Supporting Information for

Orbital Control of Photochemical Rearrangement of 4-Aryl-1,1-dicyano-1-butenes through the Hyperconjugative Substitution on the Linker Chain

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General Experimental Details

^{1}H-NMR (400 MHz) and ^{13}C-NMR (100 MHz) spectra were obtained in chloroform-*d* on JEOL JNM-ECS-400 and chemical shifts are reported in ppm relative to Me_4Si (0 ppm for ^{1}H) or residual solvent peak (77.16 ppm for ^{13}C), unless otherwise stated. Coupling constants (*J* values) are reported in Hz. Electronic absorption (UV-vis) and fluorescence (FL) spectra were measured in a conventional quartz cell (light path 1 cm) fitted with a temperature controller. The spectroscopic grade solvents were used as obtained for the spectroscopic studies. UV-vis spectra were recorded on JASCO V-670 spectrometer under the following conditions: bandwidth, 1 nm; scan rate, 100 nm min^{-1}; response, medium. Fluorescence spectra were recorded on a JASCO FP-8500 spectrometer under the following conditions: excitation bandwidth, 1 nm; emission bandwidth, 10 nm; scan rate, 100 nm min^{-1}; response, high. Fluorescence lifetime measurements were performed on a Hamamatsu C11367 employing a picosecond light emitting diode (λ_{ex} = 280 nm) as excitation source with the decay profiles being monitored at fluorescence peak maxima.

Analytical scale photoreactions were performed as follows. Sample solutions of 4-substituted-4-aryl-1,1-dicyano-2-methyl-1-butenes of an appropriate concentration were irradiated under nitrogen atmosphere with a 300-W xenon lamp (Asahi Spectra, MAX-301) through the UV mirror module and the appropriate band-path filter (HQBP254-UV, 280-UV, 300-UV, or 330-UV). Temperature was controlled with cryostat (Unisoku, CoolSpeK UV/CD USP-203-B). The yields of photoproducts were determined by HPLC with calibration (conditions: column, Kanto Mightysil, 4.6 mm × 250 mm; eluent, *n*-hexane : ethyl acetate = 95 : 5 or 97 : 3; flow rate, 2.0 mL min^{-1}; temperature, 35 °C; detector, UV-vis detectors: λ_{mon} = 275 nm).

All calculations were performed on Linux-PCs by using Gaussian 09[S1] and Turbomole 6.1 or later program suite.[S2] Geometries were fully optimized at the dispersion-corrected density functional theory (3rd generation, DFT-D3 with BJ dumping), with AO basis-set of valence triple-ξ quality (in standard notation: H, [3s1p]; C/N/B/F/O, [5s3p2d1f]) at the TPSS-D3/def2-TZVP level.[S3] The resolution of identity (RI) approximation was employed and the corresponding auxiliary basis-sets were taken from the Turbomole basis-set library. The numerical quadrature grid m5 was employed and the convergence criterion for the optimization regarding the change of total energy between two subsequent optimization cycles was set to 10^{-7} E_h. The Natural Bond Orbital analysis was performed at the CAM-B3LYP/def2-TZVP level using NBO version 3.1 implemented in Gaussian package.

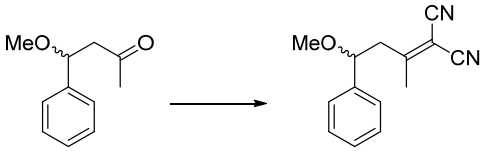
(S1) Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

(S2) Turbomole V6.1 2009, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, Turbomole GmbH, since 2007; available from http://www.turbomole.com.

(S3) (a) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104/1-18. (b) Grimme, S.; Ehrlich, S.; Goerigk, L. *J. Comput. Chem.* **2011**, *32*, 1456-1465. (c) Tao, J.; Perdew, J. P.; Staroverov, V. N.; Scuseria, G. E. *Phys. Rev. Lett.* **2003**, *91*, 146401/1-4.

