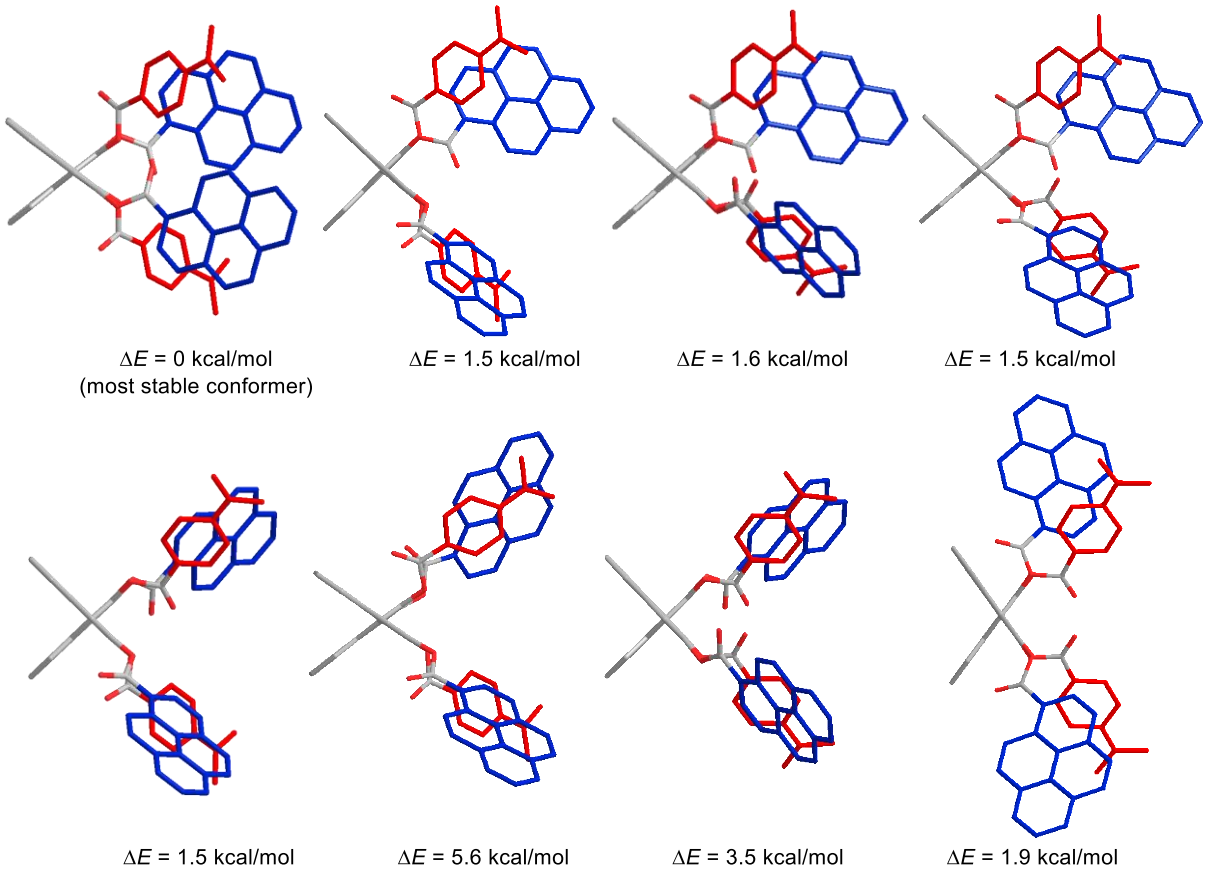


Figure S15 DFT-optimized most stable and metastable structures of (*R*)-**6** at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

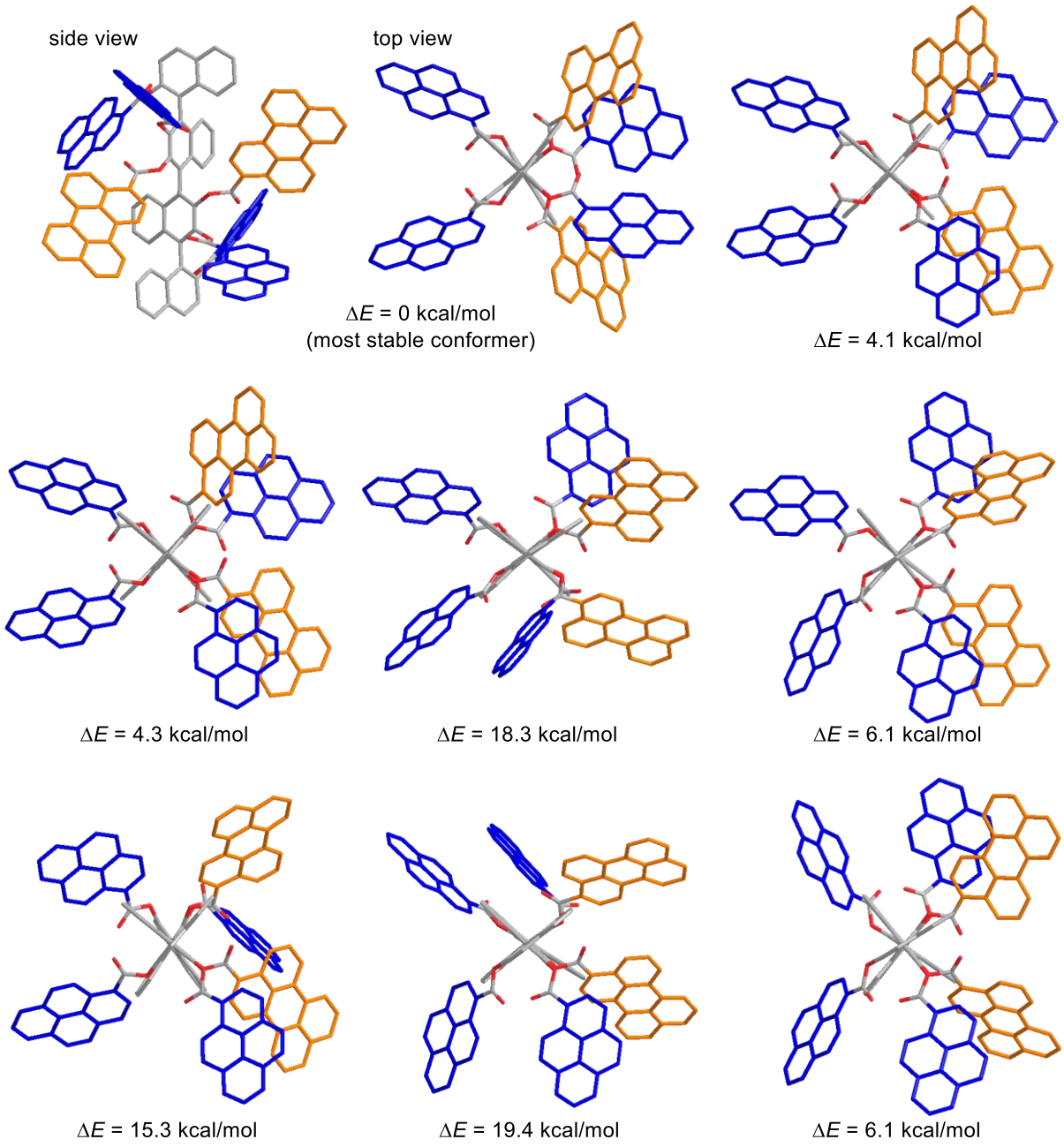


Fig. S16 DFT-optimized most stable and metastable structures of (*R*,*R*,*R*)-**7** at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

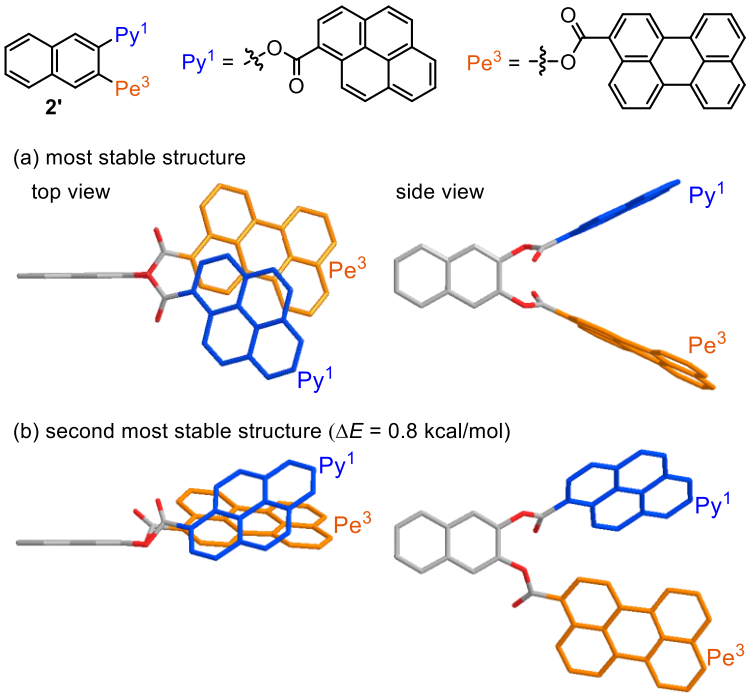
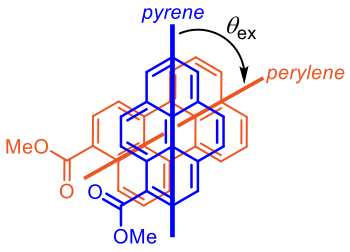


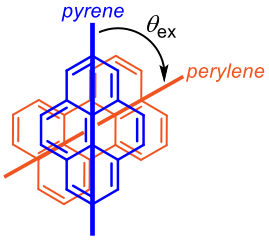
Fig. S17 DFT-optimized structures of **2'** at the CAM-B3LYP/6-31G(d,p) level. Hydrogen atoms are omitted for clarity.

Table S1 Theoretical transition dipole moments and g_{lum} values of the exciplex consisting of 1-methyl pyrenecarboxylate and 3-methyl perylenecarboxylate at each twist angle (CAM-B3LYP/6-311+G(2d,p) level)



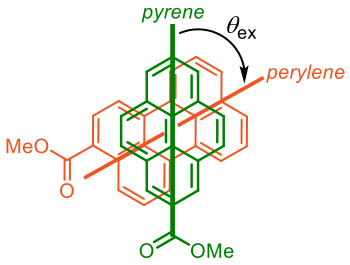
Twist angle of exciplex θ_{ex} (deg)	$\|u\|$ (10^{-18} esu·cm)	$\|m\|$ (10^{-20} erg·G^{-1})	$\theta_{\mu,m}$ (deg)	Theoretical g_{lum} (10^{-4})
15	5.18	1.15	85.3	+7.3
30	5.36	1.21	85.1	+7.7
45	5.52	1.12	86.9	+4.4
60	5.79	1.08	87.2	+3.6
75	5.94	1.08	89.4	+0.8
90	5.98	1.09	89.6	+0.1
105	5.98	1.11	91.8	–2.4
120	5.85	1.11	94.7	–6.3
135	5.68	1.11	94.2	–5.8
150	5.49	1.18	95.0	–7.5
165	5.40	1.17	95.7	–8.6
180	5.42	1.05	92.7	–3.6
195	5.42	1.10	87.5	+3.6
210	5.49	1.15	86.9	+4.5
225	5.69	1.08	88.4	+2.1
240	5.85	1.07	86.0	+5.1
255	5.99	1.06	86.4	+4.4
270	6.05	1.01	89.6	+0.5
285	5.98	1.01	91.1	–1.3
300	5.88	1.05	94.3	–5.4
315	5.66	1.10	95.4	–7.2
330	5.46	1.18	94.7	–7.1
345	5.34	1.15	95.6	–8.3

Table S2 Theoretical transition dipole moments and g_{lum} values of the exciplex consisting of pyrene and perylene at each twist angle (CAM-B3LYP/6-311+G(2d,p) level)



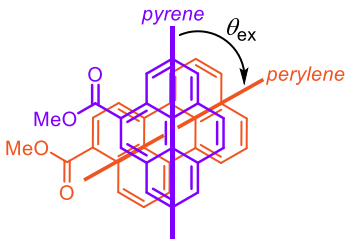
Twist angle of exciplex θ_{ex} (deg)	$\lvert u \rvert$ (10^{-18} esu·cm)	$\lvert m \rvert$ (10^{-20} erg·G^{-1})	$\theta_{\mu,m}$ (deg)	Theoretical g_{lum} (10^{-4})
15	4.85	1.03	87.3	+4.0
30	4.91	1.06	87.0	+4.6
45	5.06	1.00	88.2	+2.4
60	5.21	0.97	88.3	+2.2
75	5.27	0.96	89.0	+1.3
285	5.27	0.96	91.0	–1.3
300	5.21	0.97	91.7	–2.2
315	5.06	1.00	91.8	–2.4
330	4.91	1.06	93.0	–4.6
345	4.85	1.03	92.7	–4.0

Table S3 Theoretical transition dipole moments and g_{lum} values of the exciplex consisting of 2-methyl pyrenecarboxylate and 3-methyl perylenecarboxylate at each twist angle (CAM-B3LYP/6-311+G(2d,p) level)



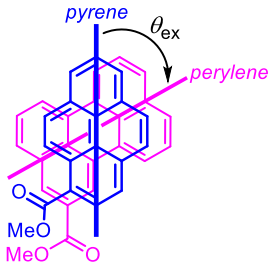
Twist angle of exciplex θ_{ex} (deg)	$\|u\|$ (10^{-18} esu·cm)	$\|m\|$ (10^{-20} erg·G^{-1})	$\theta_{\mu,m}$ (deg)	Theoretical g_{lum} (10^{-4})
15	5.61	1.14	86.9	+4.3
30	5.71	1.15	86.5	+5.0
45	5.89	1.10	87.6	+3.2
60	6.05	1.09	87.6	+3.0
75	6.06	1.11	88.4	+2.1
90	6.04	1.11	89.8	+0.3
105	6.10	1.10	92.0	–2.5
120	6.06	1.09	93.7	–4.7
135	5.87	1.09	93.8	–5.0
150	5.70	1.14	94.3	–6.1
165	5.64	1.11	93.6	–4.9
180	5.69	1.04	91.2	–1.5
195	5.67	1.08	88.6	+1.9
210	5.63	1.11	87.5	+3.5
225	5.84	1.06	88.7	+1.6
240	6.09	1.04	89.0	+1.2
255	6.14	1.03	90.3	–0.3
270	6.06	1.02	93.6	–4.3
285	6.02	1.05	95.5	–6.6
300	6.00	1.07	95.2	–6.5
315	5.83	1.10	94.6	–6.1
330	5.66	1.17	94.7	–6.8
345	5.61	1.15	93.9	–5.6

Table S4 Theoretical transition dipole moments and g_{lum} values of the exciplex consisting of 4-methyl pyrenecarboxylate and 3-methyl perylenecarboxylate at each twist angle (CAM-B3LYP/6-311+G(2d,p) level)



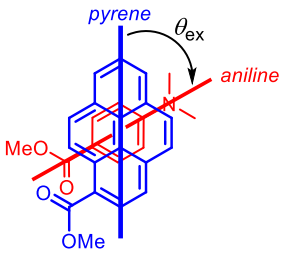
Twist angle of exciplex θ_{ex} (deg)	$\|u\|$ (10^{-18} esu·cm)	$\|m\|$ (10^{-20} erg·G^{-1})	$\theta_{\mu,m}$ (deg)	Theoretical g_{lum} (10^{-4})
15	5.67	1.08	85.4	+6.1
30	5.74	1.09	86.0	+5.3
45	5.93	1.04	88.0	+2.5
60	6.07	1.04	89.4	+0.8
75	6.06	1.06	90.4	–0.5
90	6.05	1.07	90.7	–0.8
105	5.99	1.12	93.6	–4.7
120	5.91	1.09	92.6	–3.3
135	5.72	1.11	91.7	–2.3
150	5.49	1.18	92.4	–3.6
165	5.48	1.12	90.9	–1.3
180	5.56	1.07	88.8	+1.6
195	5.56	1.13	85.8	+5.9
210	5.64	1.13	87.1	+4.1
225	5.82	1.07	91.9	–2.5
240	6.04	1.06	91.2	–1.5
255	6.11	1.07	91.9	–2.3
270	6.00	1.08	95.6	–7.0
285	5.97	1.09	95.6	–7.1
300	5.95	1.08	94.4	–5.5
315	5.77	1.09	92.4	–3.2
330	5.63	1.15	92.9	–4.0
345	5.60	1.10	92.2	–3.0

Table S5 Theoretical transition dipole moments and g_{lum} values of the exciplex consisting of 1-methyl pyrenecarboxylate and 2-methyl perylenecarboxylate at each twist angle (CAM-B3LYP/6-311+G(2d,p) level)



Twist angle of exciplex θ_{ex} (deg)	$\|u\|$ (10^{-18} esu·cm)	$\|m\|$ (10^{-20} erg·G^{-1})	$\theta_{\mu,m}$ (deg)	Theoretical g_{lum} (10^{-4})
15	4.52	1.09	87.7	+3.8
30	4.55	1.14	87.8	+3.8
45	4.71	1.06	86.8	+5.0
60	4.90	1.03	84.6	+7.9
75	4.86	1.02	85.1	+7.2
90	4.94	0.98	86.0	+5.6
105	5.09	0.98	91.3	–1.7
120	5.01	0.99	94.8	–6.6
135	4.84	1.00	96.3	–9.0
150	4.58	1.10	99.3	–15.5
165	4.42	1.10	98.3	–14.4
180	4.45	1.01	93.8	–5.9
195	4.45	1.10	88.6	+2.4
210	4.47	1.13	86.8	+5.6
225	4.69	1.06	87.6	+3.9
240	4.90	1.05	85.5	+6.8
255	5.03	1.02	86.9	+4.4
270	5.09	0.99	91.0	–1.4
285	5.07	1.01	93.7	–5.1
300	5.02	1.03	95.9	–8.5
315	4.88	1.04	97.2	–10.7
330	4.69	1.11	98.5	–14.0
345	4.56	1.11	98.4	–14.2

Table S6 Theoretical transition dipole moments and g_{lum} values of the exciplex consisting of 1-methyl pyrenecarboxylate and 4-methyl *N*,*N*-dimethylanilinecarboxylate at each twist angle (CAM-B3LYP/6-311+G(2d,p) level)

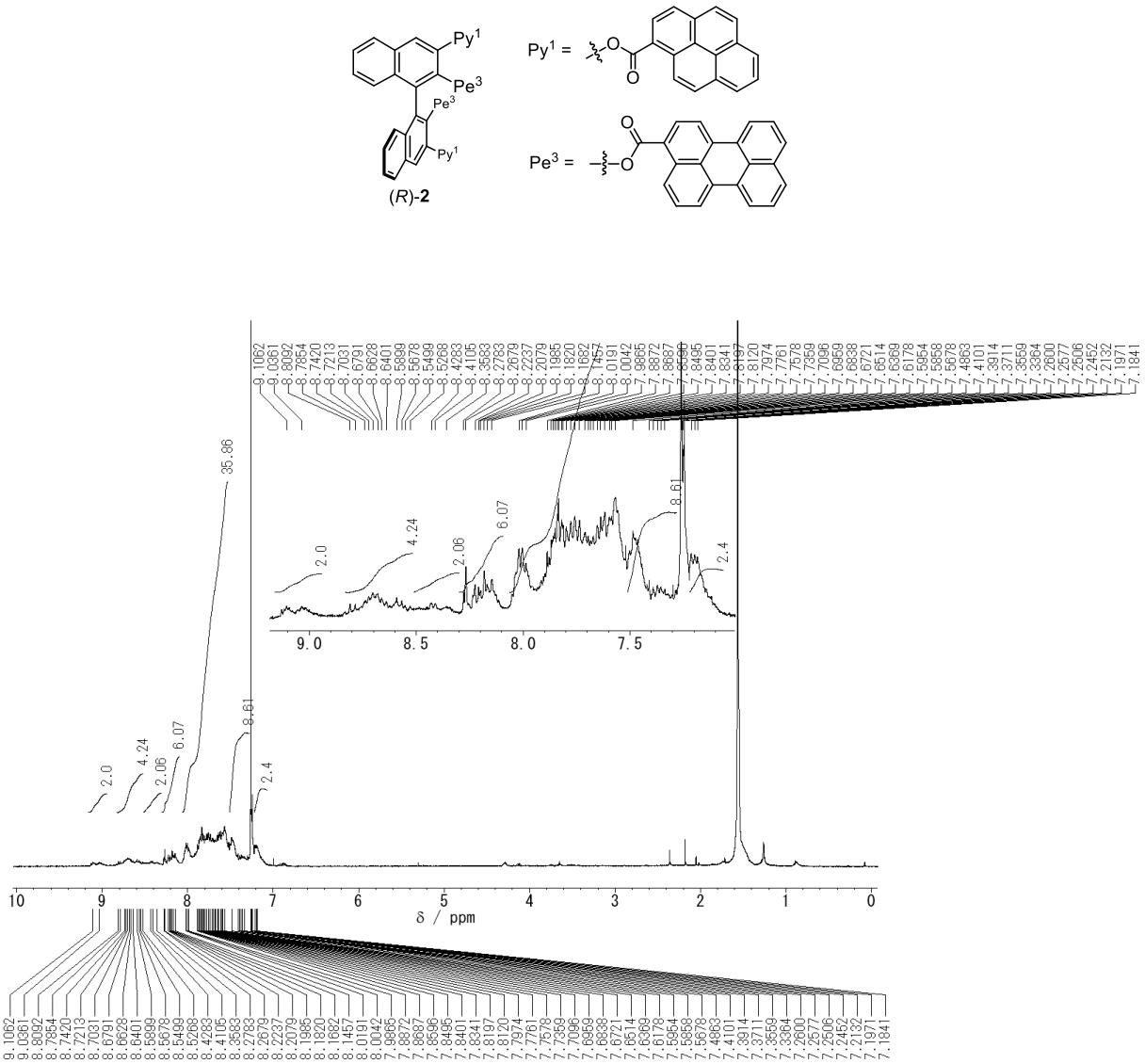


Twist angle of exciplex θ_{ex} (deg)	$\|u\|$ (10^{-18} esu·cm)	$\|m\|$ (10^{-21} erg·G^{-1})	$\theta_{\mu,m}$ (deg)	Theoretical g_{lum} (10^{-3})
15	1.35	6.59	77.7	+4.1
30	1.55	7.59	71.7	+6.1
45	1.14	4.72	63.0	+7.5
60	0.87	1.66	87.4	+0.3
75	1.45	3.89	67.7	+4.1
90	1.53	2.66	71.4	+2.2
105	1.40	2.17	108.3	–1.9
120	0.86	1.78	118.0	–3.9
135	0.98	2.33	109.9	–3.2
150	1.39	4.42	115.1	–5.4
165	1.13	4.83	112.1	–6.4
180	0.30	2.26	99.8	–5.2
195	0.98	4.66	74.0	+5.3
210	1.18	6.45	76.4	+5.1
225	0.93	3.82	86.6	+1.0
240	0.60	1.56	94.1	–0.7
255	0.55	1.21	98.1	–1.2
270	1.03	1.03	158.4	–3.7
285	1.26	1.95	129.4	–3.9
300	0.78	0.41	123.1	–1.1
315	1.00	4.01	119.9	–8.0
330	1.53	6.89	116.7	–8.1
345	1.35	6.13	110.6	–6.4

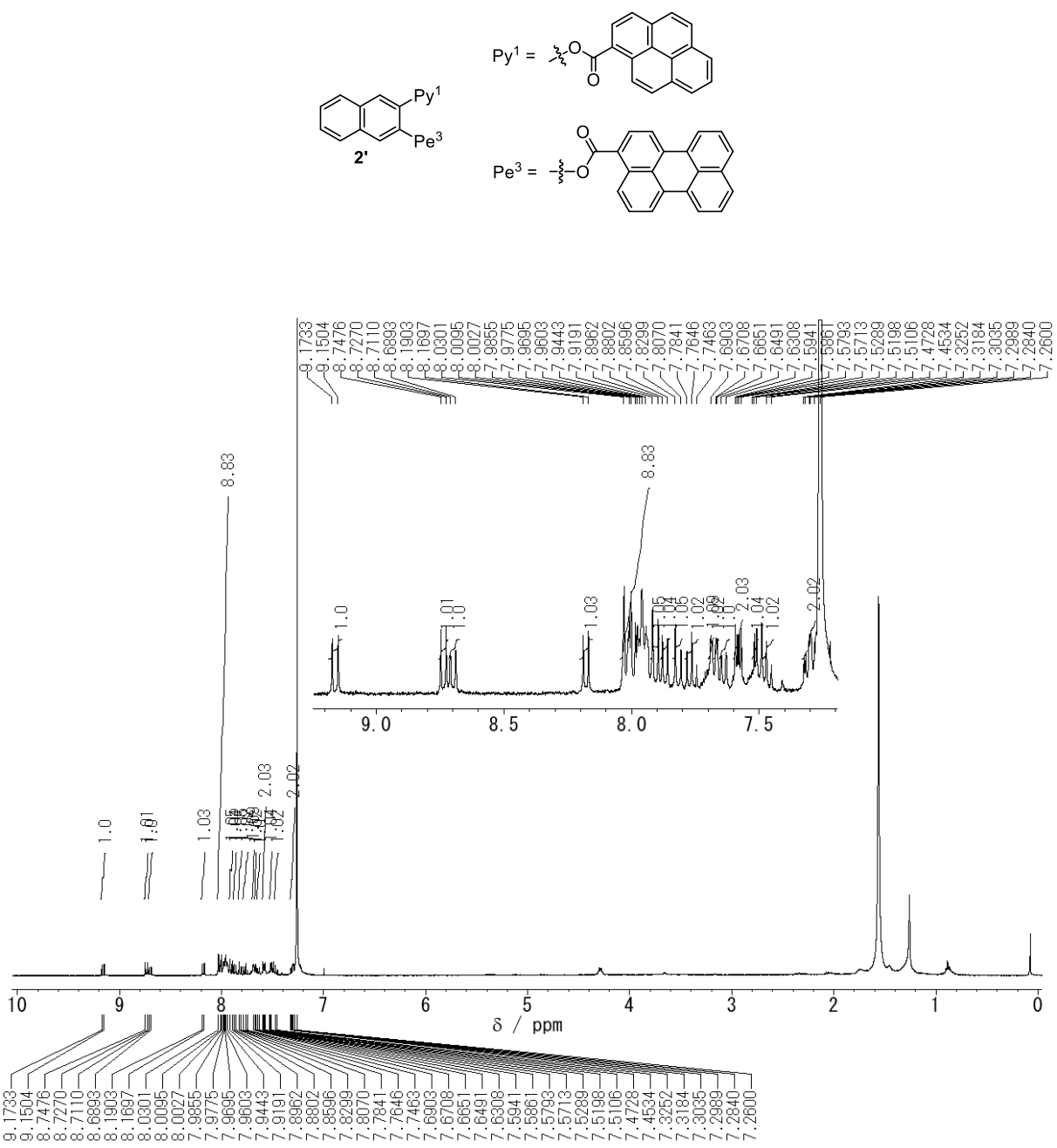
Table S7 Theoretical transition dipole moments and g_{lum} values of **2**–**7** (CAM-B3LYP/6-31G(d,p) level)

Compound	$\|u\|$ (10^{-18} esu·cm)	$\|m\|$ (10^{-20} erg·G^{-1})	$\theta_{\mu,m}$ (deg)	Theoretical g_{lum} (10^{-3})
(*R*)-**2**	5.02	1.96	88.2	+0.49
(*R*)-**3**	6.26	2.18	93.8	–0.91
(*R*)-**4**	6.59	2.16	94.1	–0.93
(*R*)-**5**	1.85	0.77	99.2	–2.7
(*R*)-**6**	1.45	0.92	98.2	–3.6
(*R*,*R*,*R*)-**7**	5.87	1.56	88.3	+0.32

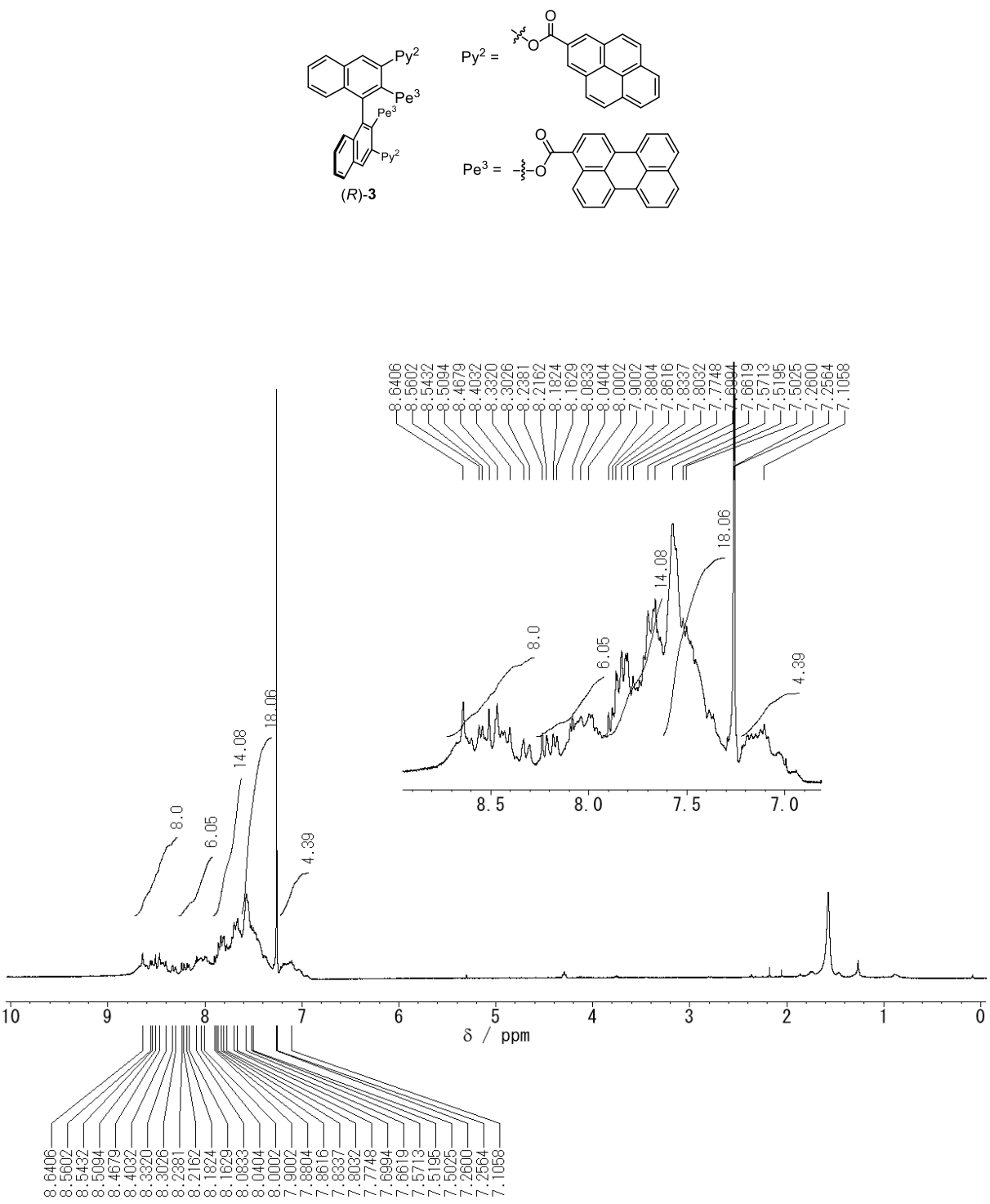
5. ^{1}H and ^{13}C NMR spectra



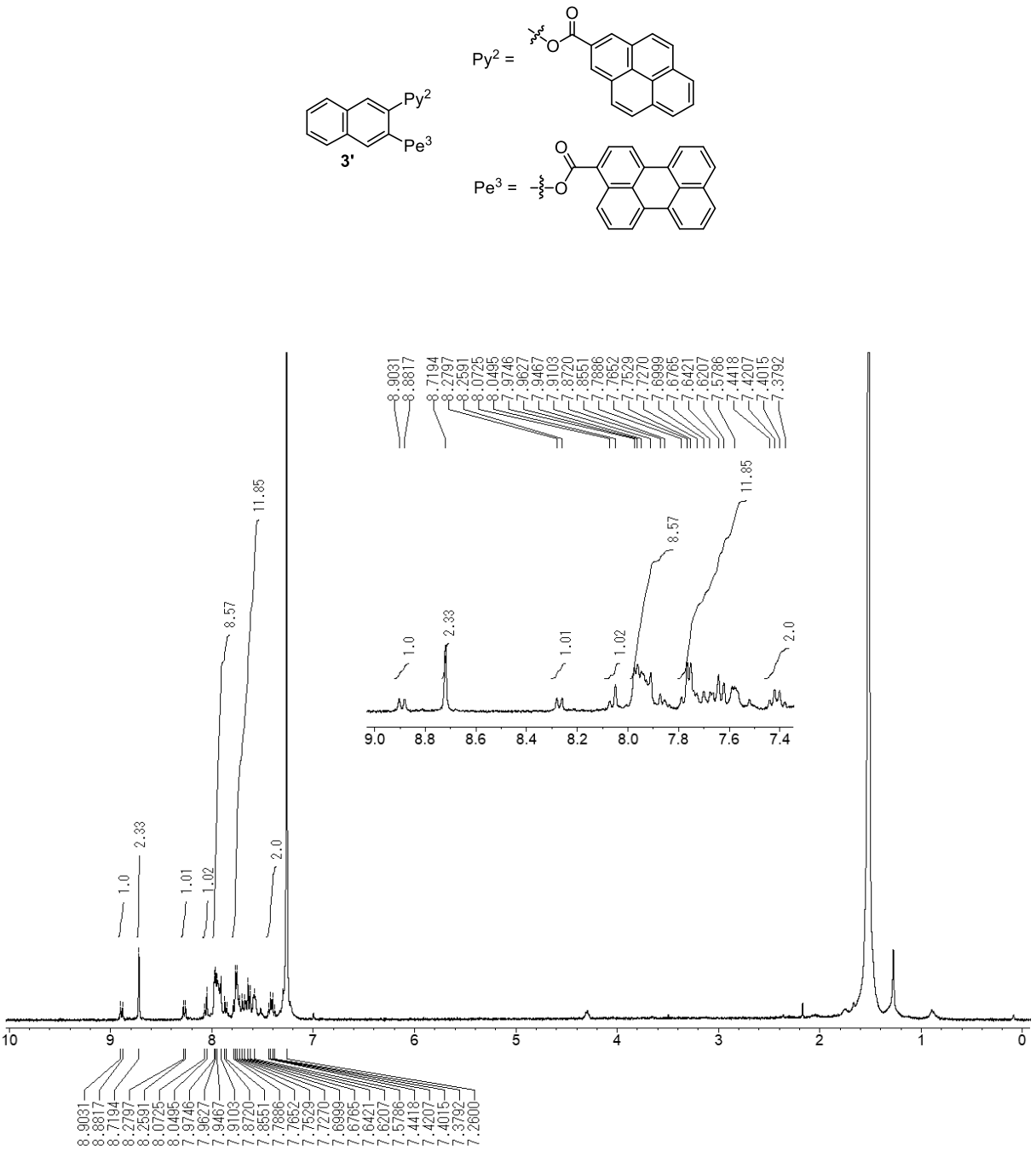
^{1}H NMR spectrum of (*R*)-**2** (400 MHz, $CDCl_3$).



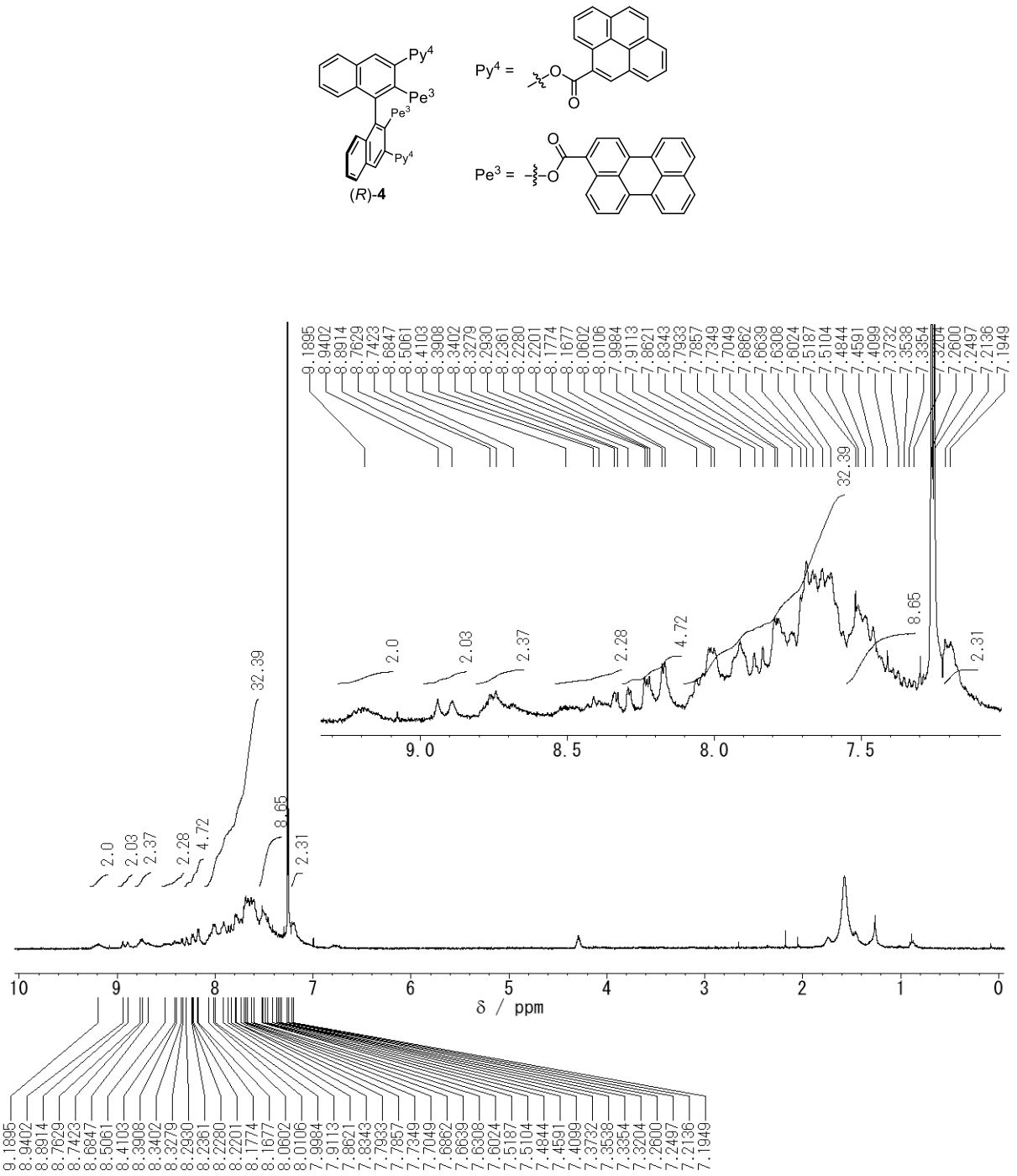
^{1}H NMR spectrum of **2'** (400 MHz, $CDCl_3$).



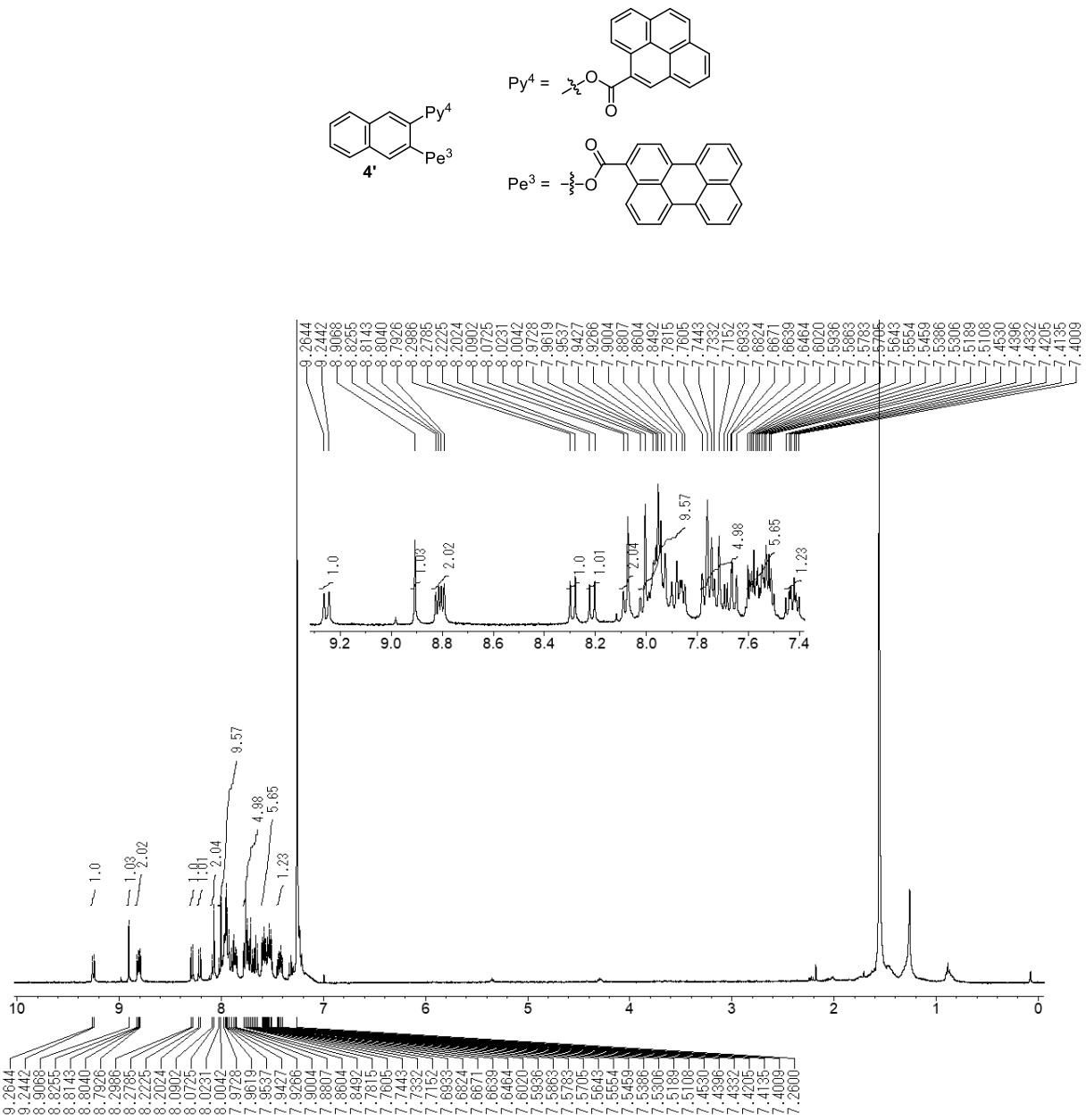
^{1}H NMR spectrum of (*R*)-**3** (400 MHz, $CDCl_3$).



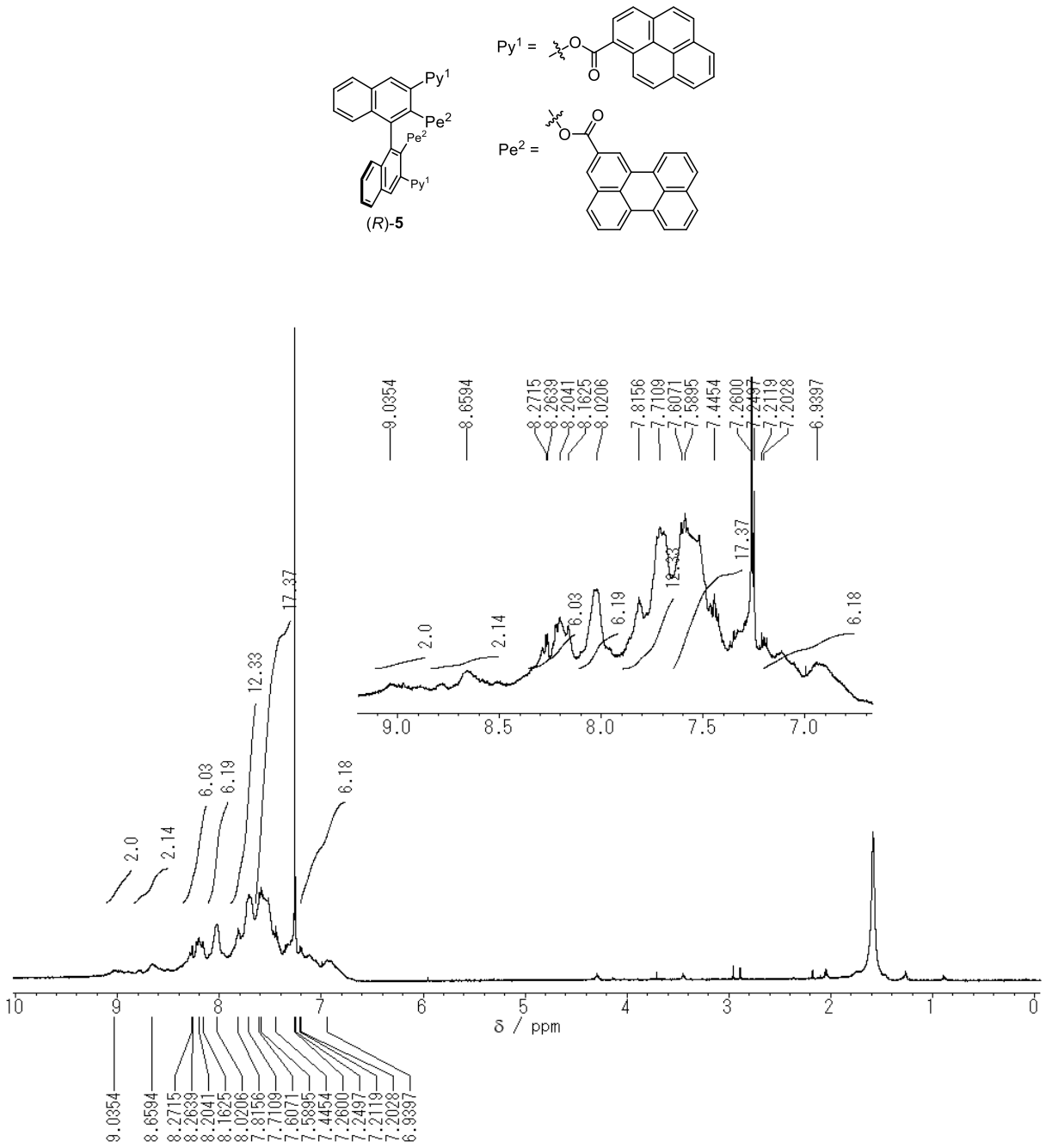
^{1}H NMR spectrum of **3'** (400 MHz, $CDCl_3$).



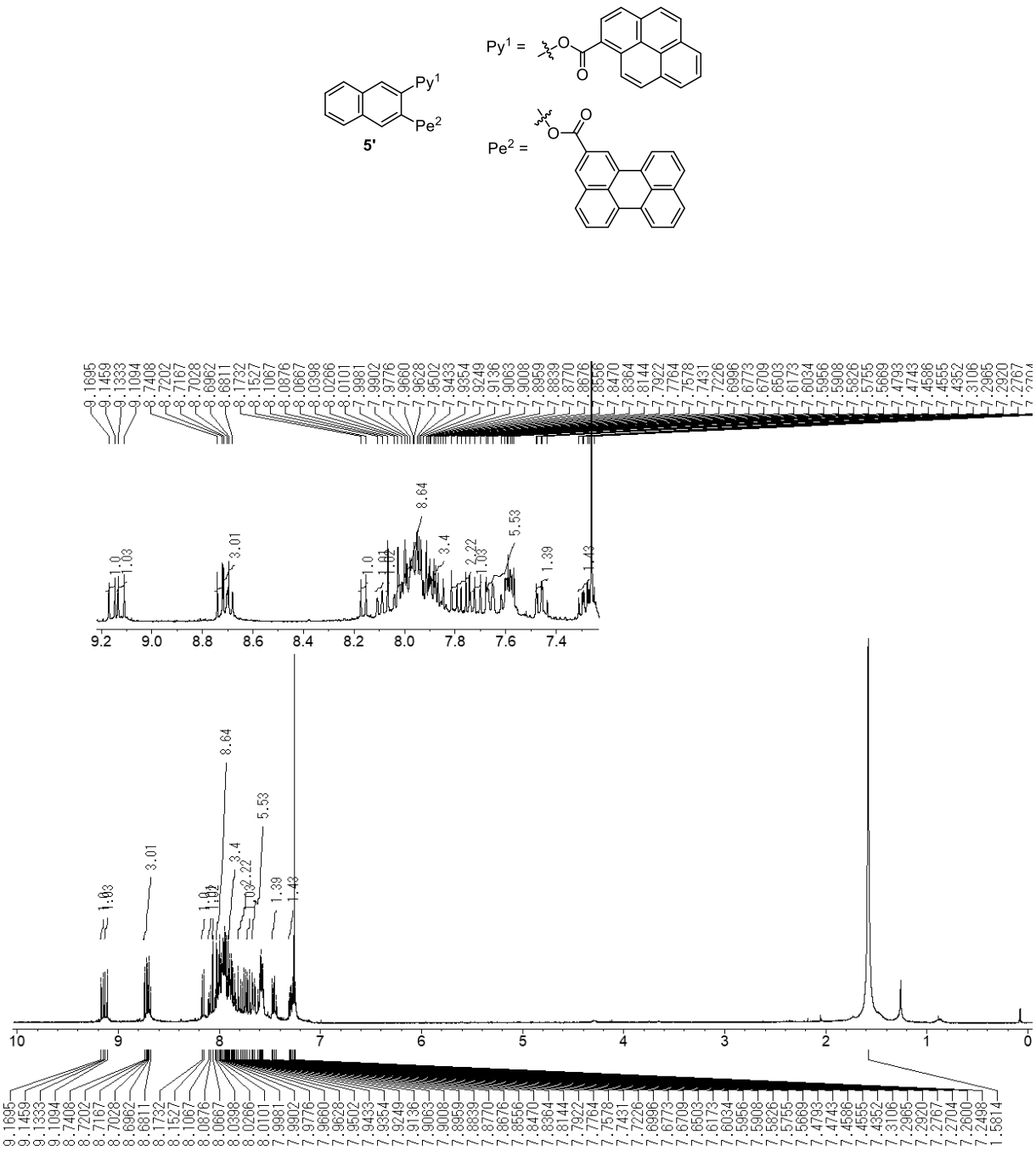
^{1}H NMR spectrum of (*R*)-**4** (400 MHz, $CDCl_3$).



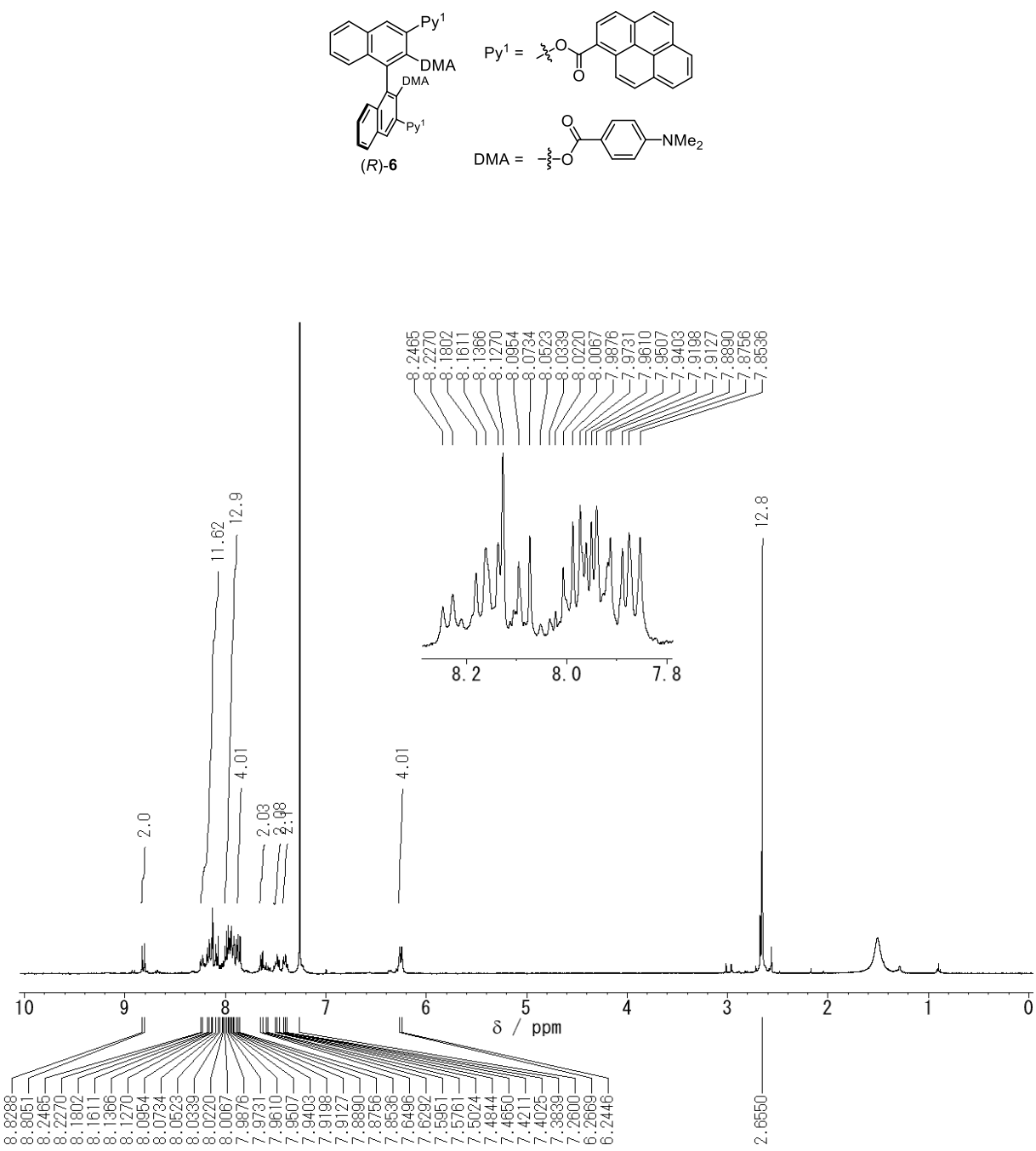
^{1}H NMR spectrum of **4'** (400 MHz, $CDCl_3$).



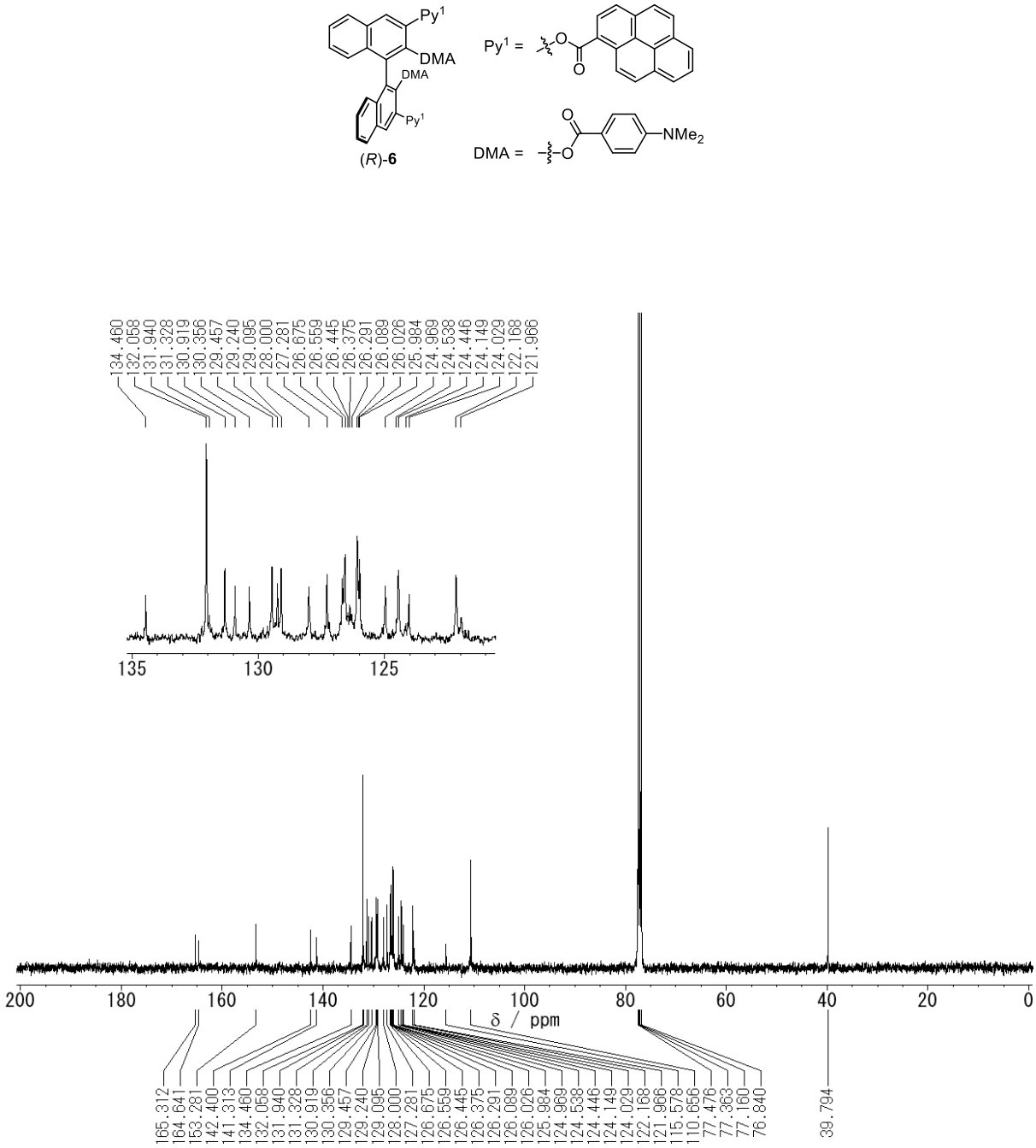
^{1}H NMR spectrum of (*R*)-**5** (400 MHz, $CDCl_3$).



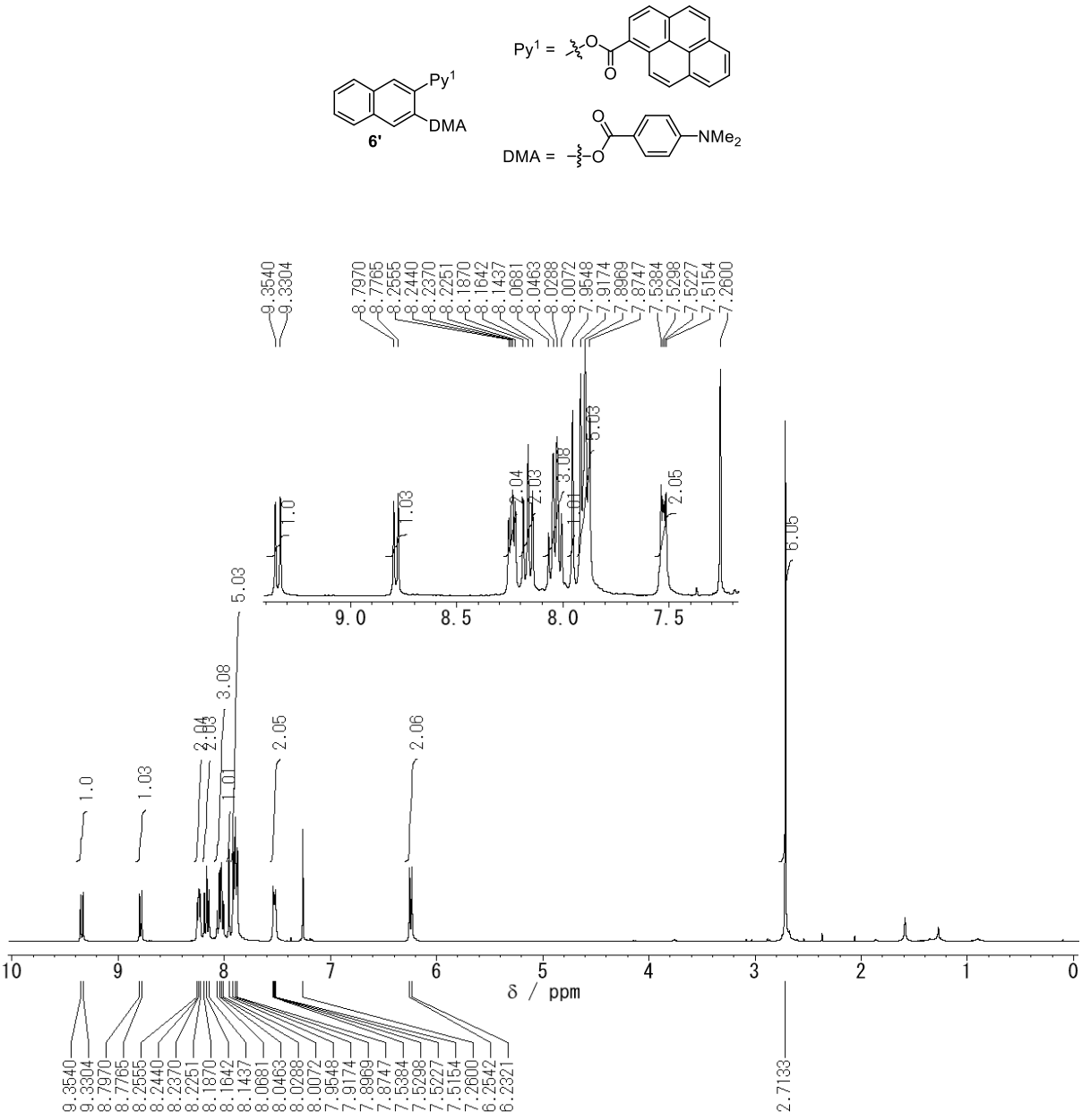
^{1}H NMR spectrum of **5'** (400 MHz, $CDCl_3$).