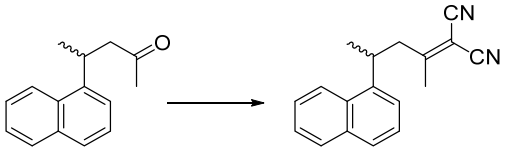
Preparation of 4-substituted-4-aryl-1,1-dicyano-2-methyl-1-butenes

1,1-Dicyano-2-methyl-4-methoxy-4-phenyl-1-butene (1c)



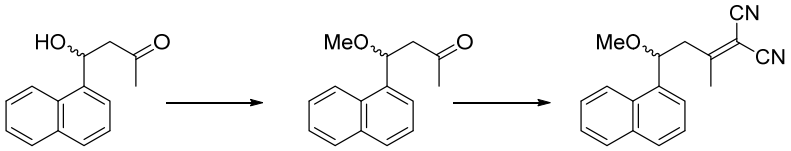
According to the literature procedures for the synthesis of similar molecule,[S4] 4-methoxy-4-phenylbutane-2-one[S5] (0.46 g, 2.6 mmol) was dissolved in a mixture of toluene and tetrahydrofuran (7.1 mL, ca. 13 : 1). To this solution was added malononitrile (0.17 g, 2.6 mmol, 1.0 eq), sodium sulfate (0.40 g), and sodium acetate (0.08 g), and the resulting mixture was stirred for 43 h at 50 °C. The crude product obtained after evaporation was purified by silica-gel column chromatography with *n*-hexane-ethyl acetate (19 : 1) as eluent to give 0.09 g (15%) of desired product as colorless oil. ^{1}H NMR: 2.34 (3H, s), 2.82 (1H, dd, J = 13.5, 4.3 Hz), 3.00 (1H, dd, J = 13.4, 9.2 Hz), 3.20 (3H, s), 4.42 (1H, dd, J = 9.2, 4.3 Hz), and 7.42-7.31 (5H, m). ^{13}C NMR: 23.9, 46.3, 56.9, 81.7, 87.5, 111.7, 111.9, 126.3, 128.7, 128.9, 139.4, and 179.4. HRMS (FAB): *m/z* = 225.1026. $C_{14}H_{13}N_2O$ requires 225.1033.

1,1-Dicyano-2-methyl-4-methyl-4-(1-naphthyl) -1-butene (2b)



According to the literature procedures for the synthesis of phenyl analog,[S6] 4-(1-naphthyl)-pentan-2-one (2.2 g, 10 mmol),[S7] malononitrile (2.0 g, 30 mmol, 10 eq), and sodium acetate (0.27 g, 3.3 mmol, 33 mol%) was dissolved in a mixture of acetic acid (0.61 mL) and toluene (23 mL). The resulting mixture was refluxed for 5 h under nitrogen atmosphere. The crude mixture was cooled down and quenched by an addition of water (50 mL), and then extracted with chloroform (3 × 50 mL). The combined crude material was purified by silica-gel column chromatography with *n*-hexane-ethyl acetate (97 : 3) as eluent to give 1.8 g (67%) of desired product as colorless crystals. M.p. 84-85 °C. ^{1}H NMR: 1.49 (3H, d, J = 6.8 Hz), 2.17 (3H, s), 3.01 (1H, dd, J = 13.5, 7.7 Hz), 3.10 (1H, dd, J = 13.5, 7.6 Hz), 4.06 (1H, sext, J = 7.3 Hz), 7.44 (1H, dd, J = 7.4, 1.2 Hz), 7.48-7.54 (2H, m), 7.57 (1H, td, J = 7.6, 1.6 Hz), 7.78 (1H, d, J = 7.9 Hz), 7.90 (1H, br d, J = 8.0 Hz), and 8.06 (1H, d, J = 8.4 Hz). ^{13}C NMR: 21.7, 22.9, 32.7, 45.7, 87.4, 111.8, 112.1, 122.0, 123.1, 125.8, 125.9, 126.6, 127.8, 129.5, 130.9, 134.1, 139.7, and 180.6. HRMS (EI): *m/z* = 260.1311. $C_{18}H_{16}N_2$ requires 260.1313.