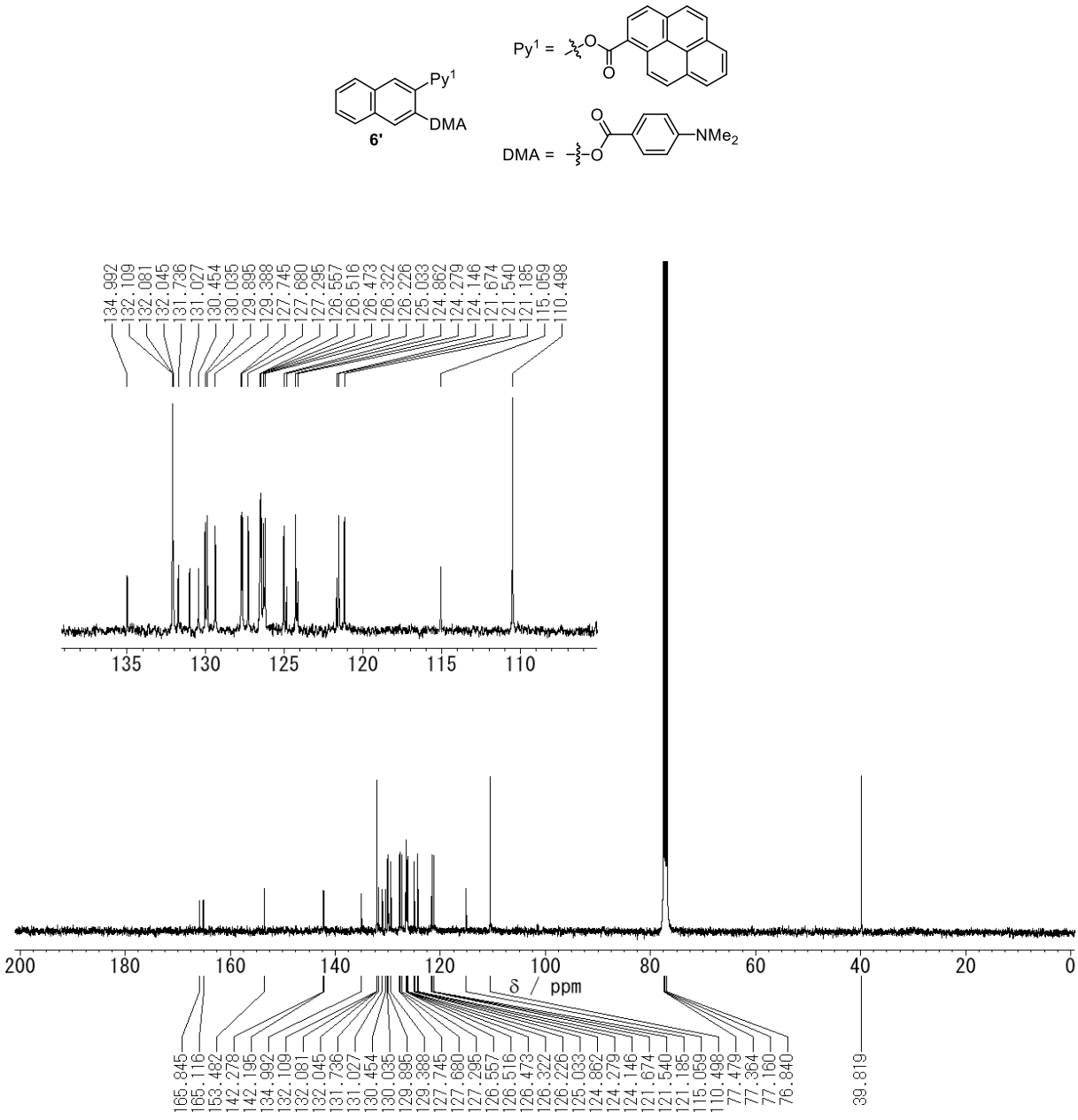
^{1}H NMR spectrum of (*R*)-**6** (400 MHz, $CDCl_3$).



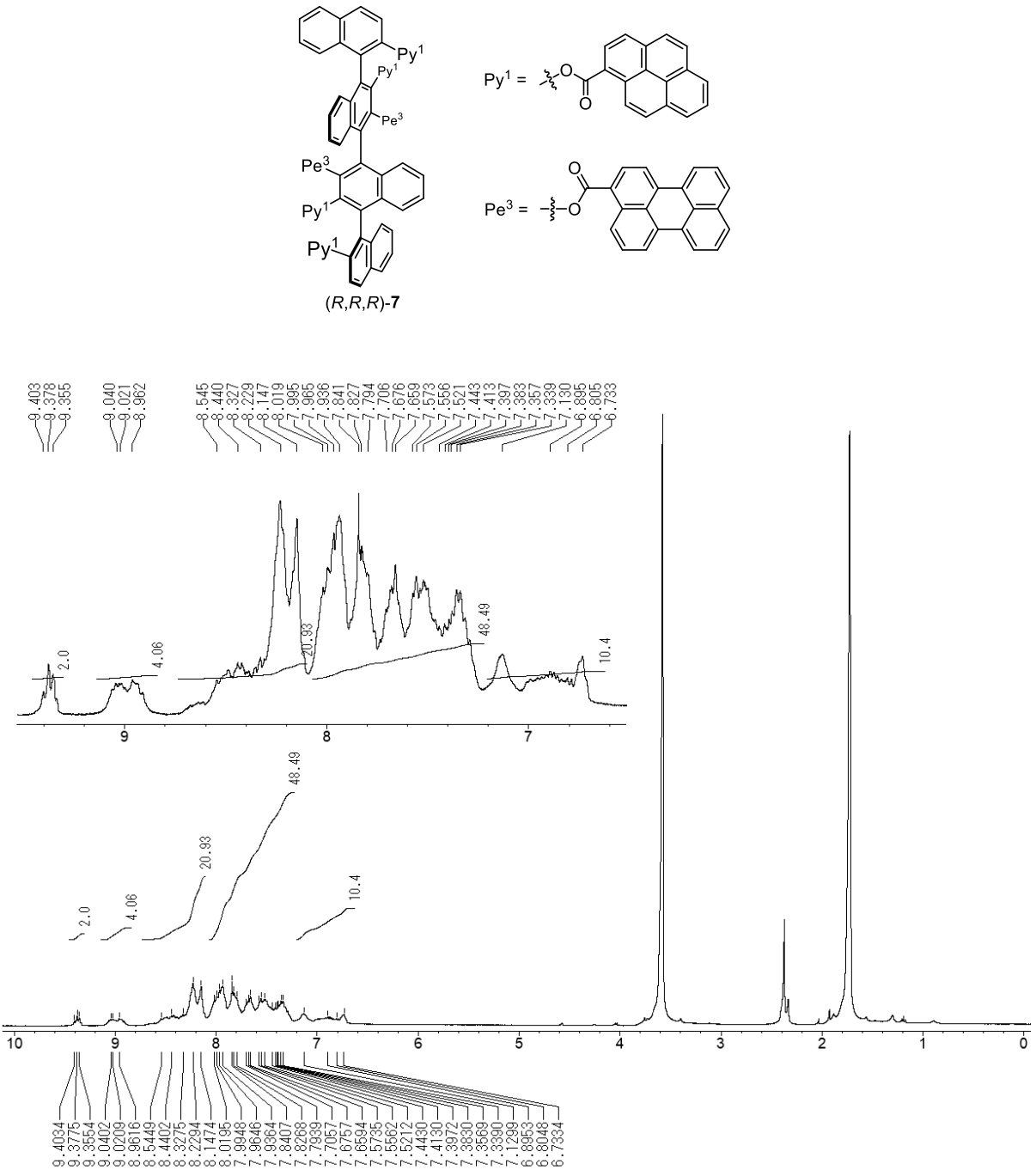
^{13}C NMR spectrum of (*R*)-**6** (101 MHz, $CDCl_3$).



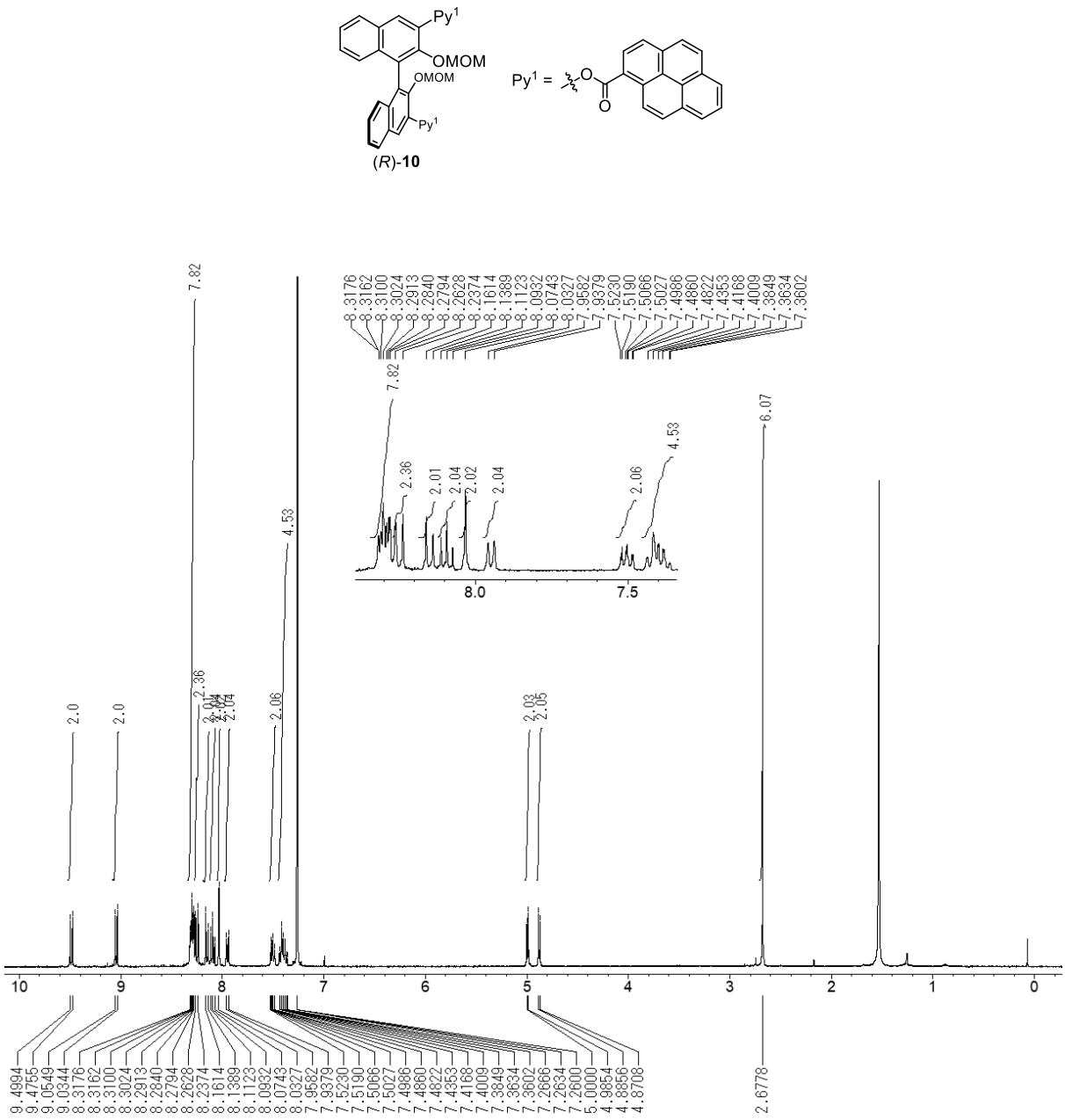
^{1}H NMR spectrum of **6'** (400 MHz, $CDCl_3$).



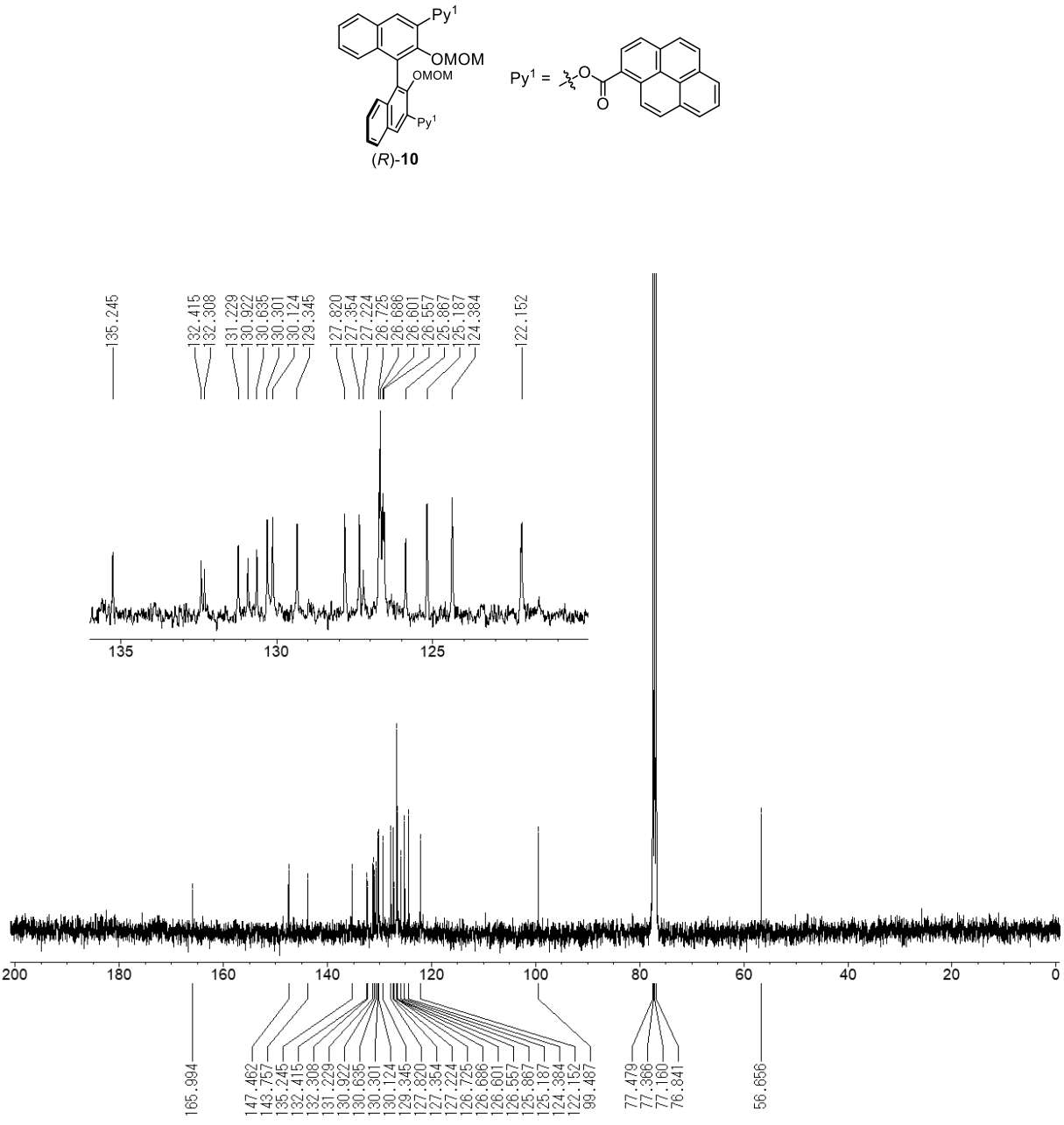
^{13}C NMR spectrum of **6'** (101 MHz, $CDCl_3$).



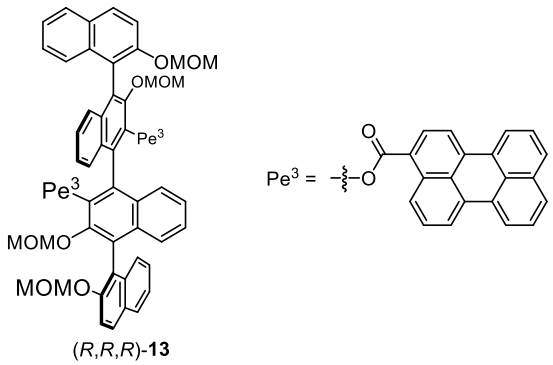
^{1}H NMR spectrum of (*R*,*R*,*R*)-**7** (400 MHz, THF-d_8).



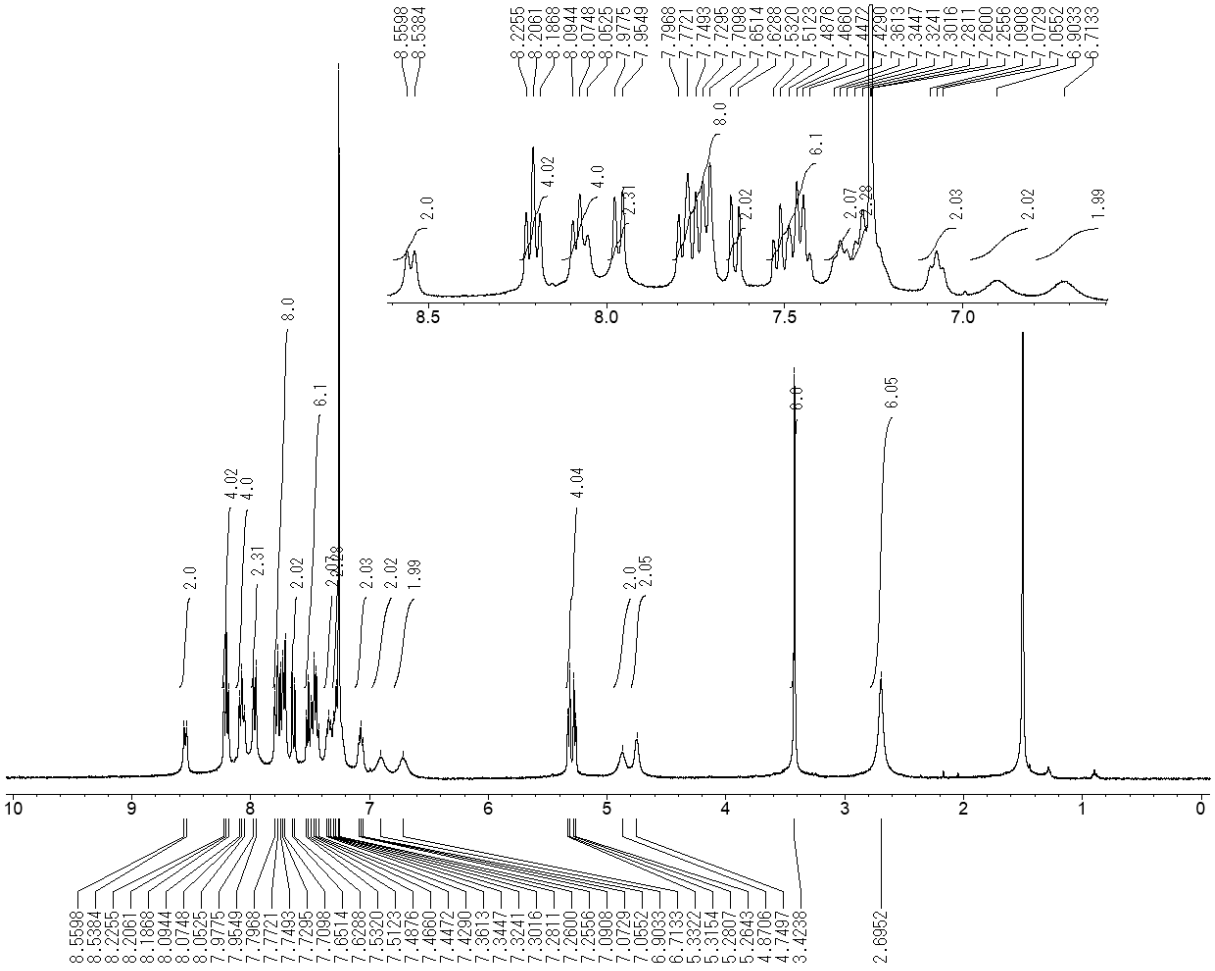
^{1}H NMR spectrum of (*R*)-**10** (400 MHz, $CDCl_3$).



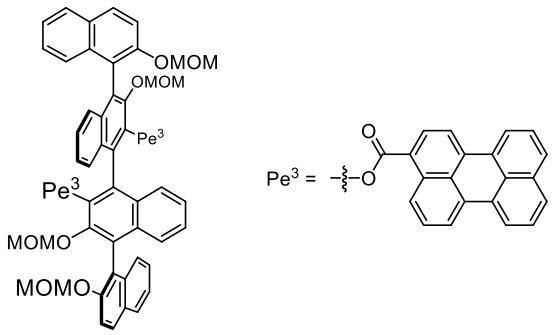
^{13}C NMR spectrum of (*R*)-**10** (101 MHz, $CDCl_3$).



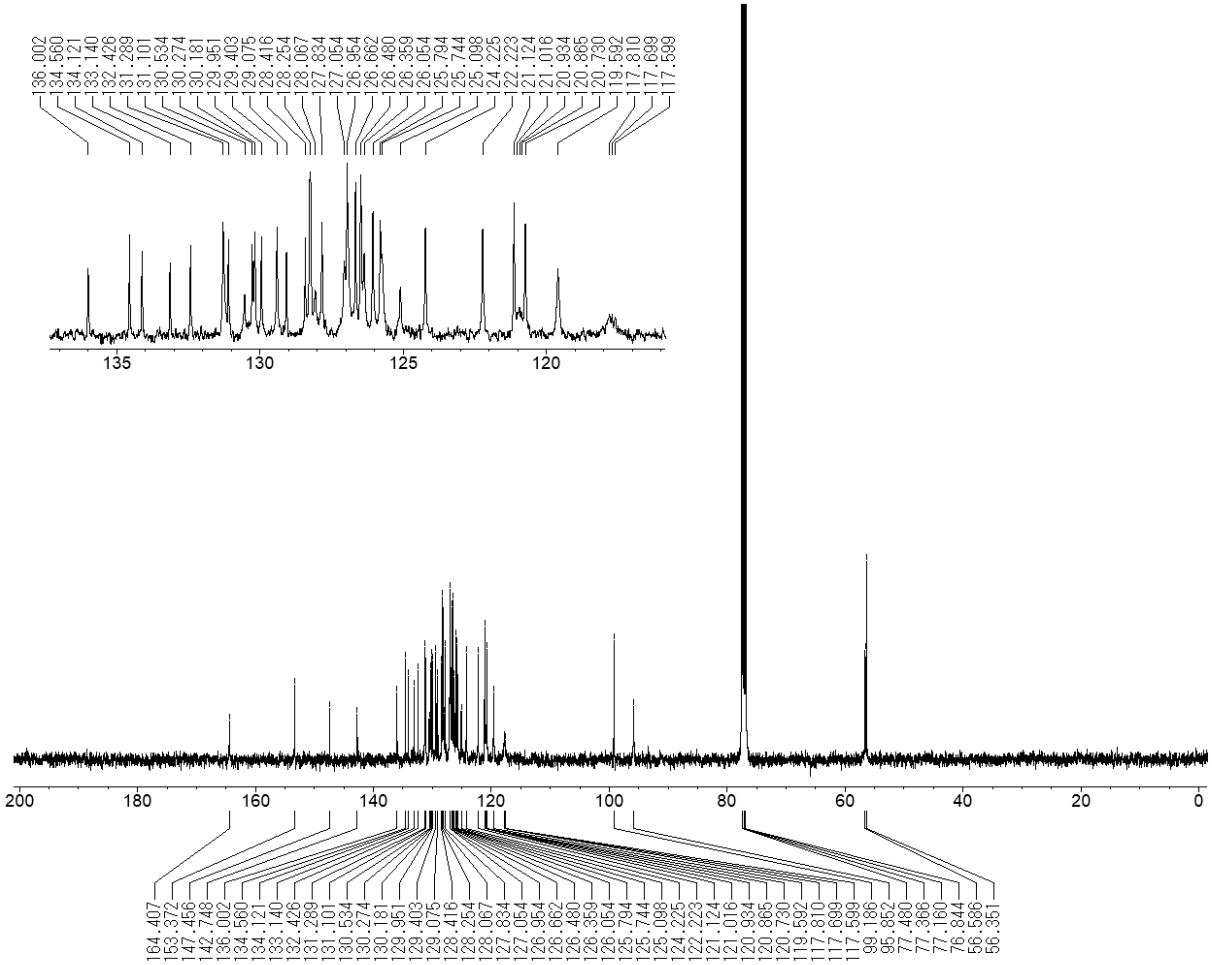
(*R*,*R*,*R*)-**13**



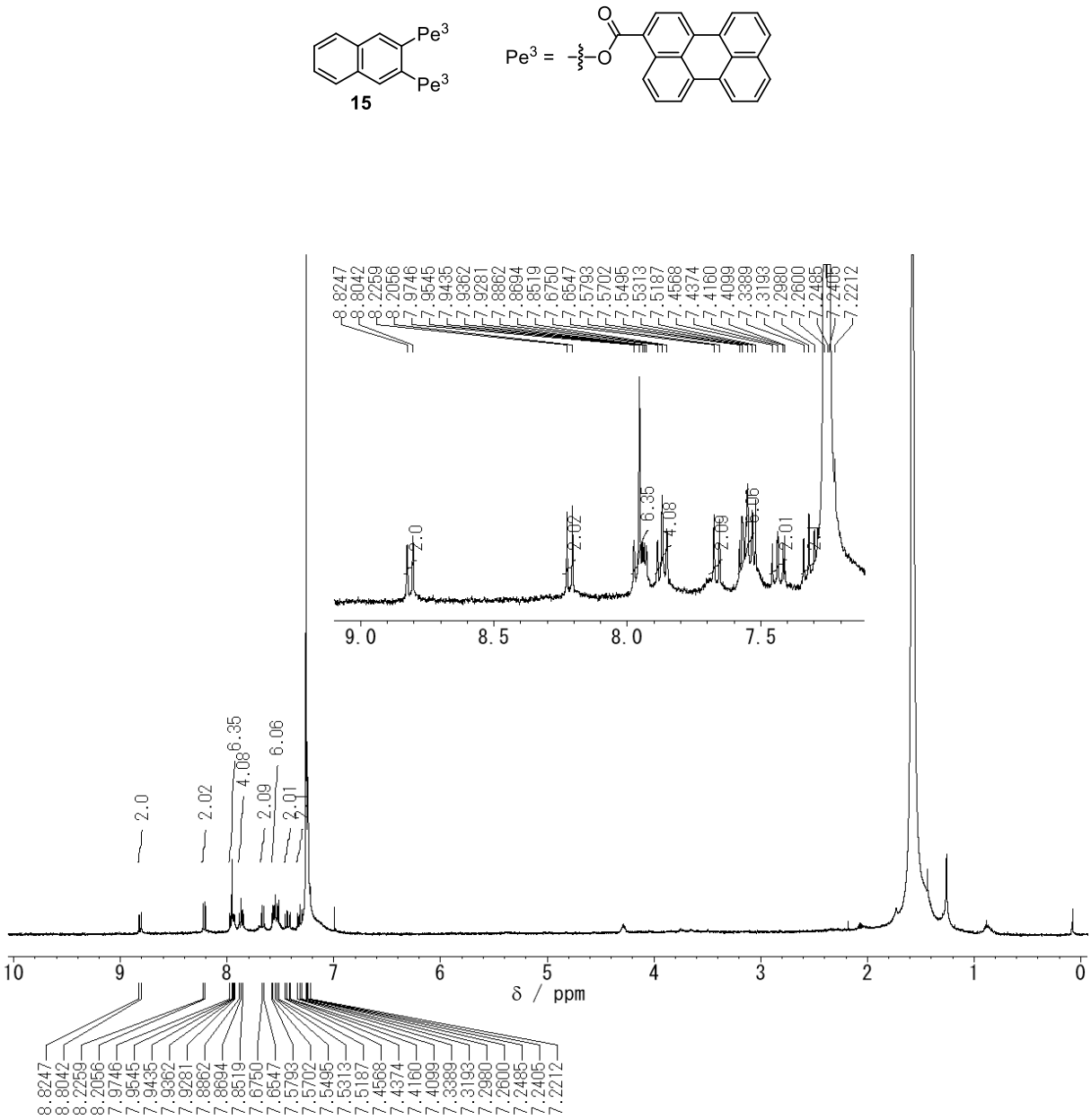
^{1}H NMR spectrum of (*R*,*R*,*R*)-**13** (400 MHz, $CDCl_3$).



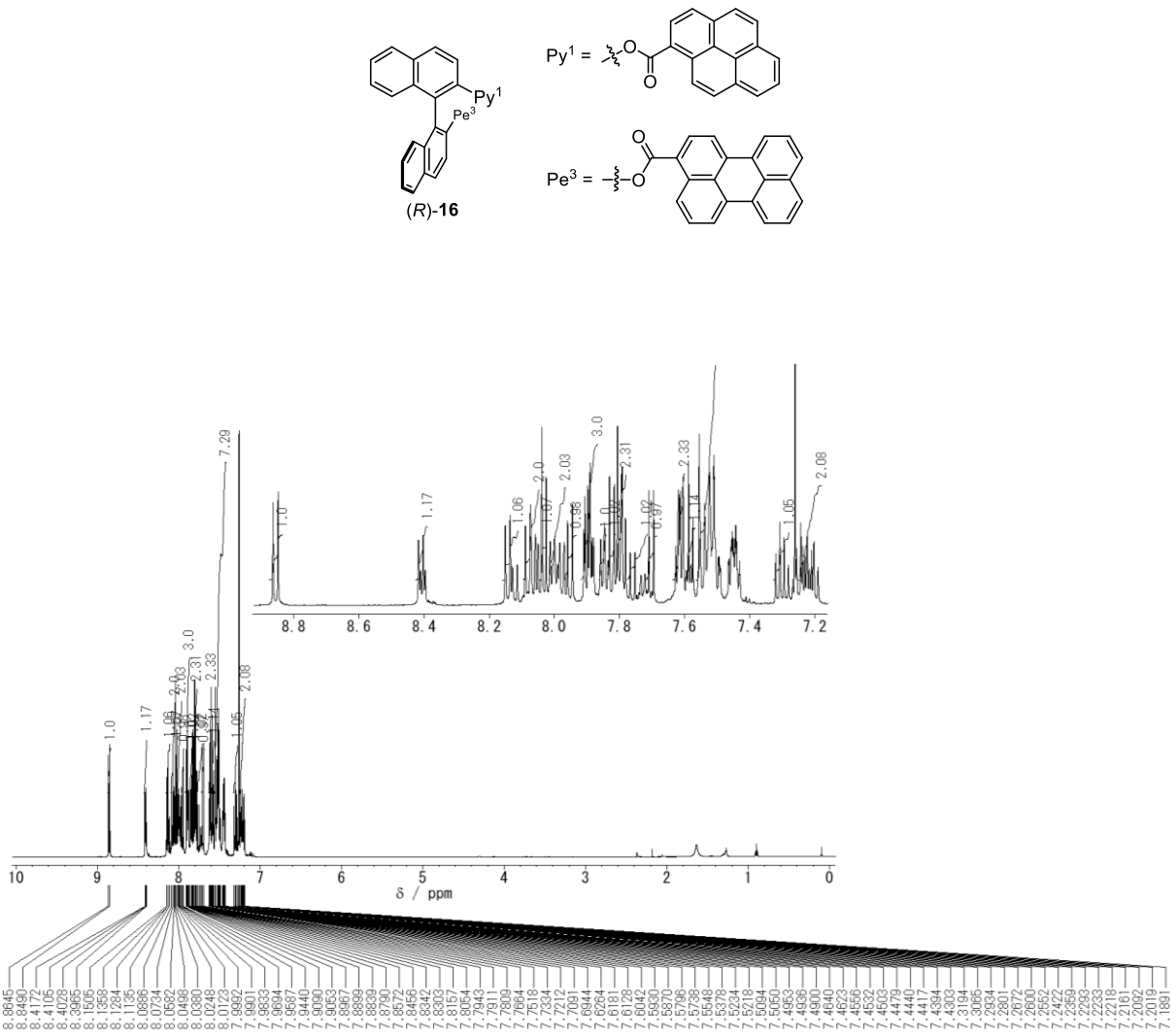
(*R*,*R*,*R*)-**13**



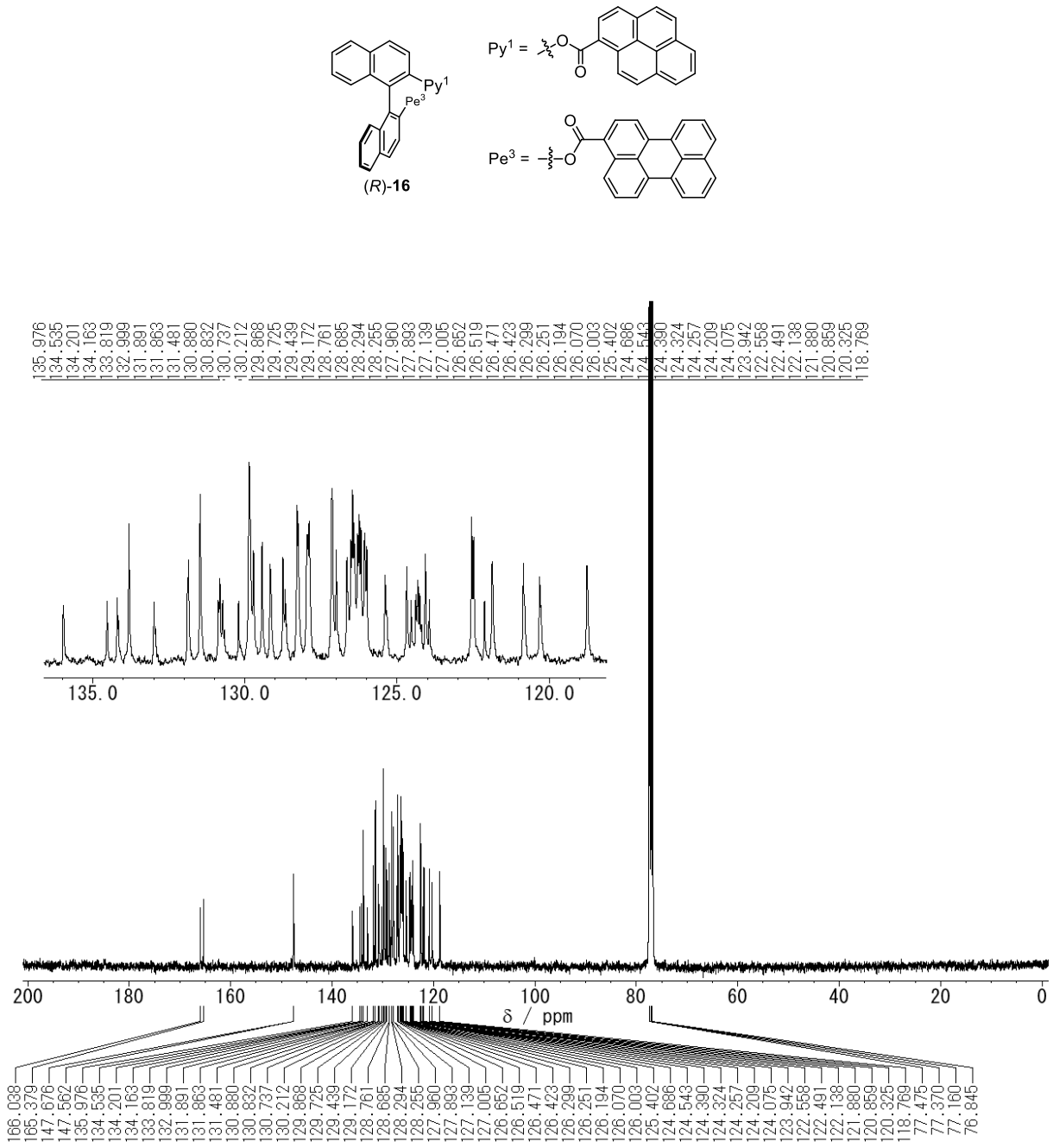
^{13}C NMR spectrum of (*R*,*R*,*R*)-**13** (101 MHz, $CDCl_3$).



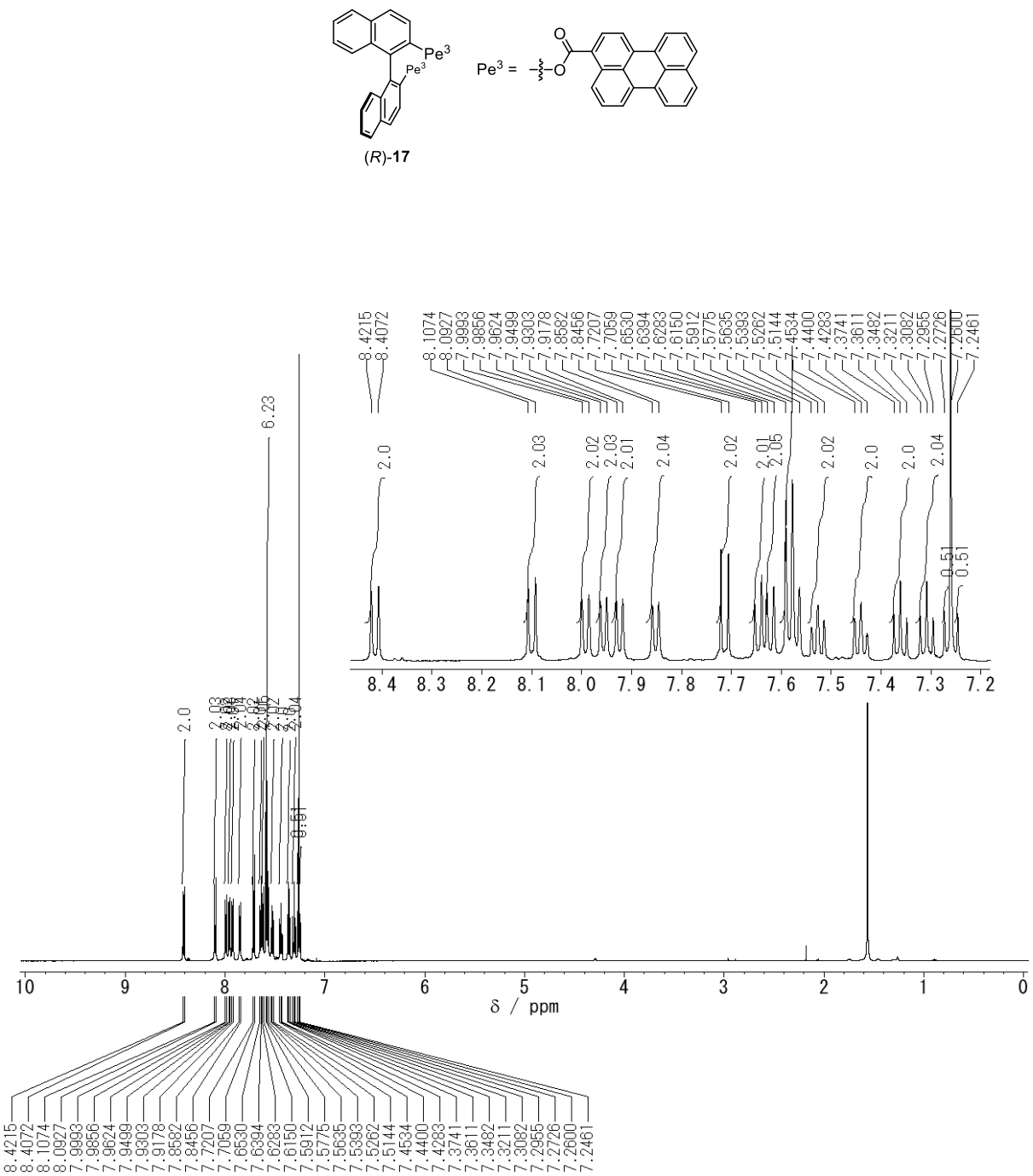
^{1}H NMR spectrum of **15** (400 MHz, $CDCl_3$)



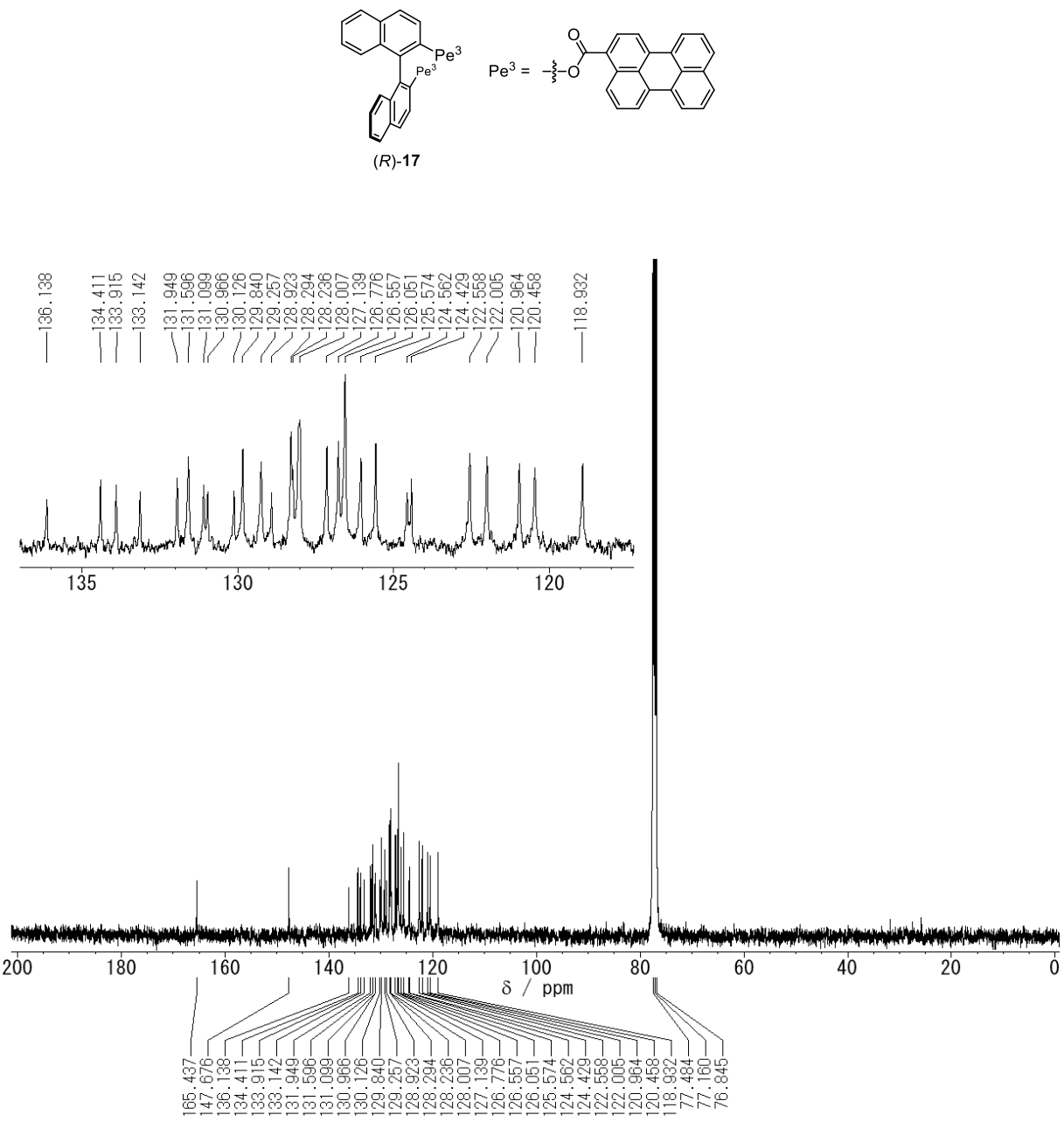
^{1}H NMR spectrum of (*R*)-**16** (600 MHz, $CDCl_3$).



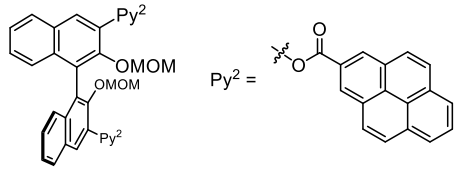
^{13}C NMR spectrum of (*R*)-**16** (101 MHz, $CDCl_3$).



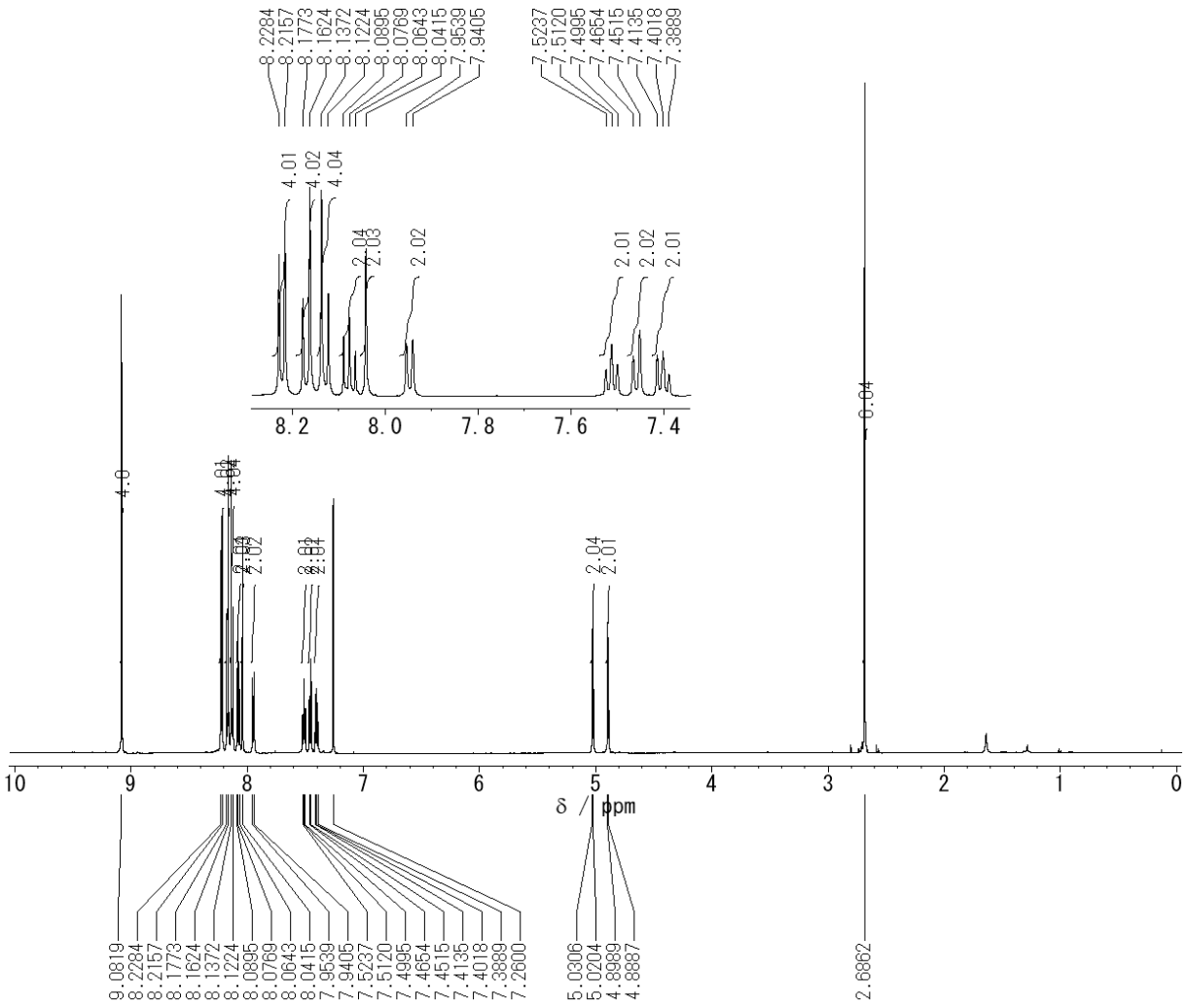
^{1}H NMR spectrum of (*R*)-**17** (600 MHz, $CDCl_3$).



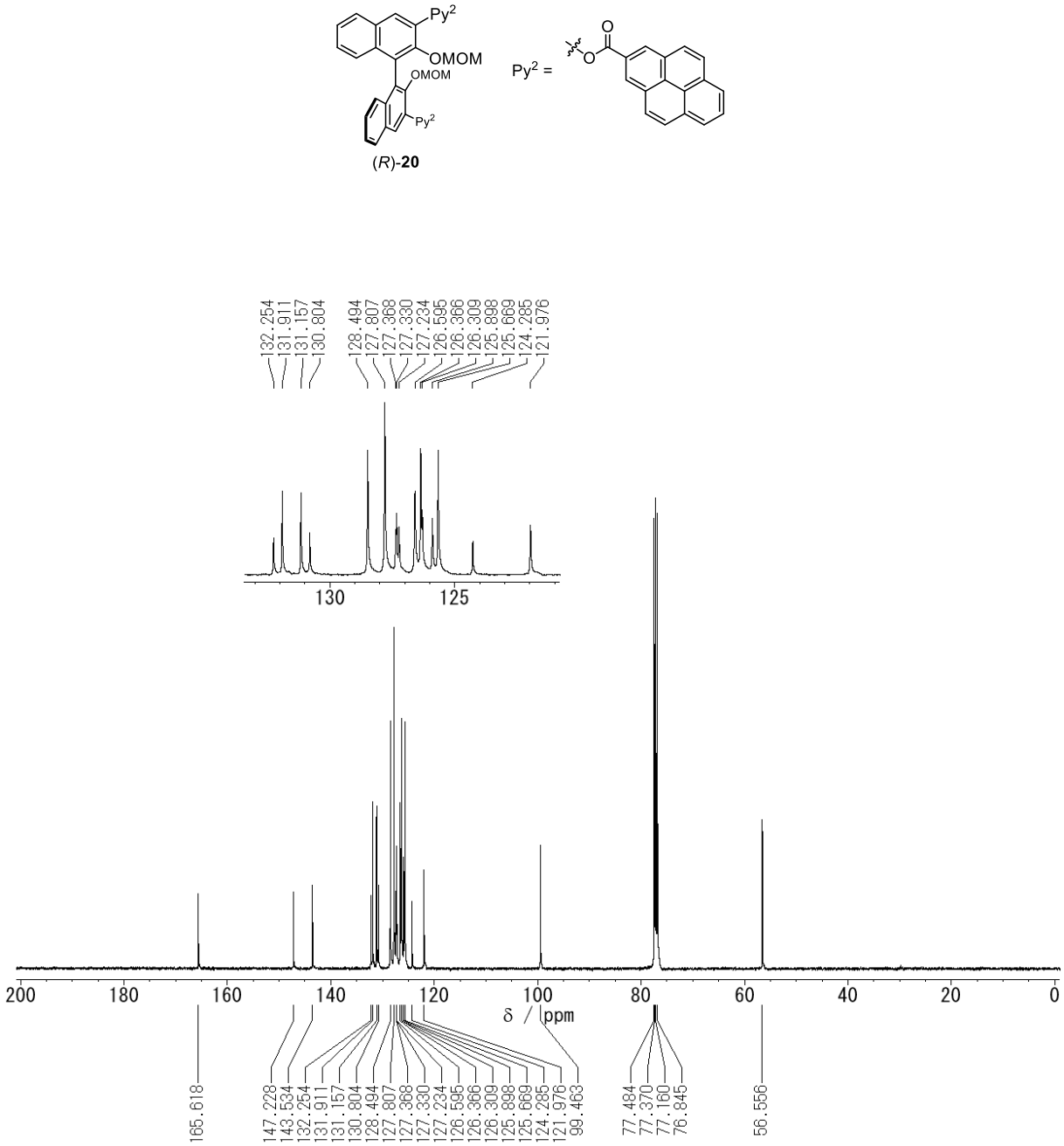
^{13}C NMR spectrum of (*R*)-**17** (101 MHz, $CDCl_3$).



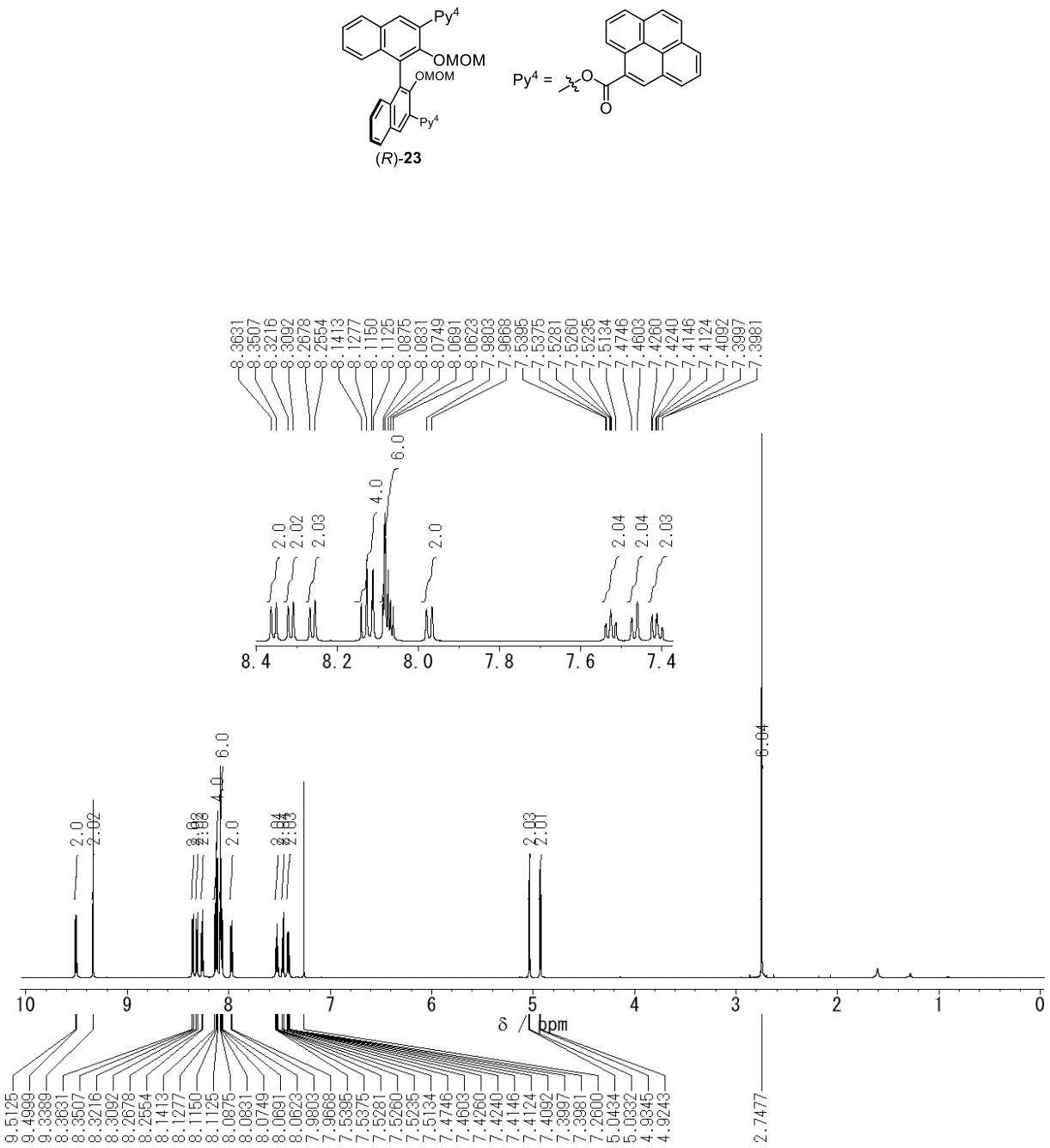
(*R*)-**20**



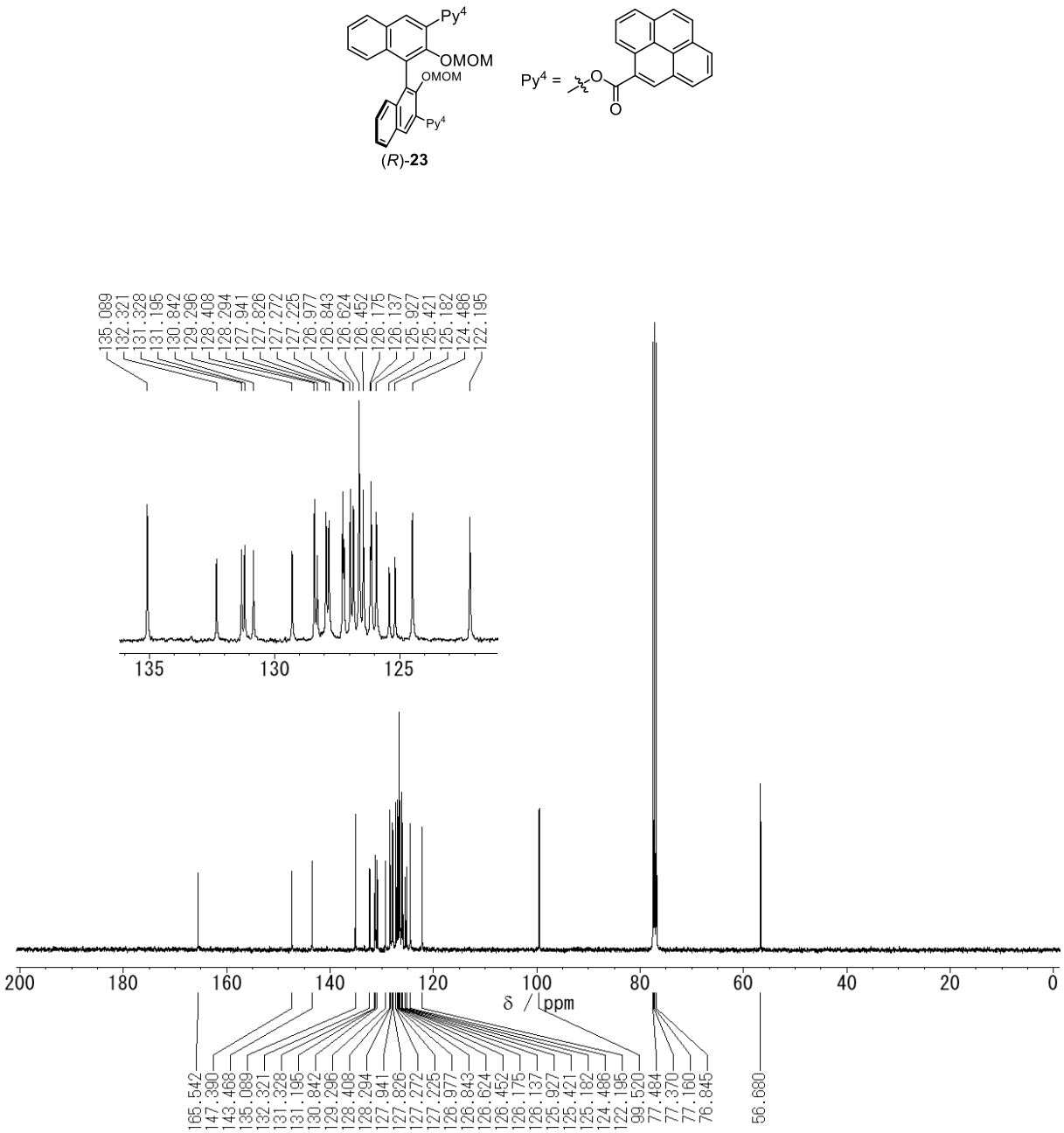
^{1}H NMR spectrum of (*R*)-**20** (600 MHz, $CDCl_3$).



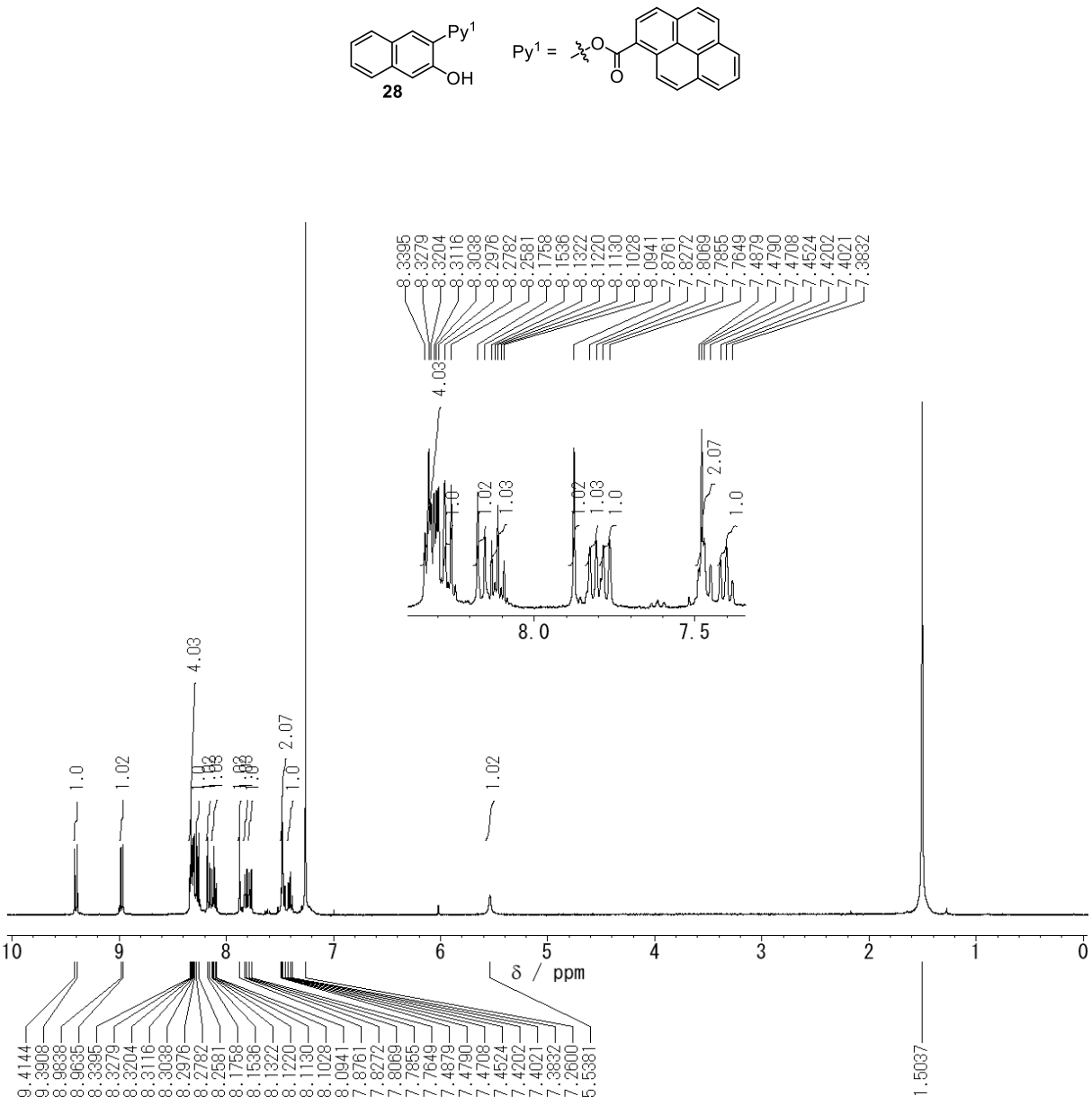
^{13}C NMR spectrum of (*R*)-**20** (101 MHz, $CDCl_3$).



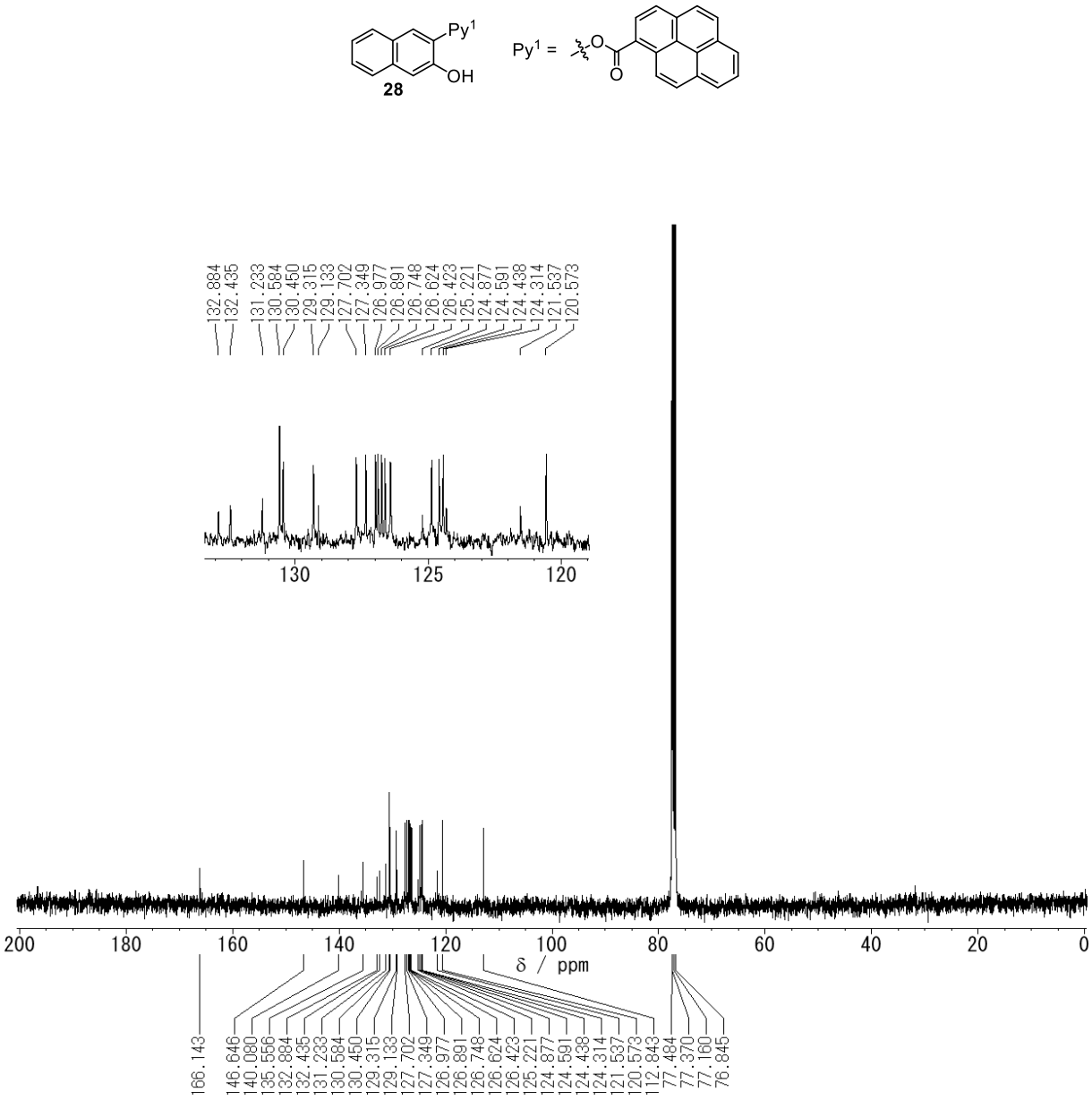
^{1}H NMR spectrum of (*R*)-**23** (600 MHz, $CDCl_3$).



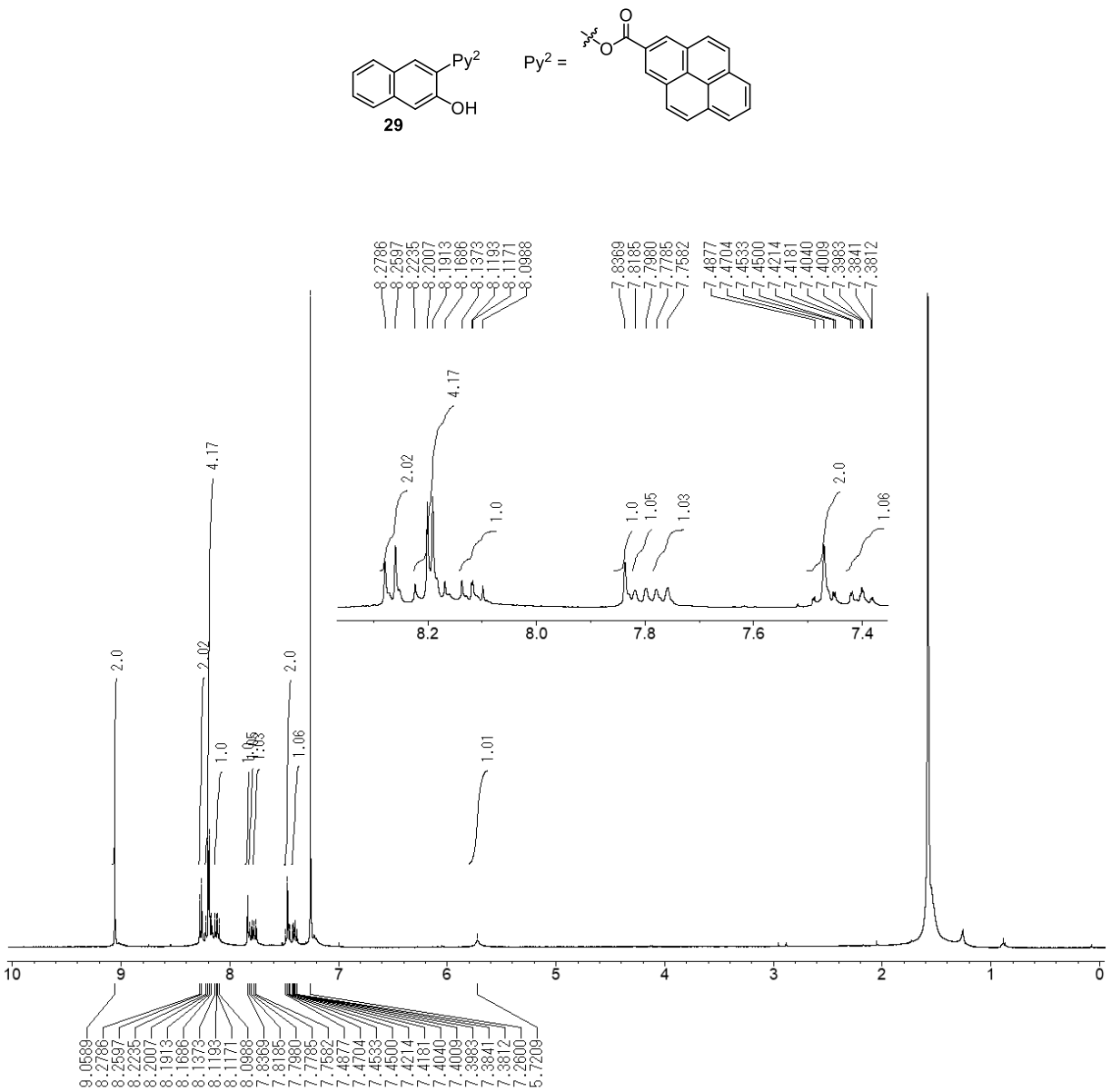
^{13}C NMR spectrum of (*R*)-**23** (101 MHz, $CDCl_3$).



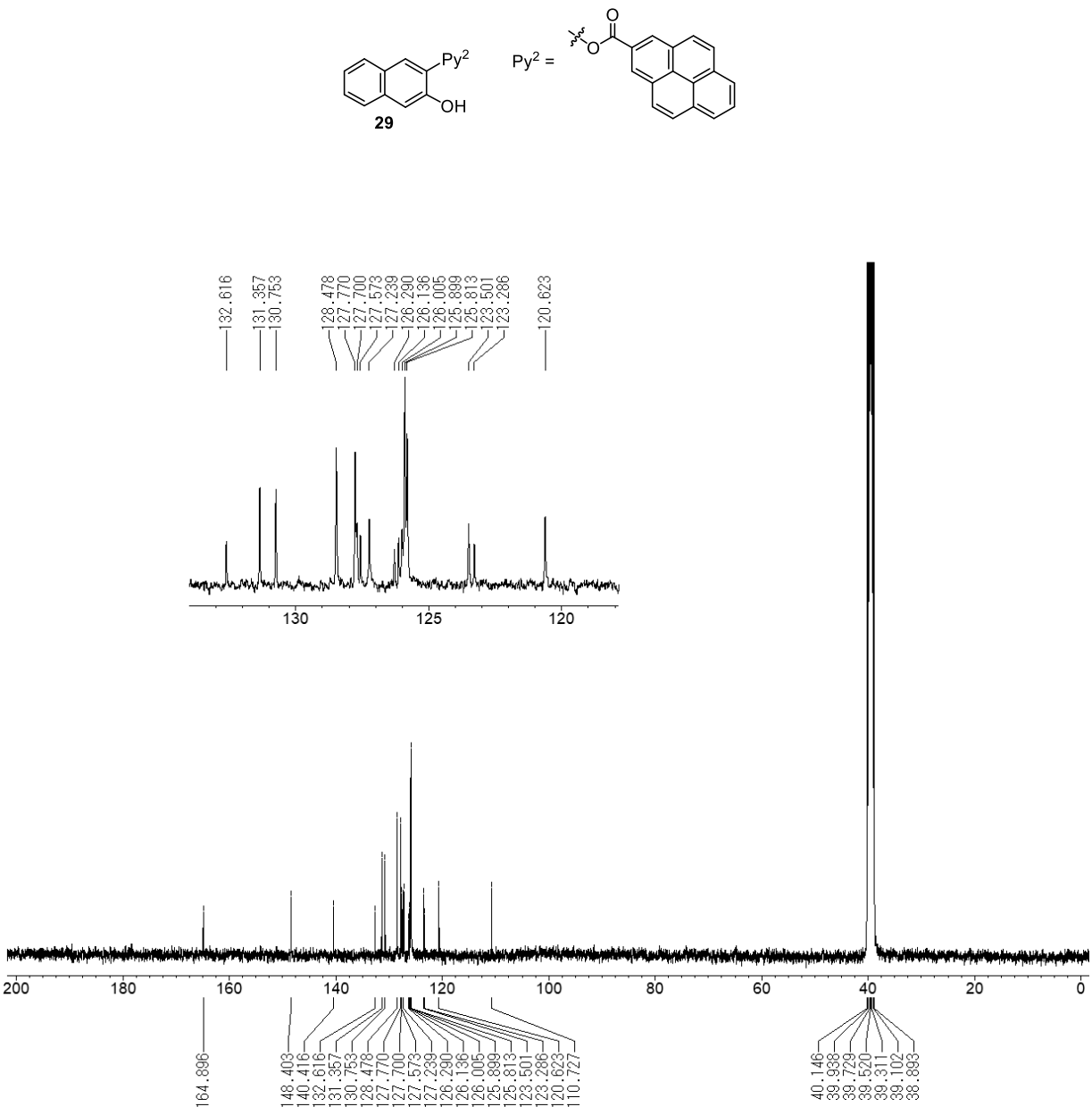
^{1}H NMR spectrum of **28** (400 MHz, $CDCl_3$).



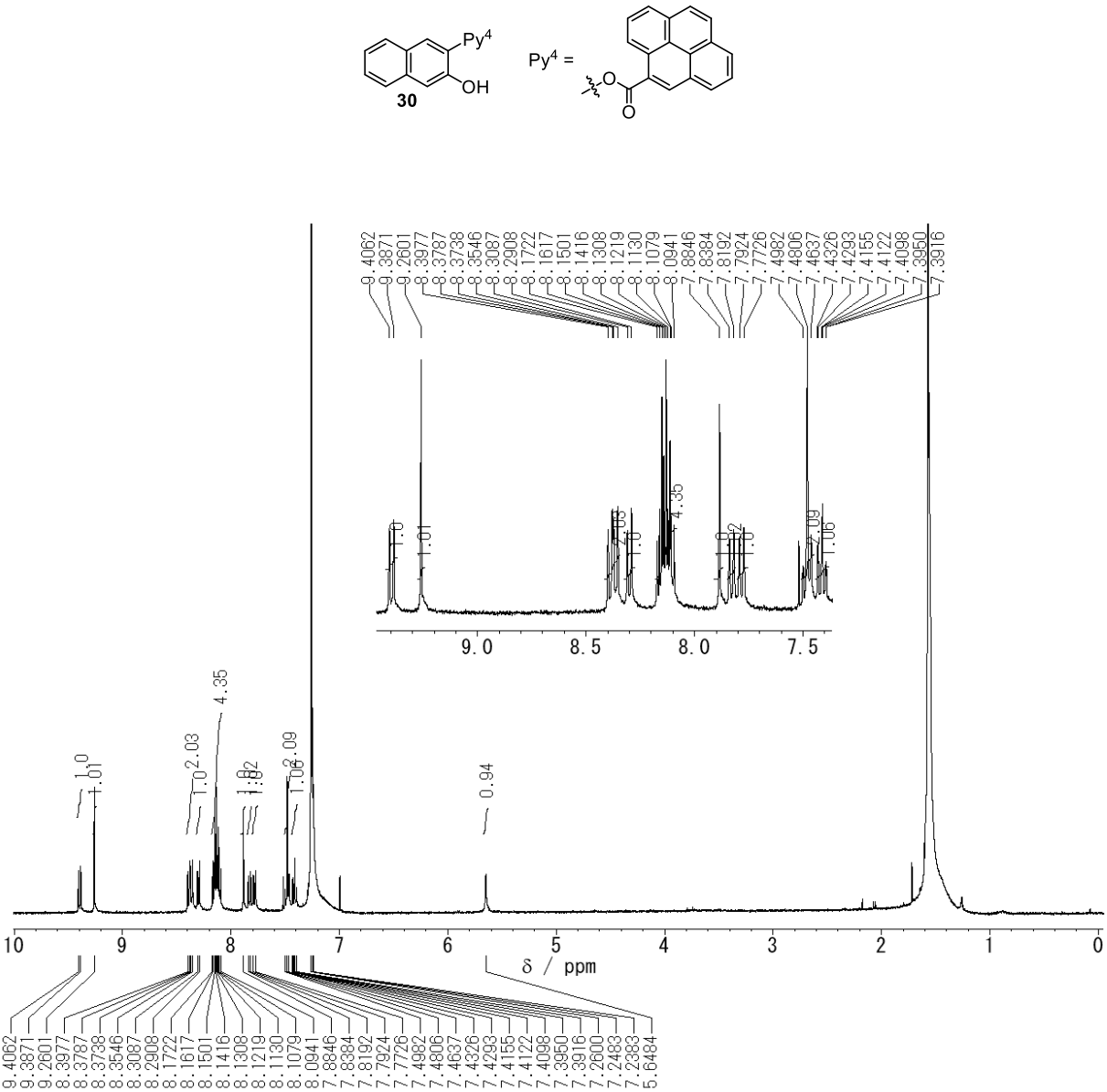
^{13}C NMR spectrum of **28** (101 MHz, $CDCl_3$).



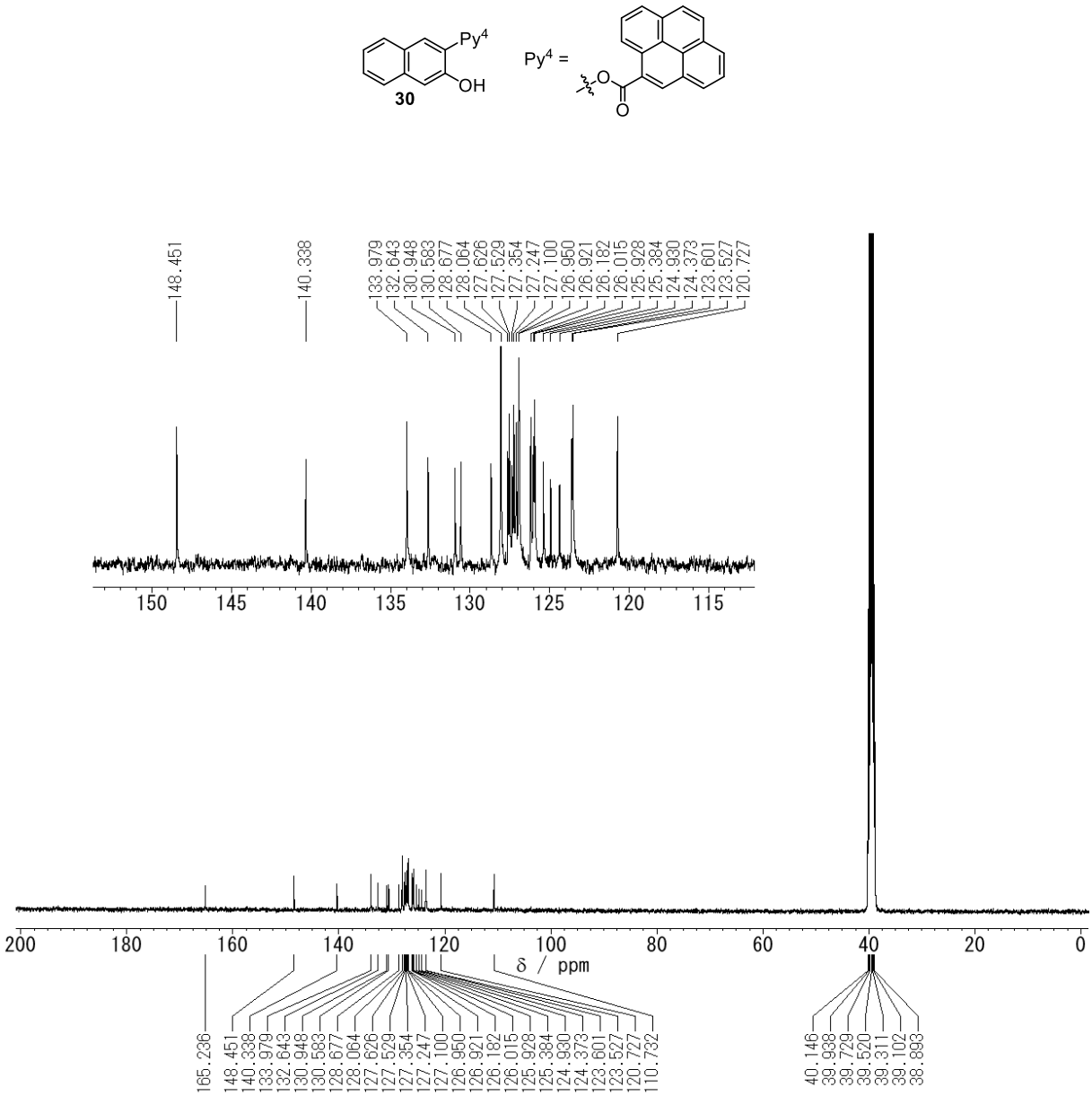
^{1}H NMR spectrum of **29** (400 MHz, $CDCl_3$).



^{13}C NMR spectrum of **29** (101 MHz, DMSO-d_6).



^{1}H NMR spectrum of **30** (400 MHz, $CDCl_3$).



^{13}C NMR spectrum of **30** (101 MHz, DMSO-d_6).

6. Coordinates of optimized structures

Coordinates of (*R*)-**2** in the ground state (0 imaginary frequencies)

C	-1.703493	2.112674	7.399875
C	-1.240562	1.223233	6.467466
C	1.050303	1.195169	3.531299
C	0.111956	2.985331	5.455740
C	-0.312950	1.628292	5.474085
C	0.196927	0.719276	4.492231
C	1.708041	-2.114519	7.397914
C	0.316153	-1.629411	5.473283
C	-0.381245	3.879252	6.437950
C	-1.266013	3.454449	7.391038
C	1.439459	2.554225	3.498689
C	-0.108780	-2.986443	5.454740
C	1.244471	-1.224730	6.466152
C	1.270537	-3.456283	7.388901
C	-1.437669	-2.554632	3.498759
C	-1.048466	-1.195588	3.531605
C	-0.194420	-0.720045	4.492108
C	-1.773396	-3.282598	1.295080
C	1.773887	3.282610	1.294946
C	-2.824211	-3.520395	0.276881
C	-2.562927	-4.271736	-0.891625
C	-4.075842	-2.930159	0.469961
C	-3.597877	-4.393297	-1.861120
C	-1.316359	-4.950474	-1.144569
C	-5.070309	-3.038187	-0.482066
C	-3.381988	-5.145825	-3.056606
C	-4.854192	-3.762821	-1.655472
C	-1.123270	-5.669462	-2.274247
C	-2.140028	-5.790812	-3.278322
C	-4.408973	-5.254328	-4.030543
C	-5.874467	-3.886950	-2.660039
C	-1.946354	-6.524272	-4.451930
C	-4.174446	-5.994061	-5.191722
C	-5.663250	-4.595834	-3.790115

C	-2.954539	-6.623353	-5.399683
C	2.824114	3.520506	0.276165
C	2.562189	4.272075	-0.892046
C	4.075820	2.930154	0.468388
C	3.596567	4.393738	-1.862140
C	1.315534	4.950988	-1.144091
C	5.069731	3.038283	-0.484211
C	3.380013	5.146500	-3.057353
C	4.852962	3.763140	-1.657360
C	1.121813	5.670187	-2.273525
C	2.137959	5.791608	-3.278211
C	4.406430	5.255135	-4.031876
C	5.872649	3.887398	-2.662507
C	1.943632	6.525292	-4.451570
C	4.171260	5.995107	-5.192772
C	5.660811	4.596519	-3.792319
C	2.951263	6.624500	-5.399898
O	-0.577973	-3.333118	1.126882
O	-2.314542	-2.965392	2.507472
O	-1.465354	-0.364582	2.511836
O	1.466652	0.364547	2.510983
O	2.315733	2.965357	2.506995
O	0.578366	3.333022	1.127374
C	0.998659	3.426355	4.442398
C	-0.996187	-3.427088	4.441856
C	0.385097	-3.880729	6.436275
C	2.788664	-0.007913	2.472422
O	3.572838	0.384474	3.301402
C	3.046389	-0.896487	1.315230
C	4.367793	-1.140041	0.813907
C	1.970937	-1.517589	0.721882
C	4.525060	-1.992922	-0.323553
C	5.520323	-0.553498	1.391816
C	2.135957	-2.365172	-0.373713
C	5.832501	-2.242016	-0.847206
C	3.377459	-2.597788	-0.927092
C	6.759479	-0.793015	0.861196

C	6.915803	-1.629365	-0.250624
C	5.999352	-3.146058	-2.005065
C	3.536870	-3.454333	-2.117719
C	4.845496	-3.718126	-2.618881
C	7.241968	-3.457972	-2.521317
C	2.450500	-4.007947	-2.768183
C	5.000673	-4.565281	-3.752201
C	7.394386	-4.303298	-3.633264
C	2.606477	-4.833895	-3.893369
C	6.297415	-4.844866	-4.243362
C	3.855477	-5.114477	-4.375007
H	-2.416306	1.785036	8.149203
H	-1.589537	0.197688	6.473322
H	2.421391	-1.787161	8.146854
H	-0.047070	4.911979	6.414474
H	-1.639567	4.148401	8.136668
H	1.593488	-0.199199	6.472126
H	1.644596	-4.150510	8.134020
H	-4.254111	-2.363556	1.375029
H	-0.531518	-4.877408	-0.405963
H	-6.024042	-2.545179	-0.324441
H	-0.176891	-6.178291	-2.434786
H	-6.825076	-3.392866	-2.485651
H	-0.993988	-7.020722	-4.613072
H	-4.962097	-6.072665	-5.934958
H	-6.442295	-4.681987	-4.541575
H	-2.789866	-7.195540	-6.306627
H	4.254590	2.363372	1.373247
H	0.531171	4.877890	-0.404975
H	6.023516	2.545168	-0.327239
H	0.175389	6.179148	-2.433381
H	6.823328	3.393217	-2.488773
H	0.991189	7.021804	-4.612071
H	4.958483	6.073819	-5.936451
H	6.439421	4.682782	-4.544217
H	2.786091	7.196874	-6.306633
H	1.316281	4.462347	4.403908

H	-1.313830	-4.463070	4.403209
H	0.050903	-4.913447	6.412652
H	0.974264	-1.367921	1.111431
H	5.407046	0.065063	2.269727
H	1.245930	-2.838137	-0.764229
H	7.636163	-0.339884	1.313061
H	7.915870	-1.789791	-0.632322
H	8.138510	-3.051989	-2.070670
H	1.444063	-3.811713	-2.421691
H	8.391378	-4.518734	-4.003126
H	1.724615	-5.242110	-4.376573
H	6.402443	-5.494507	-5.106737
H	3.988202	-5.754826	-5.241648
C	-2.787439	0.007605	2.473755
O	-3.571253	-0.385069	3.302946
C	-3.045721	0.896295	1.316777
C	-4.367363	1.139966	0.816111
C	-1.970539	1.517406	0.722932
C	-4.525151	1.992974	-0.321194
C	-5.519650	0.553411	1.394503
C	-2.136059	2.365114	-0.372483
C	-5.832832	2.242137	-0.844218
C	-3.377833	2.597902	-0.925193
C	-6.759059	0.793096	0.864551
C	-6.915885	1.629567	-0.247101
C	-6.000202	3.146152	-2.002019
C	-3.537794	3.454699	-2.115561
C	-4.846641	3.718432	-2.616190
C	-7.243032	3.457833	-2.517896
C	-2.451734	4.008586	-2.766308
C	-5.002332	4.565700	-3.749351
C	-7.395955	4.303233	-3.629716
C	-2.608227	4.834711	-3.891291
C	-6.299278	4.845106	-4.240073
C	-3.857432	5.115175	-4.372461
H	-0.973672	1.367670	1.111968
H	-5.405977	-0.065276	2.272271

H	-1.246184	2.838047	-0.763393
H	-7.635548	0.339987	1.316816
H	-7.916145	1.790165	-0.628220
H	-8.139358	3.051585	-2.067057
H	-1.445150	3.812406	-2.420217
H	-8.393101	4.518483	-3.999270
H	-1.726600	5.243166	-4.374723
H	-6.404694	5.494823	-5.103343
H	-3.990552	5.755633	-5.238960

Coordinates of (*R*)-**2** in the excited state (0 imaginary frequencies)

C	0.111545	6.897261	-3.732306
C	0.512032	6.098854	-2.694346
C	1.844651	2.664359	-2.169714
C	1.020217	4.302915	-4.268794
C	0.987511	4.784347	-2.930799
C	1.428094	3.932970	-1.868324
C	4.337707	6.660505	-0.139232
C	2.364258	5.273383	0.098453
C	0.602277	5.155150	-5.320269
C	0.161508	6.424409	-5.061012
C	1.820473	2.172978	-3.494677
C	2.270540	5.658927	1.464581
C	3.427837	5.792561	-0.681983
C	4.234338	7.054375	1.211804
C	0.350544	4.239364	1.747039
C	0.412724	3.880924	0.376212
C	1.393901	4.372848	-0.443784
C	-0.713919	2.380329	2.730118
C	1.329433	-0.108186	-3.375889
C	1.944631	-1.456874	-3.419779
C	1.153910	-2.629633	-3.450661
C	3.338124	-1.549672	-3.369724
C	1.814932	-3.890380	-3.422514
C	-0.286079	-2.624197	-3.527402
C	3.972222	-2.775725	-3.331734
C	1.059067	-5.103145	-3.449942

C	3.232305	-3.959060	-3.357541
C	-0.994258	-3.776798	-3.557505
C	-0.355673	-5.059865	-3.515215
C	1.717729	-6.360139	-3.410531
C	3.872302	-5.245214	-3.317097
C	-1.079837	-6.254943	-3.541328
C	0.957715	-7.531671	-3.436597
C	3.152664	-6.387865	-3.342772
C	-0.428114	-7.478989	-3.501923
O	0.292335	1.714909	2.658065
O	-0.688687	3.732264	2.503412
O	-0.456510	2.926703	-0.092460
O	2.217352	1.805853	-1.152913
O	2.224564	0.867009	-3.719712
O	0.193069	0.159335	-3.068097
C	1.435017	2.971331	-4.523714
C	1.242773	5.115616	2.277470
C	3.225193	6.561271	1.993989
C	3.548266	1.482971	-1.055736
O	4.350359	1.877474	-1.866684
C	3.800454	0.633541	0.131795
C	4.979032	-0.172459	0.258005
C	2.877115	0.652977	1.151893
C	5.149144	-0.961493	1.438494
C	5.970400	-0.231134	-0.752067
C	3.071362	-0.089694	2.317696
C	6.295235	-1.808031	1.564501
C	4.178987	-0.894720	2.488069
C	7.066043	-1.037287	-0.601109
C	7.227368	-1.822124	0.547036
C	6.460603	-2.644009	2.772113
C	4.378767	-1.677232	3.723428
C	5.506693	-2.544111	3.827965
C	7.516241	-3.522680	2.919307
C	3.498633	-1.601327	4.785692
C	5.681184	-3.323107	5.006418
C	7.681794	-4.298107	4.079111

C	3.679423	-2.362553	5.952051
C	6.786905	-4.199415	5.107888
C	4.745800	-3.211564	6.061661
C	-1.811476	3.214436	-0.132282
O	-2.207338	4.344256	0.052200
H	-0.251628	7.899784	-3.532097
H	0.461074	6.462333	-1.674958
H	5.147101	7.045084	-0.750785
H	0.633283	4.777808	-6.337886
H	-0.157747	7.067458	-5.874525
H	3.517440	5.483863	-1.716948
H	4.961075	7.743104	1.629770
H	3.920947	-0.637926	-3.339228
H	-0.794918	-1.672207	-3.556917
H	5.054393	-2.823201	-3.267465
H	-2.078662	-3.742076	-3.615139
H	4.956114	-5.274390	-3.264544
H	-2.163706	-6.213209	-3.597519
H	1.466021	-8.490665	-3.405325
H	3.648266	-7.353513	-3.311710
H	-1.002860	-8.398991	-3.523522
H	1.429300	2.578071	-5.534135
H	1.171610	5.384460	3.325481
H	3.143568	6.850395	3.037410
H	1.987553	1.262325	1.074493
H	5.860418	0.390874	-1.627836
H	2.313229	-0.001239	3.084001
H	7.825445	-1.066294	-1.376041
H	8.112929	-2.439833	0.623215
H	8.248548	-3.633750	2.129944
H	2.641144	-0.942779	4.738027
H	8.528329	-4.973108	4.149795
H	2.963208	-2.271506	6.761820
H	6.907265	-4.789165	6.011320
H	4.892628	-3.809161	6.956087
C	-2.087175	1.912295	3.029831
C	-2.440300	0.538250	2.965469

C	-3.063910	2.871886	3.318579
C	-3.807335	0.183405	3.157789
C	-1.510407	-0.515273	2.664616
C	-4.376415	2.515263	3.543174
C	-4.227235	-1.174431	3.018932
C	-4.777372	1.177410	3.456705
C	-1.916051	-1.803320	2.545309
C	-3.284614	-2.182846	2.699591
C	-5.595440	-1.522173	3.171301
C	-6.146280	0.795925	3.629613
C	-3.718044	-3.502389	2.525627
C	-5.987728	-2.854491	2.991786
C	-6.538508	-0.493662	3.490755
C	-5.058466	-3.832191	2.670264
H	-2.777787	3.914600	3.344642
H	-0.472372	-0.257578	2.523020
H	-5.115173	3.277581	3.768250
H	-1.190470	-2.576071	2.308580
H	-6.868257	1.571678	3.864487
H	-2.989857	-4.267810	2.276111
H	-7.036957	-3.112549	3.098541
H	-7.581993	-0.769190	3.610302
H	-5.381626	-4.857341	2.524263
C	-2.582957	1.993126	-0.382050
C	-4.009289	1.944550	-0.238665
C	-1.893430	0.827666	-0.760334
C	-4.683621	0.686624	-0.411074
C	-4.775259	3.077160	0.089663
C	-2.544222	-0.365573	-0.931053
C	-6.098116	0.618121	-0.260027
C	-3.943010	-0.488418	-0.725247
C	-6.157299	2.992049	0.241830
C	-6.811336	1.793501	0.075784
C	-6.782434	-0.640866	-0.451804
C	-4.609074	-1.755096	-0.838245
C	-6.026822	-1.814432	-0.723170
C	-8.187851	-0.746393	-0.373222

C	-3.900994	-2.960200	-1.056834
C	-6.696934	-3.067100	-0.881989
C	-8.830318	-1.961930	-0.545347
C	-4.562980	-4.172032	-1.200514
C	-8.100882	-3.112419	-0.792933
C	-5.941240	-4.236013	-1.123886
H	-0.829023	0.874826	-0.937039
H	-4.269284	4.023535	0.212109
H	-1.960600	-1.218958	-1.248538
H	-6.720225	3.884612	0.494390
H	-7.884148	1.759867	0.208250
H	-8.790301	0.132448	-0.187543
H	-2.820543	-2.950155	-1.111438
H	-9.912750	-2.008896	-0.485611
H	-3.985361	-5.075716	-1.369399
H	-8.604858	-4.065179	-0.923503
H	-6.460455	-5.181740	-1.243400

Coordinates of (*R*)-**3** in the ground state (0 imaginary frequencies)

C	1.969047	-2.021444	6.946841
C	1.403219	-1.153567	6.051604
C	-1.005146	-1.246249	3.213648
C	0.147485	-2.997304	5.056870
C	0.471413	-1.613187	5.086693
C	-0.144522	-0.730838	4.144797
C	-1.969149	2.021436	6.946833
C	-0.471505	1.613200	5.086690
C	0.746904	-3.868102	5.999887
C	1.635006	-3.392718	6.925863
C	-1.300179	-2.627574	3.170869
C	-0.147616	2.997322	5.056852
C	-1.403296	1.153565	6.051602
C	-1.635149	3.392716	6.925839
C	1.300074	2.627620	3.170868
C	1.005071	1.246282	3.213660
C	0.144462	0.730853	4.144798
C	1.769236	3.247893	0.951894

C	-1.769320	-3.247816	0.951887
C	2.887361	3.621768	0.052419
C	2.665953	4.354316	-1.134541
C	4.174732	3.196147	0.390747
C	3.780212	4.627538	-1.976729
C	1.380003	4.878109	-1.520739
C	5.248694	3.450590	-0.439686
C	3.606442	5.373111	-3.182987
C	5.075780	4.161102	-1.629061
C	1.226172	5.593176	-2.658363
C	2.325302	5.861870	-3.539827
C	4.715030	5.632881	-4.030599
C	6.179551	4.436249	-2.507425
C	2.173473	6.590560	-4.722332
C	4.520676	6.362829	-5.205297
C	6.008192	5.134966	-3.650598
C	3.261441	6.836952	-5.547142
C	-2.887429	-3.621730	0.052410
C	-2.665993	-4.354359	-1.134490
C	-4.174800	-3.196067	0.390679
C	-3.780233	-4.627619	-1.976694
C	-1.380037	-4.878192	-1.520615
C	-5.248742	-3.450554	-0.439767
C	-3.606435	-5.373261	-3.182903
C	-5.075804	-4.161150	-1.629090
C	-1.226179	-5.593317	-2.658195
C	-2.325285	-5.862042	-3.539682
C	-4.715001	-5.633079	-4.030529
C	-6.179555	-4.436349	-2.507463
C	-2.173426	-6.590795	-4.722145
C	-4.520618	-6.363093	-5.205180
C	-6.008171	-5.135139	-3.650587
C	-3.261373	-6.837232	-5.546969
O	0.612542	3.081531	0.645622
O	2.207363	3.092195	2.234384
O	1.533349	0.416182	2.243149
O	-1.533375	-0.416135	2.243137

O	-2.207453	-3.092154	2.234374
O	-0.612635	-3.081406	0.645603
C	-0.750984	-3.481978	4.074290
C	0.750849	3.482016	4.074269
C	-0.747058	3.868114	5.999855
C	2.868873	0.134086	2.295719
O	3.599834	0.593904	3.137152
C	3.283658	-0.761275	1.192154
C	4.667127	-0.961511	1.009665
C	2.376561	-1.384069	0.372523
C	5.157205	-1.756244	-0.001326
C	2.833329	-2.206022	-0.681847
C	6.605361	-1.972886	-0.196344
C	4.229939	-2.385990	-0.889538
C	1.902292	-2.839623	-1.538676
C	7.547050	-1.435162	0.657991
C	7.049547	-2.760191	-1.302183
C	4.674123	-3.192359	-1.979671
C	2.347195	-3.614613	-2.573745
C	8.924055	-1.629675	0.458861
C	6.123902	-3.364613	-2.207748
C	8.446304	-2.947571	-1.505291
C	3.724816	-3.785567	-2.789691
C	9.368730	-2.366553	-0.603394
C	6.618226	-4.096886	-3.268568
C	8.896882	-3.713564	-2.606407
C	7.997582	-4.272046	-3.471062
H	2.683529	-1.653887	7.675743
H	1.672593	-0.104064	6.063354
H	-2.683616	1.653862	7.675741
H	0.491035	-4.922774	5.969440
H	2.090136	-4.069013	7.641803
H	-1.672639	0.104054	6.063370
H	-2.090298	4.069008	7.641770
H	4.319189	2.643955	1.311493
H	0.530866	4.690319	-0.879652
H	6.238052	3.094337	-0.171570

H	0.248414	5.987393	-2.920076
H	7.160426	4.065610	-2.226749
H	1.189558	6.964073	-4.989589
H	5.370769	6.557420	-5.852181
H	6.850220	5.335949	-4.306056
H	3.128142	7.403341	-6.462848
H	-4.319274	-2.643804	1.311381
H	-0.530926	-4.690394	-0.879494
H	-6.238104	-3.094274	-0.171700
H	-0.248425	-5.987573	-2.919865
H	-7.160436	-4.065690	-2.226832
H	-1.189502	-6.964316	-4.989359
H	-5.370695	-6.557723	-5.852073
H	-6.850186	-5.336165	-4.306051
H	-3.128051	-7.403672	-6.462640
H	-1.000051	-4.536376	4.030486
H	0.999878	4.536422	4.030466
H	-0.491220	4.922793	5.969395
H	5.324923	-0.456363	1.704376
H	1.310822	-1.267391	0.528152
H	0.844292	-2.705953	-1.344395
H	7.234487	-0.847581	1.512082
H	1.637917	-4.099251	-3.236657
H	9.629099	-1.188681	1.155790
H	4.033236	-4.408211	-3.620346
H	10.430415	-2.520475	-0.769876
H	5.940464	-4.556868	-3.976619
H	9.964805	-3.846169	-2.749531
H	8.340006	-4.856695	-4.318547
C	-2.868914	-0.134005	2.295700
O	-3.599880	-0.593814	3.137131
C	-3.283669	0.761345	1.192120
C	-4.667128	0.961677	1.009655
C	-2.376543	1.384051	0.372453
C	-5.157161	1.756422	-0.001347
C	-2.833270	2.205963	-0.681965
C	-6.605298	1.973264	-0.196273

C	-4.229871	2.385984	-0.889662
C	-1.902208	2.839467	-1.538840
C	-7.546993	1.435960	0.658319
C	-7.049460	2.760316	-1.302302
C	-4.674023	3.192215	-1.979911
C	-2.347079	3.614398	-2.573969
C	-8.923987	1.630589	0.459225
C	-6.123797	3.364406	-2.208071
C	-8.446207	2.947773	-1.505399
C	-3.724696	3.785349	-2.789958
C	-9.368643	2.367155	-0.603255
C	-6.618097	4.096318	-3.269149
C	-8.896761	3.713434	-2.606756
C	-7.997447	4.271514	-3.471658
H	-5.324951	0.456589	1.704384
H	-1.310809	1.267327	0.528083
H	-0.844213	2.705801	-1.344529
H	-7.234439	0.848638	1.512592
H	-1.637769	4.098982	-3.236886
H	-9.629038	1.189924	1.156355
H	-4.033096	4.407940	-3.620662
H	-10.430321	2.521142	-0.769723
H	-5.940319	4.555967	-3.977402
H	-9.964677	3.846101	-2.749873
H	-8.339855	4.855879	-4.319345

Coordinates of (*R*)-**3** in the excited state (0 imaginary frequencies)

C	-1.568475	6.425660	-3.329798
C	-1.030115	5.707885	-2.295465
C	1.271286	2.826278	-1.800507
C	0.166270	4.299501	-3.894875
C	-0.139540	4.633933	-2.546756
C	0.452418	3.877030	-1.488644
C	2.452941	7.015685	0.756441
C	0.846418	5.204501	0.662116
C	-0.404828	5.064686	-4.941387
C	-1.248636	6.106552	-4.667095

C	1.536788	2.472281	-3.141814
C	0.533166	5.422543	2.033008
C	1.827775	6.023191	0.049373
C	2.131584	7.240676	2.111808
C	-1.022962	3.594955	1.979211
C	-0.743191	3.395213	0.605660
C	0.169933	4.168246	-0.055039
C	-1.631117	1.470963	2.756674
C	1.910543	0.153929	-3.159982
C	3.570585	-3.208071	-3.352185
C	2.987902	-0.861954	-3.255456
C	4.944186	-2.850144	-3.396172
C	3.217882	-4.602918	-3.386717
C	4.332757	-0.502203	-3.298615
C	5.943278	-3.864400	-3.470263
C	5.322261	-1.482528	-3.363184
C	4.165271	-5.563118	-3.459889
C	5.565133	-5.231935	-3.504330
C	7.316033	-3.506509	-3.509441
C	6.721764	-1.150298	-3.397913
C	6.560039	-6.209028	-3.578831
C	8.277963	-4.516534	-3.583715
C	7.668000	-2.111955	-3.468863
C	7.901289	-5.852200	-3.618311
O	-0.483323	1.112146	2.850935
O	-1.981578	2.774714	2.551241
O	-1.357755	2.335967	-0.024520
O	1.788132	2.040339	-0.789786
O	2.389824	1.411664	-3.387002
O	0.752943	-0.078052	-2.923171
C	1.012419	3.194797	-4.166688
C	-0.413851	4.585809	2.679382
C	1.195833	6.459189	2.734197
C	3.123646	2.167939	-0.501861
O	3.844752	2.873901	-1.163582
C	3.482927	1.353030	0.682540
C	4.832119	0.953757	0.953139

C	2.480534	1.001278	1.557602
C	5.098333	0.182512	2.127041
C	5.905760	1.275094	0.087411
C	2.755409	0.280424	2.720895
C	6.429387	-0.270112	2.388791
C	4.035495	-0.129235	3.032523
C	7.174256	0.846796	0.369894
C	7.435346	0.078732	1.511075
C	6.700603	-1.097453	3.582952
C	4.324136	-0.875151	4.272727
C	5.645206	-1.359788	4.506161
C	7.950145	-1.625059	3.844139
C	3.347963	-1.124947	5.217906
C	5.913074	-2.117666	5.680788
C	8.209515	-2.385285	4.996869
C	3.618635	-1.860198	6.383622
C	7.215087	-2.623375	5.904353
C	4.873287	-2.354969	6.610111
C	-2.684114	2.511912	-0.382089
O	-3.200733	3.605689	-0.284042
C	-3.288980	1.249104	-0.805110
C	-4.691084	1.137970	-1.089154
C	-2.480790	0.097085	-0.883828
C	-5.257167	-0.165817	-1.294483
C	-5.541134	2.255924	-1.163126
C	-3.027022	-1.141088	-1.090561
C	-6.651512	-0.297613	-1.544380
C	-4.430812	-1.323818	-1.232195
C	-6.900119	2.113113	-1.434354
C	-7.452406	0.867436	-1.620146
C	-7.233791	-1.611576	-1.694340
C	-5.013968	-2.630216	-1.311252
C	-6.412712	-2.761142	-1.547199
C	-8.610254	-1.791094	-1.958545
C	-4.248181	-3.808861	-1.138700
C	-6.996084	-4.062731	-1.632186
C	-9.165463	-3.056584	-2.054106

C	-4.828672	-5.064121	-1.211851
C	-8.376802	-4.181871	-1.885689
C	-6.184578	-5.202658	-1.458799
C	2.610714	-2.202039	-3.275250
H	-2.251255	7.242560	-3.121206
H	-1.294050	5.940218	-1.270633
H	3.204629	7.630726	0.273097
H	-0.163242	4.804141	-5.967388
H	-1.681206	6.684675	-5.477053
H	2.086366	5.843401	-0.987677
H	2.633929	8.030284	2.660782
H	2.165170	-4.865984	-3.353017
H	4.607886	0.545698	-3.267201
H	3.885740	-6.612016	-3.485877
H	6.999412	-0.101463	-3.364656
H	6.273103	-7.255882	-3.605145
H	9.328884	-4.245257	-3.613710
H	8.720894	-1.848047	-3.495587
H	8.661694	-6.624174	-3.675936
H	1.237464	2.913893	-5.189511
H	-0.645060	4.725926	3.729347
H	0.950053	6.618847	3.779677
H	1.458414	1.297930	1.367659
H	5.708910	1.880716	-0.784697
H	1.915996	0.058503	3.365759
H	7.992079	1.104329	-0.295425
H	8.455284	-0.234160	1.694005
H	8.766936	-1.461848	3.152791
H	2.343038	-0.749033	5.075516
H	9.207874	-2.777615	5.160115
H	2.821913	-2.033397	7.099437
H	7.405556	-3.202625	6.802525
H	5.092120	-2.931105	7.503929
H	-1.408872	0.197637	-0.776954
H	-5.116769	3.237077	-1.009164
H	-2.361928	-1.991650	-1.156610
H	-7.525710	2.997422	-1.495512

H	-8.512814	0.788889	-1.817265
H	-9.255404	-0.933979	-2.095307
H	-3.191403	-3.736076	-0.919599
H	-10.225480	-3.163259	-2.259602
H	-4.212065	-5.945967	-1.070844
H	-8.813523	-5.173537	-1.954059
H	-6.638012	-6.186688	-1.523081
H	1.555100	-2.447037	-3.229662
C	-3.610378	-1.710325	2.835106
C	-2.808435	0.572827	2.803700
C	-4.930945	-1.233970	2.618697
C	-3.390352	-3.129271	2.909876
C	-4.103232	1.049196	2.609857
C	-6.005369	-2.157706	2.465830
C	-5.175562	0.161176	2.524620
C	-4.408983	-4.004670	2.755893
C	-5.754950	-3.553695	2.523687
C	-7.322390	-1.681553	2.234625
C	-6.521832	0.614634	2.302659
C	-6.818194	-4.441816	2.346818
C	-8.356898	-2.605869	2.065647
C	-7.542097	-0.262125	2.168235
C	-8.104327	-3.969308	2.120447
C	-2.566623	-0.792633	2.929957
H	-2.378397	-3.482850	3.082030
H	-4.271983	2.113092	2.491006
H	-4.228180	-5.074184	2.804675
H	-6.697538	1.683264	2.231843
H	-6.627885	-5.509904	2.386020
H	-9.364296	-2.244740	1.882921
H	-8.553086	0.092945	1.993288
H	-8.919051	-4.672561	1.982076
H	-1.545525	-1.131497	3.065735

Coordinates of (*R*)-**4** in the ground state (0 imaginary frequencies)

C	-2.052752	1.812195	7.034641
C	-1.441001	1.007658	6.110987

C	0.845498	1.347700	3.191287
C	-0.396293	2.966487	5.094792
C	-0.588200	1.557538	5.120184
C	0.074172	0.741925	4.148412
C	2.053225	-1.812706	7.034310
C	0.588497	-1.557926	5.119996
C	-1.039580	3.770560	6.067867
C	-1.846837	3.208456	7.018669
C	1.000280	2.751640	3.149767
C	0.396711	-2.966889	5.094432
C	1.441329	-1.008103	6.110811
C	1.847432	-3.208984	7.018164
C	-1.000084	-2.751905	3.149587
C	-0.845345	-1.347968	3.191234
C	-0.073980	-0.742238	4.148357
C	-1.195586	-3.536091	0.952939
C	1.195610	3.535905	0.953145
C	-4.451947	-3.880541	-0.938999
C	-6.706960	-3.743942	-1.794442
C	-4.067210	-4.642237	-2.070050
C	-6.343117	-4.499620	-2.900845
C	-2.716786	-5.085244	-2.206773
C	-5.032742	-4.957015	-3.060947
C	-2.171173	-3.978039	-0.073864
C	-1.740591	-4.761088	-1.222738
C	-2.353387	-5.858760	-3.342064
C	-4.628247	-5.737460	-4.197931
C	-0.435432	-5.236196	-1.394533
C	-1.037356	-6.304051	-3.473855
C	-3.354597	-6.166407	-4.328118
C	-0.095196	-5.998231	-2.505256
C	4.451737	3.880726	-0.939125
C	6.706662	3.744334	-1.794836
C	4.066848	4.642580	-2.070016
C	6.342674	4.500185	-2.901075
C	2.716390	5.085549	-2.206533
C	5.032265	4.957551	-3.060966

C	2.171058	3.978045	-0.073720
C	1.740314	4.761227	-1.222435
C	2.352833	5.859198	-3.341687
C	4.627618	5.738150	-4.197792
C	0.435116	5.236310	-1.394025
C	1.036768	6.304428	-3.473290
C	3.353932	6.167045	-4.327793
C	0.094724	5.998453	-2.504622
O	-0.009809	-3.377467	0.789627
O	-1.795828	-3.300619	2.155081
O	-1.413577	-0.587783	2.188855
O	1.413694	0.587528	2.188894
O	1.795901	3.300490	2.155217
O	0.009801	3.377338	0.789898
C	0.410648	3.543585	4.083224
C	-0.410284	-3.543929	4.082876
C	1.040149	-3.771032	6.067352
C	2.777613	0.420258	2.205172
O	3.460459	0.968191	3.036311
C	3.213079	-0.472649	1.106677
C	4.588853	-0.600448	0.719208
C	2.256175	-1.223113	0.461463
C	4.920183	-1.475096	-0.363438
C	5.630498	0.110306	1.364673
C	2.591214	-2.090766	-0.577728
C	6.283633	-1.610606	-0.774126
C	3.890574	-2.220511	-1.020693
C	6.928068	-0.035294	0.951575
C	7.253402	-0.886275	-0.110966
C	6.628605	-2.521151	-1.886739
C	4.230050	-3.114429	-2.144176
C	5.591937	-3.247168	-2.545061
C	7.929352	-2.695335	-2.317645
C	3.262399	-3.826468	-2.827287
C	5.919987	-4.117153	-3.622897
C	8.252409	-3.558443	-3.378180
C	3.589039	-4.681091	-3.892724

C	7.269682	-4.257055	-4.022335
C	4.891401	-4.828782	-4.283484
C	-2.777493	-0.420342	2.205359
O	-3.460278	-0.968158	3.036609
C	-3.212980	0.472654	1.106939
C	-4.588755	0.600481	0.719508
C	-2.256086	1.223170	0.461782
C	-4.920093	1.475109	-0.363147
C	-5.630396	-0.110201	1.365055
C	-2.591139	2.090859	-0.577380
C	-6.283558	1.610698	-0.773750
C	-3.890482	2.220506	-1.020422
C	-6.927996	0.035547	0.952103
C	-7.253347	0.886554	-0.110413
C	-6.628519	2.521155	-1.886441
C	-4.229947	3.114329	-2.143979
C	-5.591848	3.247131	-2.544803
C	-7.929255	2.695245	-2.317424
C	-3.262269	3.826173	-2.827251
C	-5.919892	4.117056	-3.622689
C	-8.252309	3.558325	-3.377982
C	-3.588909	4.680774	-3.892708
C	-7.269586	4.256952	-4.022127
C	-4.891288	4.828582	-4.283365
H	-2.705126	1.374072	7.782566
H	-1.612435	-0.062044	6.121461
H	2.705618	-1.374627	7.782242
H	-0.883610	4.844614	6.039414
H	-2.336702	3.834100	7.757362
H	1.612667	0.061612	6.121409
H	2.337409	-3.834686	7.756734
H	-7.727758	-3.390900	-1.694019
H	-7.080311	-4.740367	-3.661048
H	-5.372760	-5.975497	-4.951458
H	0.315292	-5.004751	-0.652474
H	-0.763029	-6.897372	-4.340916
H	-3.056921	-6.757240	-5.189085

H	0.924065	-6.357303	-2.608058
H	7.727486	3.391322	-1.694580
H	7.079782	4.741095	-3.661310
H	5.372048	5.976354	-4.951348
H	-0.315493	5.004795	-0.651871
H	0.762319	6.897844	-4.340249
H	3.056146	6.757995	-5.188642
H	-0.924566	6.357482	-2.607281
H	0.548255	4.618158	4.037886
H	-0.547824	-4.618505	4.037452
H	0.884271	-4.845096	6.038775
H	1.222380	-1.164069	0.769559
H	5.386429	0.747552	2.201504
H	1.786555	-2.668339	-1.010018
H	7.719265	0.507025	1.459758
H	8.293568	-0.969652	-0.398122
H	8.740047	-2.161362	-1.838867
H	2.218879	-3.736957	-2.554263
H	9.289223	-3.662601	-3.680386
H	2.795748	-5.217674	-4.402847
H	7.506676	-4.924814	-4.844762
H	5.155725	-5.487194	-5.105263
H	-1.222292	1.164167	0.769876
H	-5.386304	-0.747470	2.201865
H	-1.786495	2.668531	-1.009566
H	-7.719205	-0.506652	1.460395
H	-8.293547	0.970123	-0.397389
H	-8.739931	2.161188	-1.838711
H	-2.218729	3.736483	-2.554360
H	-9.289115	3.662435	-3.680230
H	-2.795605	5.217236	-4.402938
H	-7.506581	4.924681	-4.844579
H	-5.155612	5.486977	-5.105158
C	3.464933	3.579414	0.052103
H	3.764548	3.001758	0.919385
C	5.770875	3.435468	-0.818708
H	6.050211	2.832239	0.038946

C	-3.465024	-3.579392	0.052158
H	-3.764523	-3.001852	0.919557
C	-5.771057	-3.435267	-0.818362
H	-6.050294	-2.832186	0.039427

Coordinates of (*R*)-**4** in the excited state (0 imaginary frequencies)

C	2.923741	6.970405	-0.736624
C	2.272698	5.882703	-1.254879
C	-0.477791	3.555784	-0.305622
C	0.857619	5.779871	0.733072
C	1.216295	5.261375	-0.541947
C	0.511331	4.130739	-1.060948
C	-0.724981	5.897451	-4.828828
C	0.410218	4.134647	-3.613447
C	1.548084	6.908334	1.238813
C	2.555892	7.493715	0.521309
C	-0.800455	4.053853	0.982820
C	0.737692	3.508833	-4.848168
C	-0.338950	5.338032	-3.640153
C	-0.385882	5.283615	-6.053660
C	1.814946	1.714671	-3.665984
C	1.536422	2.356893	-2.439078
C	0.840189	3.534725	-2.388200
C	1.775895	-0.597816	-3.323192
C	4.821120	-2.664140	-2.448899
C	6.979563	-3.510454	-1.769525
C	4.329206	-3.989247	-2.543984
C	6.510535	-4.813318	-1.870280
C	2.973235	-4.221118	-2.926594
C	5.192590	-5.076726	-2.251796
C	2.640521	-1.785234	-3.109979
C	2.099200	-3.133422	-3.210545
C	2.500270	-5.558024	-3.019627
C	4.679687	-6.415020	-2.357148
C	0.782224	-3.417547	-3.590741
C	1.176886	-5.791301	-3.396041
C	3.399834	-6.640778	-2.723274

C	0.333623	-4.729638	-3.680817
O	0.573096	-0.563610	-3.228416
O	2.505149	0.512342	-3.639669
O	1.908047	1.731801	-1.264270
O	-1.074689	2.400672	-0.741510
O	-1.833489	3.459264	1.682811
C	-0.164050	5.144960	1.484009
C	1.440588	2.277730	-4.844341
C	0.325838	4.114984	-6.060538
C	3.240484	1.757477	-0.934053
O	4.060851	2.217976	-1.691212
C	3.467195	1.168600	0.405844
C	4.771662	0.788272	0.865123
C	2.382686	1.017007	1.240231
C	4.902744	0.224000	2.172994
C	5.933362	0.942622	0.069052
C	2.525874	0.498809	2.527763
C	6.189110	-0.195288	2.637595
C	3.752056	0.093282	3.013647
C	7.156003	0.550187	0.543879
C	7.284137	-0.017601	1.816772
C	6.323540	-0.801965	3.978576
C	3.894752	-0.460444	4.374132
C	5.175128	-0.905274	4.818033
C	7.531387	-1.274639	4.453894
C	2.818795	-0.569430	5.234090
C	5.306814	-1.464036	6.120487
C	7.658404	-1.832505	5.736984
C	2.953479	-1.111792	6.522507
C	6.570504	-1.922997	6.559944
C	4.171349	-1.554812	6.959070
C	3.937237	-1.581620	-2.754121
C	6.143572	-2.441459	-2.055966
H	3.731951	7.431199	-1.294732
H	2.566488	5.476748	-2.215787
H	-1.299901	6.817493	-4.830141
H	1.265045	7.297203	2.212286

H	3.079293	8.356258	0.920347
H	-0.610287	5.807217	-2.701913
H	-0.697367	5.737662	-6.988549
H	8.003973	-3.327893	-1.462919
H	7.169379	-5.647060	-1.646404
H	5.346598	-7.242295	-2.134390
H	0.107788	-2.602913	-3.811842
H	0.818786	-6.813951	-3.468091
H	3.019212	-7.654732	-2.801092
H	-0.692931	-4.918250	-3.979526
H	-0.434553	5.516952	2.465982
H	1.669117	1.773086	-5.776428
H	0.582366	3.629492	-6.997209
H	1.396447	1.317218	0.915445
H	5.840731	1.399831	-0.904706
H	1.629716	0.435066	3.129788
H	8.041549	0.686838	-0.068899
H	8.272183	-0.308142	2.149605
H	8.418657	-1.225543	3.835851
H	1.837146	-0.233945	4.925956
H	8.628657	-2.188563	6.067192
H	2.081447	-1.177896	7.164465
H	6.656834	-2.348155	7.555060
H	4.286492	-1.980589	7.951101
H	4.317288	-0.568883	-2.681017
H	6.503469	-1.422018	-1.963481
C	-1.675423	2.170972	2.114524
C	-5.365925	1.862377	2.903426
C	-7.718402	2.200668	3.346441
C	-5.542625	0.461939	3.020809
C	-7.903095	0.828648	3.458260
C	-4.427448	-0.411721	2.846444
C	-6.834915	-0.057756	3.295101
C	-2.983305	1.549224	2.447170
C	-3.126758	0.104195	2.571908
C	-4.633335	-1.814975	2.935545
C	-7.002212	-1.481681	3.386272

C	-2.076995	-0.803702	2.393718
C	-3.553949	-2.679609	2.747923
C	-5.953430	-2.314231	3.210118
C	-2.293994	-2.172893	2.480538
O	-0.585227	1.657388	2.189211
C	-4.064086	2.364493	2.597623
C	-6.461327	2.716167	3.068307
H	-8.561504	2.871216	3.476140
H	-8.889781	0.428834	3.673161
H	-7.992840	-1.873757	3.595942
H	-1.087931	-0.429958	2.176714
H	-3.715644	-3.751528	2.808311
H	-6.087370	-3.390040	3.270631
H	-1.460530	-2.850882	2.328799
H	-3.944551	3.433474	2.473024
H	-6.315241	3.787764	2.974033
C	-2.445758	2.372014	-0.940019
O	-3.096407	3.393370	-0.929552
C	-2.895337	0.987466	-1.105493
C	-4.269646	0.608225	-0.963659
C	-1.933132	-0.003574	-1.370713
C	-4.610749	-0.786965	-0.999382
C	-5.294625	1.546980	-0.751762
C	-2.274291	-1.326366	-1.460252
C	-5.959526	-1.184943	-0.778903
C	-3.607963	-1.766891	-1.246391
C	-6.614666	1.143004	-0.562631
C	-6.946636	-0.191207	-0.565722
C	-6.301260	-2.588167	-0.769238
C	-3.948713	-3.159811	-1.274427
C	-5.293654	-3.557152	-1.026677
C	-7.616774	-3.032255	-0.505420
C	-2.985408	-4.165781	-1.529707
C	-5.632406	-4.945878	-1.032092
C	-7.935904	-4.380599	-0.509406
C	-3.329691	-5.507783	-1.538800
C	-6.963586	-5.329978	-0.772098

C	-4.633159	-5.905955	-1.292970
H	-0.904065	0.282751	-1.529704
H	-5.038486	2.596571	-0.743437
H	-1.489728	-2.032314	-1.695465
H	-7.382249	1.891237	-0.397877
H	-7.978795	-0.473126	-0.410280
H	-8.398647	-2.317883	-0.287317
H	-1.955180	-3.896008	-1.720064
H	-8.955272	-4.690972	-0.304935
H	-2.564026	-6.251145	-1.737001
H	-7.214856	-6.386208	-0.778414
H	-4.901517	-6.957638	-1.297400

Coordinates of (*R*)-**5** in the ground state (0 imaginary frequencies)

C	1.969047	-2.021444	6.946841
C	1.403219	-1.153567	6.051604
C	-1.005146	-1.246249	3.213648
C	0.147485	-2.997304	5.056870
C	0.471413	-1.613187	5.086693
C	-0.144522	-0.730838	4.144797
C	-1.969149	2.021436	6.946833
C	-0.471505	1.613200	5.086690
C	0.746904	-3.868102	5.999887
C	1.635006	-3.392718	6.925863
C	-1.300179	-2.627574	3.170869
C	-0.147616	2.997322	5.056852
C	-1.403296	1.153565	6.051602
C	-1.635149	3.392716	6.925839
C	1.300074	2.627620	3.170868
C	1.005071	1.246282	3.213660
C	0.144462	0.730853	4.144798
C	1.769236	3.247893	0.951894
C	-1.769320	-3.247816	0.951887
C	2.887361	3.621768	0.052419
C	2.665953	4.354316	-1.134541
C	4.174732	3.196147	0.390747
C	3.780212	4.627538	-1.976729

C	1.380003	4.878109	-1.520739
C	5.248694	3.450590	-0.439686
C	3.606442	5.373111	-3.182987
C	5.075780	4.161102	-1.629061
C	1.226172	5.593176	-2.658363
C	2.325302	5.861870	-3.539827
C	4.715030	5.632881	-4.030599
C	6.179551	4.436249	-2.507425
C	2.173473	6.590560	-4.722332
C	4.520676	6.362829	-5.205297
C	6.008192	5.134966	-3.650598
C	3.261441	6.836952	-5.547142
C	-2.887429	-3.621730	0.052410
C	-2.665993	-4.354359	-1.134490
C	-4.174800	-3.196067	0.390679
C	-3.780233	-4.627619	-1.976694
C	-1.380037	-4.878192	-1.520615
C	-5.248742	-3.450554	-0.439767
C	-3.606435	-5.373261	-3.182903
C	-5.075804	-4.161150	-1.629090
C	-1.226179	-5.593317	-2.658195
C	-2.325285	-5.862042	-3.539682
C	-4.715001	-5.633079	-4.030529
C	-6.179555	-4.436349	-2.507463
C	-2.173426	-6.590795	-4.722145
C	-4.520618	-6.363093	-5.205180
C	-6.008171	-5.135139	-3.650587
C	-3.261373	-6.837232	-5.546969
O	0.612542	3.081531	0.645622
O	2.207363	3.092195	2.234384
O	1.533349	0.416182	2.243149
O	-1.533375	-0.416135	2.243137
O	-2.207453	-3.092154	2.234374
O	-0.612635	-3.081406	0.645603
C	-0.750984	-3.481978	4.074290
C	0.750849	3.482016	4.074269
C	-0.747058	3.868114	5.999855

C	2.868873	0.134086	2.295719
O	3.599834	0.593904	3.137152
C	3.283658	-0.761275	1.192154
C	4.667127	-0.961511	1.009665
C	2.376561	-1.384069	0.372523
C	5.157205	-1.756244	-0.001326
C	2.833329	-2.206022	-0.681847
C	6.605361	-1.972886	-0.196344
C	4.229939	-2.385990	-0.889538
C	1.902292	-2.839623	-1.538676
C	7.547050	-1.435162	0.657991
C	7.049547	-2.760191	-1.302183
C	4.674123	-3.192359	-1.979671
C	2.347195	-3.614613	-2.573745
C	8.924055	-1.629675	0.458861
C	6.123902	-3.364613	-2.207748
C	8.446304	-2.947571	-1.505291
C	3.724816	-3.785567	-2.789691
C	9.368730	-2.366553	-0.603394
C	6.618226	-4.096886	-3.268568
C	8.896882	-3.713564	-2.606407
C	7.997582	-4.272046	-3.471062
H	2.683529	-1.653887	7.675743
H	1.672593	-0.104064	6.063354
H	-2.683616	1.653862	7.675741
H	0.491035	-4.922774	5.969440
H	2.090136	-4.069013	7.641803
H	-1.672639	0.104054	6.063370
H	-2.090298	4.069008	7.641770
H	4.319189	2.643955	1.311493
H	0.530866	4.690319	-0.879652
H	6.238052	3.094337	-0.171570
H	0.248414	5.987393	-2.920076
H	7.160426	4.065610	-2.226749
H	1.189558	6.964073	-4.989589
H	5.370769	6.557420	-5.852181
H	6.850220	5.335949	-4.306056

H	3.128142	7.403341	-6.462848
H	-4.319274	-2.643804	1.311381
H	-0.530926	-4.690394	-0.879494
H	-6.238104	-3.094274	-0.171700
H	-0.248425	-5.987573	-2.919865
H	-7.160436	-4.065690	-2.226832
H	-1.189502	-6.964316	-4.989359
H	-5.370695	-6.557723	-5.852073
H	-6.850186	-5.336165	-4.306051
H	-3.128051	-7.403672	-6.462640
H	-1.000051	-4.536376	4.030486
H	0.999878	4.536422	4.030466
H	-0.491220	4.922793	5.969395
H	5.324923	-0.456363	1.704376
H	1.310822	-1.267391	0.528152
H	0.844292	-2.705953	-1.344395
H	7.234487	-0.847581	1.512082
H	1.637917	-4.099251	-3.236657
H	9.629099	-1.188681	1.155790
H	4.033236	-4.408211	-3.620346
H	10.430415	-2.520475	-0.769876
H	5.940464	-4.556868	-3.976619
H	9.964805	-3.846169	-2.749531
H	8.340006	-4.856695	-4.318547
C	-2.868914	-0.134005	2.295700
O	-3.599880	-0.593814	3.137131
C	-3.283669	0.761345	1.192120
C	-4.667128	0.961677	1.009655
C	-2.376543	1.384051	0.372453
C	-5.157161	1.756422	-0.001347
C	-2.833270	2.205963	-0.681965
C	-6.605298	1.973264	-0.196273
C	-4.229871	2.385984	-0.889662
C	-1.902208	2.839467	-1.538840
C	-7.546993	1.435960	0.658319
C	-7.049460	2.760316	-1.302302
C	-4.674023	3.192215	-1.979911

C	-2.347079	3.614398	-2.573969
C	-8.923987	1.630589	0.459225
C	-6.123797	3.364406	-2.208071
C	-8.446207	2.947773	-1.505399
C	-3.724696	3.785349	-2.789958
C	-9.368643	2.367155	-0.603255
C	-6.618097	4.096318	-3.269149
C	-8.896761	3.713434	-2.606756
C	-7.997447	4.271514	-3.471658
H	-5.324951	0.456589	1.704384
H	-1.310809	1.267327	0.528083
H	-0.844213	2.705801	-1.344529
H	-7.234439	0.848638	1.512592
H	-1.637769	4.098982	-3.236886
H	-9.629038	1.189924	1.156355
H	-4.033096	4.407940	-3.620662
H	-10.430321	2.521142	-0.769723
H	-5.940319	4.555967	-3.977402
H	-9.964677	3.846101	-2.749873
H	-8.339855	4.855879	-4.319345

Coordinates of (*R*)-**5** in the excited state (0 imaginary frequencies)

C	-3.417158	-6.904308	-0.248527
C	-2.781970	-5.888935	-0.912401
C	0.249103	-3.760395	-0.511003
C	-1.063661	-5.824658	0.824260
C	-1.585033	-5.326802	-0.401158
C	-0.890024	-4.274489	-1.070738
C	-0.327664	-6.136117	-4.951211
C	-1.176083	-4.306508	-3.608303
C	-1.743602	-6.878160	1.484106
C	-2.891380	-7.408554	0.960654
C	0.744394	-4.222006	0.736845
C	-1.646580	-3.670428	-4.790004
C	-0.506238	-5.550621	-3.726518
C	-0.806470	-5.509613	-6.122212
C	-2.453132	-1.819690	-3.482426

C	-2.022503	-2.463889	-2.301227
C	-1.387454	-3.676782	-2.342809
C	-2.368636	0.509075	-3.142891
C	-3.239331	1.682699	-2.887574
C	-2.799609	3.000087	-3.144008
C	-4.502465	1.454654	-2.334993
C	-3.662188	4.079057	-2.802837
C	-1.540114	3.313303	-3.770766
C	-5.329902	2.507521	-1.995368
C	-3.259958	5.428490	-3.044849
C	-4.930192	3.826914	-2.214756
C	-1.169855	4.593204	-4.005596
C	-2.005644	5.701761	-3.644693
C	-4.113968	6.505078	-2.688910
C	-5.773468	4.936367	-1.863025
C	-1.628395	7.027479	-3.874795
C	-3.698465	7.815902	-2.932699
C	-5.385036	6.210433	-2.086778
C	-2.467322	8.073905	-3.520361
O	-1.158495	0.490634	-3.136947
O	-3.111023	-0.604001	-3.383967
O	-2.170427	-1.819526	-1.086931
O	0.843753	-2.676603	-1.118174
O	1.910091	-3.723277	1.263295
C	0.105756	-5.243538	1.373692
C	-2.283049	-2.407946	-4.696184
C	-1.448344	-4.303953	-6.041686
C	-3.431061	-1.727461	-0.565969
O	-4.410341	-2.091743	-1.169135
C	-3.432778	-1.118960	0.782461
C	-4.686777	-0.762624	1.320651
C	-2.282564	-0.927982	1.507017
C	-4.805333	-0.190346	2.565872
C	-2.357870	-0.352386	2.796730
C	-6.115788	0.189350	3.132690
C	-3.618608	0.038576	3.330696
C	-1.177556	-0.163996	3.555531

C	-7.299240	-0.043884	2.461012
C	-6.164757	0.820872	4.412967
C	-3.671868	0.643472	4.621224
C	-1.251454	0.405808	4.796922
C	-8.541730	0.332939	2.997451
C	-4.976813	1.070543	5.167254
C	-7.425485	1.209304	4.948976
C	-2.491233	0.807577	5.320313
C	-8.607243	0.951462	4.214958
C	-5.089925	1.703583	6.388956
C	-7.482864	1.848528	6.210105
C	-6.335112	2.092614	6.911049
H	-4.333685	-7.322137	-0.651545
H	-3.194208	-5.496961	-1.835098
H	0.188357	-7.087630	-5.023939
H	-1.337686	-7.253089	2.418722
H	-3.404409	-8.213292	1.476805
H	-0.131241	-6.030557	-2.830252
H	-0.659207	-5.985241	-7.086204
H	-4.819697	0.434473	-2.155331
H	-0.891159	2.498726	-4.058805
H	-6.298800	2.312484	-1.547334
H	-0.220030	4.801244	-4.489969
H	-6.735980	4.722538	-1.409165
H	-0.667526	7.230356	-4.338211
H	-4.353489	8.636715	-2.656813
H	-6.030883	7.040031	-1.815558
H	-2.161241	9.098352	-3.704425
H	0.500477	-5.598963	2.319073
H	-2.633645	-1.901829	-5.588757
H	-1.813472	-3.810960	-6.937524
H	-5.552707	-0.964061	0.704210
H	-1.313680	-1.222315	1.118868
H	-0.232768	-0.490021	3.133933
H	-7.289317	-0.532282	1.494677
H	-0.352586	0.551535	5.386641
H	-9.447049	0.128632	2.435225

H	-2.502698	1.252781	6.307546
H	-9.561285	1.250620	4.638003
H	-4.205799	1.916211	6.976611
H	-8.451000	2.140083	6.605450
H	-6.375209	2.586154	7.876570
C	1.996842	-2.372599	1.586716
C	3.355019	-1.990090	1.933092
C	3.720443	-0.626744	2.199090
C	4.341035	-3.001039	2.047757
C	5.074611	-0.339767	2.552745
C	2.817480	0.472337	2.094557
C	5.629225	-2.717181	2.403252
C	5.490262	1.007132	2.790568
C	6.037564	-1.385521	2.659990
C	3.221285	1.757591	2.317095
C	4.559673	2.074685	2.671585
C	6.843914	1.295292	3.135646
C	7.371009	-1.072059	3.022033
C	4.988565	3.397021	2.901032
C	7.227658	2.628929	3.350444
C	7.767444	0.215365	3.245445
C	6.303485	3.661274	3.240285
O	0.997176	-1.675581	1.543576
H	4.052736	-4.024217	1.847606
H	1.794897	0.269244	1.816078
H	6.358699	-3.516487	2.492892
H	2.504754	2.568614	2.222987
H	8.082561	-1.887790	3.115241
H	4.267009	4.204203	2.819265
H	8.256658	2.841808	3.624222
H	8.793023	0.435614	3.526726
H	6.618310	4.684749	3.420867
C	2.166904	-2.703993	-1.424270
O	2.817316	-3.709380	-1.534256
C	2.685621	-1.315973	-1.524788
C	4.045218	-1.134530	-1.300481
C	1.848623	-0.227176	-1.701635

C	4.607289	0.150104	-1.200093
C	2.377351	1.080323	-1.665265
C	6.000347	0.348559	-0.886074
C	3.759767	1.280972	-1.378957
C	1.537497	2.188915	-1.871959
C	6.890879	-0.730578	-0.720301
C	6.490816	1.674081	-0.707045
C	4.259320	2.603890	-1.252515
C	2.046699	3.474355	-1.791700
C	8.216880	-0.528981	-0.374997
C	5.643455	2.801636	-0.874873
C	7.851702	1.868623	-0.327320
C	3.382205	3.680999	-1.481256
C	8.694940	0.751853	-0.163628
C	6.175653	4.084114	-0.644571
C	8.330752	3.174467	-0.105808
C	7.497914	4.265617	-0.269534
H	4.641676	-2.025406	-1.160323
H	0.787841	-0.365599	-1.874545
H	0.491750	2.012211	-2.099224
H	6.541338	-1.744793	-0.855533
H	1.393094	4.322868	-1.963278
H	8.873178	-1.382382	-0.249375
H	3.745191	4.698414	-1.417501
H	9.728284	0.912938	0.125455
H	5.545839	4.957265	-0.748768
H	9.365472	3.310780	0.191172
H	7.873025	5.267600	-0.093327

Coordinates of (*R*)-**6** in the ground state (0 imaginary frequencies)

C	-0.553734	6.669562	2.714532
C	-0.159019	5.756702	1.773498
C	-1.592914	2.868972	-0.094673
C	-2.383240	4.750810	1.813446
C	-1.061964	4.776288	1.288663
C	-0.683093	3.815818	0.298806
C	0.554262	6.669446	-2.714845

C	1.062359	4.776183	-1.288916
C	-2.761927	5.712355	2.782652
C	-1.870662	6.652612	3.222409
C	-2.895578	2.832770	0.454294
C	2.383635	4.750599	-1.813696
C	0.159482	5.756644	-1.773782
C	1.871189	6.652391	-3.222721
C	2.895853	2.832577	-0.454472
C	1.593185	2.868876	0.094471
C	0.683421	3.815764	-0.299034
C	3.694368	0.618302	-0.493191
C	1.733472	1.871299	2.238308
C	-1.733362	1.871412	-2.238498
C	-3.694217	0.618554	0.493211
C	4.608354	-0.304100	0.227621
C	5.049595	-1.513932	-0.354014
C	5.004531	0.041633	1.522729
C	5.896797	-2.363061	0.412672
C	4.714835	-1.925281	-1.694560
C	5.816718	-0.793569	2.264918
C	6.374364	-3.592903	-0.136162
C	6.275297	-1.999413	1.732224
C	5.176668	-3.087317	-2.208882
C	6.016717	-3.971075	-1.453939
C	7.211675	-4.444039	0.631917
C	7.123071	-2.880795	2.487436
C	6.492550	-5.176954	-1.975478
C	7.665125	-5.641608	0.074493
C	7.568283	-4.044057	1.965163
C	7.308435	-6.004030	-1.217312
C	1.127895	0.820159	3.063751
C	0.010576	0.089204	2.652999
C	-0.542743	-0.874668	3.470930
C	0.011183	-1.157105	4.736229
C	-1.127936	0.820222	-3.063975
C	-0.010656	0.089167	-2.653319
C	0.542493	-0.874784	-3.471287

C	-0.011530	-1.157083	-4.736567
C	-4.608199	-0.303892	-0.227547
C	-5.049485	-1.513663	0.354184
C	-5.004321	0.041724	-1.522704
C	-5.896659	-2.362857	-0.412462
C	-4.714795	-1.924891	1.694785
C	-5.816488	-0.793535	-2.264847
C	-6.374256	-3.592647	0.136462
C	-6.275101	-1.999328	-1.732064
C	-5.176656	-3.086878	2.209192
C	-6.016670	-3.970703	1.454289
C	-7.211539	-4.443849	-0.631577
C	-7.122846	-2.880773	-2.487233
C	-6.492532	-5.176532	1.975916
C	-7.665018	-5.641365	-0.074065
C	-7.568087	-4.043986	-1.964875
C	-7.308388	-6.003672	1.217789
O	2.946523	0.341483	-1.400117
H	0.152187	7.409572	3.076619
H	0.856417	5.767310	1.395697
H	-0.151609	7.409493	-3.076957
H	-3.774448	5.684329	3.173780
H	-2.170877	7.382770	3.966728
H	-0.855954	5.767334	-1.395985
H	2.171455	7.382505	-3.967063
O	3.790961	1.882657	0.005905
O	1.199359	1.882526	0.971756
O	-1.199173	1.882601	-0.971963
O	-3.790735	1.882862	-0.006011
H	-0.452643	0.293040	1.696447
O	2.597883	2.642683	2.579269
O	-2.597768	2.642837	-2.579379
O	-2.946436	0.341805	1.400215
H	4.648637	0.972063	1.948333
H	4.079738	-1.279857	-2.283501
H	6.102355	-0.514572	3.274111
H	4.914328	-3.372687	-3.223769

H	7.398702	-2.584819	3.494875
H	6.215488	-5.460604	-2.986384
H	8.304317	-6.290086	0.666085
H	8.208712	-4.701113	2.545924
H	7.670016	-6.937614	-1.635493
H	-1.422283	-1.395669	3.118926
H	0.452636	0.292917	-1.696783
H	1.421893	-1.396026	-3.119285
H	-4.648393	0.972106	-1.948385
H	-4.079739	-1.279406	2.283703
H	-6.102079	-0.514626	-3.274078
H	-4.914371	-3.372152	3.224120
H	-7.398433	-2.584884	-3.494710
H	-6.215517	-5.460091	2.986860
H	-8.304188	-6.289893	-0.665627
H	-8.208495	-4.701090	-2.545603
H	-7.669992	-6.937216	1.636038
C	-3.288717	3.754680	1.372772
H	-4.296836	3.714932	1.770135
C	3.289051	3.754431	-1.372982
H	4.297172	3.714617	-1.770333
C	2.762390	5.712087	-2.782932
H	3.774909	5.683979	-3.174058
C	1.668143	0.566487	4.326106
H	2.522033	1.150105	4.652637
C	1.130561	-0.401567	5.149274
H	1.577128	-0.570216	6.120046
C	-1.130998	-0.401564	-5.149467
H	-1.577711	-0.570278	-6.120161
C	-1.668388	0.566545	-4.326259
H	-2.522301	1.150204	-4.652654
N	0.524106	-2.133179	-5.544596
N	-0.524442	-2.133392	5.544132
C	1.736914	-2.813643	-5.143505
H	2.591510	-2.129072	-5.052800
H	1.608839	-3.321590	-4.181948
H	1.984797	-3.569999	-5.887719

C	0.023677	-2.311574	-6.890290
H	0.562573	-3.129496	-7.367379
H	-1.040559	-2.571732	-6.890137
H	0.152062	-1.412777	-7.508332
C	-0.026076	-2.309658	6.890903
H	1.038403	-2.568684	6.892713
H	-0.156423	-1.410319	7.507777
H	-0.564811	-3.127700	7.367977
C	-1.738046	-2.812774	5.143539
H	-1.611221	-3.318990	4.180958
H	-1.984934	-3.570555	5.886646
H	-2.592737	-2.127964	5.055187

Coordinates of (*R*)-**6** in the excited state (0 imaginary frequencies)

C	5.839983	-0.745654	-4.389325
C	5.299458	-0.600190	-3.139733
C	2.517337	-2.028998	-1.113002
C	3.633744	-2.307563	-3.659596
C	4.188135	-1.381931	-2.732898
C	3.610312	-1.263056	-1.429375
C	7.295037	-1.841844	0.817559
C	5.345617	-0.501569	0.291991
C	4.218823	-2.437213	-4.943434
C	5.298899	-1.677374	-5.301226
C	1.939865	-2.904724	-2.061102
C	5.777193	0.481453	1.225124
C	6.131939	-1.667849	0.115993
C	7.731425	-0.859580	1.732356
C	3.814837	1.820502	0.778340
C	3.413572	0.853110	-0.179682
C	4.130629	-0.285198	-0.429456
C	1.985912	-2.909820	1.018798
C	-0.365267	-2.983119	-1.634211
C	1.473051	-2.517571	2.333229
C	1.182458	-1.190849	2.662342
C	0.740182	-0.858345	3.926171
C	0.556220	-1.847272	4.914817

C	-1.418658	-3.834652	-1.027948
C	-2.791524	-3.587821	-1.254891
C	-1.018139	-4.871847	-0.181336
C	-3.744926	-4.413072	-0.595395
C	-3.284436	-2.565972	-2.145341
C	-1.950096	-5.661847	0.463694
C	-5.144243	-4.205514	-0.798369
C	-3.316722	-5.451457	0.274120
C	-4.610665	-2.382760	-2.339949
C	-5.594452	-3.184557	-1.671617
C	-6.094357	-5.022161	-0.130716
C	-4.301011	-6.261777	0.937891
C	-6.966183	-2.997284	-1.861143
C	-7.456531	-4.800513	-0.344540
C	-5.622245	-6.057475	0.746986
C	-7.887896	-3.797633	-1.202223
O	3.090253	2.965318	0.942186
O	2.182137	1.013611	-0.793343
O	1.917205	-1.868139	0.115988
O	0.821471	-3.640381	-1.700855
O	2.415739	-3.995009	0.707819
O	-0.494675	-1.844861	-2.024800
C	2.488233	-3.057572	-3.295097
C	4.985352	1.634900	1.451507
C	6.987898	0.271923	1.931303
C	0.864535	-3.184113	4.575402
C	1.317576	-3.502425	3.311994
N	0.097108	-1.520863	6.168403
C	-0.100443	-0.129990	6.522799
C	0.044258	-2.529552	7.204080
H	6.689460	-0.137987	-4.682801
H	5.714958	0.121078	-2.446348
H	7.883355	-2.741876	0.673048
H	3.788878	-3.150139	-5.640509
H	5.738413	-1.784223	-6.287453
H	5.794701	-2.428354	-0.578779
H	8.655246	-1.007826	2.281915

H	1.324381	-0.394255	1.943587
H	0.559413	0.186752	4.137602
H	0.040416	-5.034323	-0.017431
H	-2.564565	-1.948526	-2.662577
H	-1.620722	-6.452704	1.129810
H	-4.956829	-1.620304	-3.032921
H	-3.952466	-7.047662	1.600564
H	-7.304915	-2.216461	-2.535694
H	-8.179711	-5.426457	0.169326
H	-6.355882	-6.676673	1.254201
H	-8.949961	-3.641082	-1.358849
H	2.034551	-3.745142	-4.000264
H	5.297635	2.380308	2.174268
H	7.311620	1.028017	2.640090
H	0.756573	-3.973521	5.307222
H	1.566131	-4.528427	3.062783
H	0.831644	0.448530	6.485081
H	-0.821704	0.351574	5.854874
H	-0.496591	-0.072415	7.536142
H	-0.349765	-2.084680	8.117170
H	-0.619030	-3.355794	6.924993
H	1.032894	-2.951365	7.429970
C	1.741381	2.856784	1.353775
C	0.972477	4.003555	0.969409
C	-0.461197	4.071742	1.169217
C	1.621593	5.096896	0.327491
C	-1.169775	5.211218	0.665408
C	-1.218739	3.054503	1.795039
C	0.939976	6.184223	-0.124056
C	-2.593487	5.285980	0.777847
C	-0.476965	6.274231	0.015679
C	-2.589222	3.127023	1.905653
C	-3.320637	4.230013	1.405072
C	-3.303308	6.408410	0.246337
C	-1.202140	7.373659	-0.484549
C	-4.730277	4.315881	1.490114
C	-4.713221	6.439087	0.340878

C	-2.567877	7.446895	-0.379245
C	-5.402955	5.407984	0.967009
O	1.387165	1.839923	1.931950
H	2.693654	5.043953	0.192451
H	-0.690283	2.197695	2.186952
H	1.469766	7.002227	-0.602753
H	-3.129691	2.331535	2.412399
H	-0.650396	8.177830	-0.963960
H	-5.275087	3.520938	1.990982
H	-5.246604	7.298839	-0.052994
H	-3.105884	8.305328	-0.770243
H	-6.484954	5.462812	1.051228
C	1.954750	2.049378	-1.626738
C	0.485543	2.216883	-1.818384
C	-0.413628	1.212985	-1.423249
C	-1.759963	1.439936	-1.477703
C	-2.265253	2.700015	-1.923880
O	2.796101	2.750930	-2.119799
C	0.009771	3.427529	-2.344068
C	-1.334602	3.681368	-2.390837
N	-3.589082	2.937847	-1.886154
C	-4.213211	4.135556	-2.428021
C	-4.492336	2.008596	-1.210071
H	-0.041276	0.259831	-1.076658
H	-2.434554	0.648395	-1.185691
H	0.727473	4.182205	-2.637526
H	-1.675792	4.656963	-2.703002
H	-3.591378	4.590266	-3.193279
H	-5.162770	3.847802	-2.882134
H	-4.405633	4.856925	-1.625886
H	-4.093759	1.756609	-0.228181
H	-5.451718	2.500280	-1.075430
H	-4.626867	1.098454	-1.802312

Coordinates of (*R*,*R*,*R*)-**7** in the ground state (0 imaginary frequencies)

C	4.165123	-0.122572	-2.979922
C	3.330458	0.060975	-1.910740

C	0.428645	-1.610020	-0.309086
C	2.105959	-1.974115	-2.506371
C	2.288195	-0.860596	-1.637619
C	1.428477	-0.699448	-0.508439
C	4.315181	-0.704296	2.711920
C	3.612172	1.492625	3.415695
C	2.530527	0.408510	1.508518
C	2.997618	-2.141011	-3.596352
C	4.002320	-1.239864	-3.824872
C	1.036224	-2.894563	-2.272043
C	2.631825	1.520870	2.391513
C	1.748599	2.634417	2.236267
C	3.388401	-0.703297	1.704516
C	4.434071	0.408934	3.569519
C	0.839890	2.612907	1.215270
C	0.763668	1.528138	0.317872
C	1.577612	0.436826	0.444691
C	-1.267652	3.630486	1.436716
C	0.067585	2.227374	-1.817114
C	-1.995941	4.897770	1.188654
C	-3.408590	4.964776	1.223175
C	-1.243919	6.051308	0.944636
C	-4.029628	6.229956	1.015238
C	-4.260914	3.821087	1.429632
C	-1.852379	7.274706	0.751472
C	-5.453461	6.348275	1.038600
C	-3.243370	7.389701	0.784393
C	-5.607732	3.940994	1.443632
C	-6.259410	5.204079	1.257118
C	-6.072402	7.610581	0.841478
C	-3.895793	8.654811	0.588113
C	-7.650362	5.336582	1.277554
C	-7.465778	7.701395	0.870635
C	-5.242046	8.760831	0.616213
C	-8.246998	6.574357	1.086783
C	-0.816784	-5.048374	-6.385701
C	-0.541256	-2.773860	-4.787251

C	0.823531	-4.075256	-3.157165
C	-1.389394	-3.866235	-6.768171
C	-1.249813	-2.717697	-5.957726
C	1.373041	-5.282444	-2.810424
C	-0.074906	-5.140968	-5.181432
C	0.069251	-3.983850	-4.366904
C	3.395380	-5.434226	-1.596167
C	0.523380	-6.359005	-4.770344
C	3.937217	-5.278658	-0.221567
C	5.271596	-5.622059	0.099579
C	3.099646	-4.732636	0.755875
C	5.725068	-5.398511	1.431568
C	6.197146	-6.203461	-0.839908
C	3.549413	-4.504515	2.041733
C	7.062241	-5.736604	1.805583
C	4.857610	-4.830750	2.403043
C	7.458409	-6.527314	-0.475383
C	7.944743	-6.306731	0.855089
C	7.518600	-5.503768	3.129962
C	5.346818	-4.603236	3.735813
C	9.248928	-6.632624	1.237218
C	8.829675	-5.842588	3.471541
C	6.613024	-4.922588	4.082078
C	9.686274	-6.402546	2.533367
C	10.553171	4.611662	-3.150912
C	7.173809	3.677679	-4.470750
C	9.551197	4.206753	-4.022516
C	10.251862	4.910872	-1.830379
C	5.898782	3.577704	-4.035561
C	8.228425	4.095193	-3.588752
C	8.940802	4.810829	-1.356746
C	8.591981	5.108894	0.001446
C	5.548517	3.883416	-2.674996
C	7.910836	4.400387	-2.238764
C	4.231822	3.784252	-2.222534
C	7.322224	5.003523	0.454535
C	6.564749	4.294078	-1.770907

C	3.917226	4.084008	-0.911435
C	6.248888	4.589366	-0.413496
C	4.900655	4.477746	0.001236
C	2.058258	6.087730	4.783206
C	4.491048	4.718012	1.408117
C	1.144645	3.845924	4.397016
C	1.270376	4.995050	5.225844
C	2.563128	4.908586	2.763427
C	-0.289010	2.820771	6.060531
C	-0.160174	3.960283	6.885149
C	1.823898	3.817144	3.140634
C	0.345009	2.764083	4.848182
C	0.600275	5.020903	6.474544
C	2.692936	6.052138	3.574850
C	1.233501	-6.434888	-3.606866
C	-0.955532	1.959646	-2.853450
C	-1.161033	2.837635	-3.966885
C	-1.684973	0.795841	-2.759119
C	-2.118124	2.471236	-4.963446
C	-0.469958	4.066106	-4.100510
C	-2.596823	0.431826	-3.752232
C	-2.369591	3.352785	-6.060879
C	-2.817019	1.227672	-4.857983
C	-0.713838	4.883981	-5.170001
C	-1.654733	4.530015	-6.144829
C	-3.383561	2.991442	-7.073402
C	-3.751508	0.819466	-5.924905
C	-4.030160	1.722505	-6.993288
C	-3.725151	3.839939	-8.108326
C	-4.371279	-0.415858	-5.918998
C	-4.968906	1.348697	-7.995561
C	-4.664780	3.476416	-9.087667
C	-5.283631	-0.789199	-6.920013
C	-5.271527	2.252140	-9.041061
C	-5.585961	0.077062	-7.934072
C	-0.299078	-2.200087	1.855139
C	-1.170956	-1.730269	2.955333

C	-1.512080	-2.562328	4.071561
C	-1.622476	-0.430049	2.911974
C	-2.323282	-2.014385	5.113972
C	-1.095425	-3.912424	4.168571
C	-2.382077	0.107932	3.952519
C	-2.716736	-2.840427	6.213266
C	-2.732494	-0.644631	5.055240
C	-1.469217	-4.677367	5.240250
C	-2.274411	-4.146911	6.255398
C	-3.582396	-2.284973	7.274543
C	-3.512945	-0.063458	6.164703
C	-3.938061	-0.904334	7.235432
C	-4.057274	-3.057998	8.316076
C	-3.852033	1.276238	6.194833
C	-4.730910	-0.354232	8.281403
C	-4.852732	-2.517031	9.340105
C	-4.620839	1.819743	7.237643
C	-5.179276	-1.189413	9.331254
C	-5.060063	1.021508	8.257506
H	-1.248798	8.159027	0.574231
O	-1.693873	2.634343	1.973714
O	0.019486	3.705248	0.990577
O	-0.211158	1.546520	-0.663330
O	-0.458505	-1.427855	0.737972
O	2.030596	-5.371033	-1.591284
O	4.017969	-5.579693	-2.620667
O	5.197491	4.744652	2.386990
O	3.137938	4.897805	1.499830
O	1.053534	2.918593	-1.919218
H	4.957222	0.593353	-3.173726
H	3.455467	0.921719	-1.264751
H	4.962890	-1.564338	2.846756
H	3.709461	2.350792	4.069839
H	2.878985	-3.003509	-4.241032
H	4.677838	-1.386569	-4.660973
H	3.298718	-1.560729	1.048260
H	5.181796	0.406604	4.355536

H	-0.164702	5.975361	0.920336
H	-3.799147	2.856028	1.573202
H	10.701913	-6.660043	2.815169
H	-6.226406	3.061549	1.596058
H	-3.274855	9.528201	0.414846
H	-8.261634	4.454813	1.444120
H	-7.934407	8.669323	0.720430
H	-5.723554	9.722493	0.466234
H	-9.328218	6.662069	1.105261
H	-0.920330	-5.937568	-7.000594
H	-0.450846	-1.893090	-4.163106
H	-1.953113	-3.806129	-7.693412
H	-1.710013	-1.784257	-6.264868
H	0.408563	-7.236807	-5.398637
H	2.082881	-4.464987	0.504437
H	5.861689	-6.364815	-1.853527
H	2.875692	-4.061071	2.767526
H	8.135711	-6.965090	-1.202880
H	4.665892	-4.168074	4.460872
H	9.919702	-7.069173	0.503343
H	9.174057	-5.661553	4.485337
H	6.970630	-4.747118	5.092345
H	11.575827	4.693138	-3.504141
H	7.425883	3.445247	-5.501153
H	9.789021	3.971190	-5.055518
H	11.036068	5.225940	-1.148585
H	5.105327	3.265730	-4.707727
H	9.382316	5.424042	0.676504
H	3.443311	3.462806	-2.894830
H	7.090375	5.217830	1.487163
H	2.889373	3.991801	-0.589636
H	2.150626	6.959618	5.423335
H	-0.898342	1.985476	6.389673
H	-0.668109	3.990448	7.843493
H	0.232249	1.891287	4.216022
H	0.703371	5.902484	7.100356
H	3.298416	6.878689	3.223499

H	1.695682	-7.358016	-3.279126
H	-1.542093	0.126189	-1.922016
H	0.257613	4.342984	-3.352258
H	-3.118153	-0.505346	-3.615361
H	-0.175460	5.821175	-5.266313
H	-1.809674	5.207362	-6.974809
H	-3.268986	4.818612	-8.185013
H	-4.156621	-1.129258	-5.133652
H	-4.899683	4.176061	-9.882945
H	-5.747200	-1.769301	-6.877722
H	-5.992192	1.956911	-9.797291
H	-6.296451	-0.197216	-8.707775
O	0.482009	-3.123657	1.878290
H	-1.374784	0.209323	2.075988
H	-0.460181	-4.321767	3.397365
H	-2.678503	1.143380	3.855019
H	-1.136188	-5.707963	5.309698
H	-2.539327	-4.788949	7.085559
H	-3.823235	-4.113826	8.363434
H	-3.523991	1.941459	5.406476
H	-5.201009	-3.163303	10.138939
H	-4.865524	2.876466	7.220933
H	-5.786333	-0.758529	10.121329
H	-5.662439	1.428944	9.063606
C	-2.050976	-3.280918	-1.252514
C	-3.027650	-4.228303	-0.662746
C	-4.311601	-4.417622	-1.221607
C	-2.663689	-4.901090	0.507185
C	-5.216528	-5.291189	-0.554672
C	-4.747412	-3.800480	-2.448371
C	-3.550782	-5.735983	1.156948
C	-6.524672	-5.515232	-1.083689
C	-4.833011	-5.945167	0.646306
C	-5.984220	-4.023735	-2.946513
C	-6.925302	-4.879715	-2.284822
C	-7.432398	-6.375323	-0.411775
C	-5.772774	-6.808994	1.306526

C	-8.208734	-5.108597	-2.787832
C	-8.706611	-6.576921	-0.946726
C	-7.009649	-7.013705	0.803966
C	-9.090469	-5.948967	-2.123885
O	-2.292036	-2.331357	-1.960664
H	-1.671699	-4.747223	0.912287
H	-4.057615	-3.151891	-2.967782
H	-3.254790	-6.228521	2.077506
H	-6.288264	-3.548943	-3.874898
H	-5.460507	-7.295985	2.225022
H	-8.509653	-4.618564	-3.708884
H	-9.398298	-7.234283	-0.428580
H	-7.710666	-7.668999	1.312166
H	-10.084089	-6.116587	-2.526060
C	0.224583	-2.691606	-1.191276
O	-0.777586	-3.592627	-0.876154

Coordinates of (*R*,*R*,*R*)-**7** in the excited state (0 imaginary frequencies)

C	-0.960243	-1.893671	-7.784495
C	-0.753904	-0.564069	-5.335476
C	1.107714	-2.077661	-4.663092
C	-1.788676	-0.842333	-7.500947
C	-1.684831	-0.174757	-6.260847
C	1.899725	-3.151655	-4.978878
C	0.012382	-2.325626	-6.848647
C	0.123140	-1.646895	-5.603386
C	4.112744	-3.373473	-4.166145
C	0.871896	-3.419892	-7.122340
C	4.857490	-3.688596	-2.920341
C	6.263769	-3.843457	-2.908913
C	4.132735	-3.783005	-1.728094
C	6.905570	-4.097326	-1.662640
C	7.086151	-3.777278	-4.090600
C	4.761990	-4.015376	-0.520726
C	8.323011	-4.268557	-1.602005
C	6.147228	-4.176668	-0.463797
C	8.425996	-3.948080	-4.025147

C	9.100042	-4.196948	-2.784557
C	8.964885	-4.510441	-0.358618
C	6.823282	-4.419996	0.781575
C	10.485024	-4.367796	-2.708180
C	10.351340	-4.674619	-0.324855
C	8.164012	-4.578058	0.832401
C	11.103849	-4.604510	-1.489500
C	9.203672	7.439226	-1.468007
C	5.849703	6.465425	-2.823609
C	8.158668	7.230471	-2.357974
C	9.056200	7.112616	-0.127975
C	4.681676	5.947078	-2.385122
C	6.945746	6.692385	-1.922574
C	7.858827	6.570871	0.347555
C	7.670955	6.217887	1.724335
C	4.490539	5.601576	-1.002507
C	6.785588	6.356279	-0.552192
C	3.284251	5.069843	-0.544309
C	6.511928	5.687356	2.175820
C	5.553919	5.804654	-0.082181
C	3.122632	4.743892	0.788236
C	5.398814	5.455757	1.290202
C	4.158730	4.919785	1.710344
C	1.793576	3.744734	6.879334
C	3.929249	4.474935	3.108930
C	1.273491	1.727400	5.587205
C	1.298369	2.416852	6.831043
C	2.214182	3.674869	4.525378
C	0.315565	-0.204572	6.692771
C	0.345043	0.478560	7.928805
C	1.757609	2.386727	4.416760
C	0.765581	0.403284	5.551301
C	0.823224	1.758835	7.993112
C	2.242122	4.368092	5.750348
C	1.797094	-3.832995	-6.207024
O	2.776564	-3.614658	-4.007729
O	4.557891	-2.942956	-5.202934

O	4.761053	4.234687	3.950744
O	2.593911	4.330138	3.361559
C	3.909325	1.932885	-2.962611
C	3.225701	1.476810	-1.867656
C	0.845474	-1.229131	-0.983075
C	2.210047	-0.288781	-3.225390
C	2.370109	0.350711	-1.963363
C	1.675338	-0.155058	-0.822733
C	4.980192	-0.817001	1.919323
C	2.859640	0.241706	1.416369
C	2.944074	0.200587	-4.335550
C	3.774417	1.281351	-4.205905
C	0.637056	-1.821076	-2.245380
C	2.878319	0.881819	2.688868
C	3.929363	-0.618481	1.064126
C	5.013676	-0.161092	3.166738
C	0.753761	1.897171	2.209441
C	0.766707	1.316396	0.919073
C	1.774951	0.485867	0.519092
C	-1.548009	2.157741	2.596059
C	-1.565192	-2.612679	-2.295754
C	-2.391466	-3.838304	-2.412024
C	-3.763741	-3.841504	-2.068203
C	-1.789985	-4.996333	-2.912339
C	-4.506582	-5.040366	-2.265612
C	-4.452463	-2.708032	-1.502010
C	-2.516483	-6.154554	-3.102455
C	-5.897569	-5.090980	-1.940963
C	-3.876588	-6.199580	-2.791302
C	-5.767679	-2.766356	-1.192527
C	-6.546650	-3.950890	-1.406184
C	-6.640284	-6.282672	-2.149630
C	-4.652137	-7.392808	-2.990567
C	-7.907471	-4.016740	-1.096139
C	-7.999294	-6.307184	-1.828398
C	-5.967535	-7.432722	-2.686881
C	-8.626666	-5.184163	-1.306624

O	-1.681936	0.983764	2.848634
O	-0.307329	2.731214	2.508300
O	-0.327754	1.507419	0.107347
O	0.127734	-1.714164	0.095586
O	-0.230609	-2.899473	-2.325486
O	-1.966674	-1.476453	-2.205449
C	1.303870	-1.388266	-3.356168
C	1.781112	1.711518	3.088298
C	3.988127	0.664672	3.543387
C	0.627230	-2.818164	0.731835
O	1.573569	-3.427195	0.290824
C	-0.120269	-3.096130	1.979835
C	-0.093020	-4.377294	2.620621
C	-0.817682	-2.059905	2.557831
C	-0.792589	-4.542440	3.856895
C	0.580444	-5.489879	2.061013
C	-1.476598	-2.222732	3.778179
C	-0.806618	-5.821903	4.495722
C	-1.471595	-3.430064	4.447404
C	0.563611	-6.700568	2.698224
C	-0.122324	-6.865929	3.907600
C	-1.548797	-6.001752	5.761076
C	-2.147684	-3.590243	5.749766
C	-2.184577	-4.876728	6.365068
C	-1.645238	-7.228062	6.389468
C	-2.753498	-2.527352	6.393072
C	-2.868198	-5.038197	7.602990
C	-2.330438	-7.388281	7.605469
C	-3.416431	-2.687546	7.621326
C	-2.926999	-6.315582	8.207555
C	-3.480062	-3.918344	8.213769
C	-0.564160	2.768067	-0.407076
O	0.239824	3.665502	-0.252977
C	-2.616053	3.146785	2.317503
C	-3.920285	2.746199	1.929686
C	-2.292125	4.505034	2.392205
C	-4.861484	3.758877	1.585141

C	-4.334980	1.374364	1.811639
C	-3.222644	5.479691	2.097232
C	-6.161761	3.404969	1.112582
C	-4.511741	5.132362	1.680354
C	-5.572658	1.048024	1.367613
C	-6.527992	2.041955	0.987695
C	-7.089558	4.413598	0.741599
C	-5.474406	6.130052	1.319552
C	-7.792705	1.712119	0.488424
C	-8.346633	4.041251	0.251343
C	-6.704921	5.787519	0.869351
C	-8.692024	2.704261	0.123424
C	-1.859304	2.804899	-1.084892
C	-2.517923	4.033728	-1.419644
C	-2.471047	1.583151	-1.422764
C	-3.828290	3.980605	-2.008537
C	-1.945921	5.292852	-1.165950
C	-3.709120	1.541754	-2.006272
C	-4.507053	5.191504	-2.325980
C	-4.448339	2.725607	-2.270771
C	-2.623887	6.468699	-1.480174
C	-3.877457	6.428001	-2.044258
C	-5.820509	5.143348	-2.927448
C	-5.783114	2.673928	-2.795504
C	-6.448579	3.885286	-3.138234
C	-6.510030	6.314769	-3.309108
C	-6.472015	1.452367	-2.980070
C	-7.761734	3.835201	-3.700294
C	-7.776367	6.255910	-3.868578
C	-7.751090	1.418120	-3.516815
C	-8.402297	5.036086	-4.060620
C	-8.394354	2.585861	-3.881929
H	-1.035725	-2.416645	-8.733323
H	-0.691942	-0.058860	-4.378642
H	-2.530299	-0.521022	-8.224905
H	-2.351607	0.651479	-6.037453
H	0.782093	-3.929772	-8.076550

H	3.059319	-3.655328	-1.738375
H	6.605935	-3.573978	-5.036196
H	4.166446	-4.063766	0.384948
H	9.022732	-3.893983	-4.931049
H	6.222723	-4.476471	1.684282
H	11.074112	-4.311472	-3.618629
H	10.837488	-4.858260	0.628609
H	8.663284	-4.762453	1.778989
H	12.180183	-4.734318	-1.445660
H	10.139588	7.858182	-1.822717
H	5.981561	6.723487	-3.870211
H	8.276466	7.484670	-3.407112
H	9.874446	7.274220	0.567347
H	3.855937	5.781009	-3.070162
H	8.494332	6.383309	2.413062
H	2.463148	4.898553	-1.232633
H	6.403181	5.413709	3.214777
H	2.177287	4.329355	1.109347
H	1.811468	4.262432	7.833405
H	-0.069293	-1.218057	6.648252
H	-0.014370	-0.016433	8.825052
H	0.729158	-0.122027	4.604235
H	0.847492	2.293214	8.938328
H	2.622247	5.382265	5.770174
H	2.458530	-4.668561	-6.400659
H	4.559422	2.796903	-2.870822
H	3.328640	1.979409	-0.913236
H	5.791646	-1.477645	1.631526
H	2.846469	-0.302239	-5.290243
H	4.331512	1.638879	-5.065452
H	3.903678	-1.124110	0.105938
H	5.857023	-0.310782	3.832568
H	-0.738035	-4.969645	-3.165136
H	-3.890952	-1.803868	-1.322196
H	-2.032059	-7.039644	-3.502054
H	-6.259599	-1.898025	-0.762339
H	-4.150170	-8.266628	-3.394074

H	-8.397911	-3.139831	-0.684119
H	-8.563190	-7.220702	-1.991102
H	-6.543069	-8.340255	-2.842379
H	-9.682755	-5.220742	-1.060814
H	4.019305	1.174260	4.499030
H	-0.847347	-1.088641	2.084173
H	1.114273	-5.365485	1.130777
H	-1.985798	-1.355922	4.177486
H	1.086166	-7.546409	2.263468
H	-0.102879	-7.841596	4.375845
H	-1.187990	-8.104789	5.949099
H	-2.724511	-1.536818	5.957884
H	-2.377883	-8.371356	8.062080
H	-3.879361	-1.825946	8.090643
H	-3.453740	-6.425836	9.150321
H	-3.995628	-4.055399	9.159331
H	-1.286841	4.786378	2.677066
H	-3.632588	0.601286	2.083179
H	-2.951869	6.528036	2.169202
H	-5.855348	0.002156	1.285508
H	-5.187670	7.173255	1.407077
H	-8.065424	0.665472	0.392754
H	-9.048914	4.816569	-0.039296
H	-7.422172	6.552257	0.586973
H	-9.666396	2.433315	-0.268819
H	-1.948496	0.655323	-1.239189
H	-0.959322	5.333451	-0.728315
H	-4.104230	0.573994	-2.284938
H	-2.154119	7.424756	-1.273993
H	-4.380435	7.358513	-2.269337
H	-6.049797	7.284736	-3.178360
H	-6.002425	0.519142	-2.697829
H	-8.277908	7.173864	-4.156997
H	-8.246713	0.461916	-3.650498
H	-9.396292	4.990925	-4.495038
H	-9.391233	2.558864	-4.310552

Coordinates of **2'** (Figure S17a) (0 imaginary frequencies)

C	8.375453	-2.906147	-1.003324
C	7.042362	-3.134078	-1.215541
C	3.770249	-1.543466	-0.461333
C	6.493767	-1.067011	-0.030793
C	6.067717	-2.224177	-0.736895
C	7.880115	-0.858576	0.172986
C	8.799028	-1.755599	-0.301433
C	4.195669	-0.382627	0.228612
C	2.531777	1.248934	-0.121770
C	1.451747	1.982112	0.584733
C	0.841767	3.127849	0.023362
C	1.026583	1.495752	1.824980
C	-0.199453	3.766154	0.756227
C	1.228993	3.702437	-1.240555
C	0.005955	2.110635	2.522105
C	-0.836734	4.934587	0.236308
C	-0.619570	3.248803	2.010257
C	0.623691	4.811416	-1.722565
C	-0.431696	5.471028	-1.010732
C	-1.878704	5.567667	0.963644
C	-1.678663	3.907810	2.723810
C	-1.064376	6.614990	-1.504646
C	-2.486095	6.708848	0.435177
C	-2.278046	5.011334	2.226551
C	-2.081885	7.227358	-0.787602
O	2.423763	-1.723767	-0.718726
O	3.249574	0.478993	0.753210
O	2.788229	1.274687	-1.300577
C	5.519669	-0.151665	0.443255
C	1.608712	-2.036439	0.336662
O	2.055453	-2.278442	1.430909
C	0.183214	-2.008272	-0.073745
C	-0.837016	-2.683929	0.671524
C	-0.159172	-1.284278	-1.193846
C	-2.192261	-2.590727	0.224853
C	-0.547174	-3.457929	1.821686

C	-1.488893	-1.174655	-1.604600
C	-3.219376	-3.294339	0.928938
C	-2.513610	-1.796267	-0.919878
C	-1.550534	-4.104393	2.490385
C	-2.876836	-4.023998	2.048673
C	-4.614613	-3.230591	0.446748
C	-3.919978	-1.655777	-1.344943
C	-4.932356	-2.395348	-0.664700
C	-5.631935	-3.951186	1.041420
C	-4.289347	-0.830353	-2.389361
C	-6.282548	-2.296293	-1.103642
C	-6.962053	-3.863913	0.597467
C	-5.624608	-0.722807	-2.811295
C	-7.287020	-3.047699	-0.450015
C	-6.603220	-1.446536	-2.188049
H	9.113106	-3.610093	-1.374135
H	6.712436	-4.017366	-1.753898
H	8.201306	0.027256	0.712448
H	9.858337	-1.585596	-0.139778
H	1.499472	0.609839	2.229456
H	2.012530	3.218475	-1.804505
H	-0.317797	1.708203	3.476512
H	0.935507	5.225392	-2.677016
H	-1.985862	3.493360	3.678902
H	-0.748554	7.021097	-2.460865
H	-3.283042	7.189238	0.994770
H	-3.076862	5.500782	2.775586
H	-2.563911	8.115032	-1.183609
H	5.821142	0.740250	0.981368
H	0.613569	-0.772763	-1.753841
H	0.473366	-3.517148	2.169009
H	-1.694676	-0.582370	-2.486020
H	-1.319269	-4.689834	3.374274
H	-3.635706	-4.550852	2.612687
H	-5.420140	-4.610015	1.873778
H	-3.546302	-0.238258	-2.907788
H	-7.727611	-4.448180	1.097094

H	-5.869457	-0.063231	-3.637018
H	-8.312327	-2.965941	-0.797033
H	-7.637558	-1.377706	-2.510490
C	4.679848	-2.437888	-0.935813
H	4.330906	-3.315854	-1.468137

Coordinates of **2'** (Figure S17b) (0 imaginary frequencies)

C	8.669784	-2.216295	0.078063
C	7.354745	-2.567085	-0.066920
C	4.038073	-0.941800	-0.470974
C	6.729480	-0.206972	-0.168759
C	6.349898	-1.575539	-0.193993
C	8.098290	0.125769	-0.017248
C	9.046016	-0.854456	0.103494
C	4.418203	0.424062	-0.435999
C	2.498321	1.577002	0.305832
C	1.529001	2.628562	-0.099789
C	0.293117	2.802055	0.569106
C	1.867139	3.465149	-1.168631
C	-0.577065	3.839889	0.123262
C	-0.150444	1.973728	1.662463
C	1.025806	4.475539	-1.586947
C	-1.840386	4.046613	0.758829
C	-0.202470	4.682731	-0.956448
C	-1.350341	2.173414	2.253147
C	-2.241272	3.214356	1.832627
C	-2.704515	5.084256	0.320048
C	-1.094845	5.726489	-1.379156
C	-3.480268	3.428072	2.442501
C	-3.934100	5.266364	0.957076
C	-2.285758	5.918658	-0.771383
C	-4.317903	4.445153	2.008449
O	2.700049	-1.175201	-0.704545
O	3.465065	1.406852	-0.646832
O	2.492839	0.927414	1.322032
C	5.723908	0.783430	-0.294766
C	1.997636	-2.069246	0.061166

O	2.543637	-2.812229	0.837357
C	0.542000	-1.973766	-0.222482
C	-0.395935	-2.948915	0.256751
C	0.082110	-0.901383	-0.954545
C	-1.785349	-2.772364	-0.037494
C	0.001258	-4.088939	0.998316
C	-1.277861	-0.720210	-1.208166
C	-2.731874	-3.758374	0.384630
C	-2.224437	-1.613238	-0.749637
C	-0.927753	-5.001620	1.418248
C	-2.284403	-4.840510	1.113647
C	-4.158589	-3.604570	0.032577
C	-3.664679	-1.392914	-0.981242
C	-4.593479	-2.410723	-0.614312
C	-5.096217	-4.578049	0.317328
C	-4.144455	-0.228923	-1.549944
C	-5.976135	-2.228955	-0.897055
C	-6.458311	-4.407038	0.017583
C	-5.512383	-0.042494	-1.808733
C	-6.896136	-3.252082	-0.568823
C	-6.411468	-1.026020	-1.500892
H	9.429778	-2.984493	0.175426
H	7.060649	-3.612003	-0.084578
H	8.382171	1.173657	0.003310
H	10.091464	-0.588742	0.220419
H	2.813849	3.312814	-1.669232
H	0.503346	1.186949	2.006365
H	1.315541	5.116952	-2.413134
H	-1.660820	1.531780	3.072327
H	-0.785356	6.360144	-2.204481
H	-3.781207	2.785064	3.263896
H	-4.590498	6.062495	0.618827
H	-2.951726	6.711173	-1.099392
H	-5.276635	4.599407	2.492246
H	5.984840	1.835998	-0.281568
H	0.787614	-0.176100	-1.335954
H	1.045398	-4.217950	1.237058

H	-1.571670	0.150243	-1.779292
H	-0.611025	-5.865490	1.993515
H	-2.981921	-5.587769	1.469765
H	-4.793790	-5.507836	0.781986
H	-3.466272	0.575752	-1.803369
H	-7.158580	-5.199012	0.261537
H	-5.846016	0.886677	-2.258328
H	-7.947627	-3.104262	-0.794473
H	-7.469567	-0.897447	-1.707142
C	4.983496	-1.919329	-0.353985
H	4.688659	-2.959575	-0.370748

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