1,1-Dicyano-2-methyl-4-methoxy-4-(1-naphthyl) -1-butene (2c)



A typical methylation procedure was used as described in literature.[S8] Thus, in diethyl ether solution of 4-hydroxy-4-(1-naphthyl)-butane-2-one[S9] (4.5 g, 21 mmol in 17 mL), silver oxide (3.7 g, 16 mmol) and iodomethane (1.54 mL, 21 mmol) were added. The resultant mixture was refluxed for 72 h. After filtration, the crude product was purified by silica-gel column chromatography with *n*-hexane-ethyl acetate (97 : 3) as eluent to give 1.7 g (25%) of 4-methoxy-4-(1-naphthyl)-butane-2-one as colorless oil. ^{1}H NMR: 2.21 (3H, s). 2.74 (1H, dd, J = 16.5, 3.2 Hz), 3.09 (1H, dd, J = 16.4, 9.6 Hz), 3.30 (3H, s), 5.45 (1H, dd, J = 9.6, 3.2 Hz), 7.46-7.54 (3H, m), 7.59 (1H, d, J = 6.6 Hz), 7.79 (1H, d, J = 8.2 Hz), 7.87-7.89 (1H, m), 8.13-8.15 (1H, m) ^{13}C NMR: 31.1, 51.3, 57.2, 77.3, 123.0, 124.8, 125.5, 125.7, 126.2, 128.2, 129.0, 130.6, 134.0, 136.5, 206.7. HRMS (FAB): *m/z* = 228.1153. $C_{15}H_{16}O_2$ requires 228.1150. Then, this ketone was converted to dicyanoethene according to the literature procedure.[S4] Thus, 4-methoxy-4-(1-naphthyl)-butane-2-one (1.21 g, 5.3 mmol),

(S4) Manimekalai, A.; Anusuya, J. *Indian J. Chem.* **2005**, *44B*, 2087-2092.
(S5) Keck, G. E.; Wager, C. A. *Org. Lett.* **2000**, *2*, 2307-2309.
(S6) Goudie, A. C.; Gaster, L. M.; Lake, A. W.; Rose, C. J.; Freeman, P. C.; Hughes, B. O.; Miller, D. *J. Med. Chem.* **1978**, *21*, 1260-1264.
(S7) Umeda, R.; Takahashi, Y.; Nishiyama, Y. *Tetrahedron Lett.* **2015**, *55*, 6113-6116.
(S8) Kenyon, J.; Phillips, H.; Shutt, G. R. *J. Chem. Soc.* **1935**, 1663-1668.
(S9) Kawamura, Y.; Nagasawa, T.; Nakai, H. *J. Chem. Phys.* **2001**, *114*, 8357-8363.

malononitrile (2.4 g, 40 mmol, 7.5 eq), and sodium acetate (0.24 g, 3.0 mmol, 57 mol%) was dissolved in toluene (22 mL) containing sodium sulfate (1.2 g, 8.4 mmol) and molecular sieves 4A (1.0 g). The resulting mixture was stirred at 80 °C for 120 h. The crude mixture was concentrated *in vacuo* and was purified by silica-gel column chromatography with *n*-hexane-ethyl acetate (97 : 3) as eluent to give 1.1 g (75%) of desired product as pale yellow crystals. The analytical sample was obtained by recrystallization from toluene. M.p. 115-116 °C. ^{1}H NMR: 2.40 (3H, s). 3.02 (1H, dd, *J* = 13.5, 4.0 Hz), 3.18 (1H, dd, *J* = 13.5, 9.5 Hz), 3.28 (3H, s), 5.16 (1H, dd, *J* = 9.6, 4.0 Hz), 7.48-7.60 (4H, m), 7.85 (1H, d, *J* = 8.5 Hz), 7.91 (1H, d, *J* = 8.0 Hz), and 8.22 (1H, d, *J* = 8.0 Hz). ^{13}C NMR: 24.1, 45.3, 57.1, 79.8, 87.4, 111.9, 112.0, 122.5, 124.4, 125.5, 126.0, 126.7, 129.1, 129.2, 130.5, 134.0, 134.8, 179.6. HRMS (FAB): *m/z* = 276.1264. $C_{18}H_{16}N_2O$ requires 276.1263.

Preparative photolysis of 4-substituted-4-aryl-1,1-dicyano-2-methyl-1-butenes

Photoreaction of 1c

In a donut-shaped cylindrical Quartz vessel, **1c** (0.29 g, 1.3 mmol) was dissolved in acetonitrile (350 mL, 3.6 mM) and was irradiated under nitrogen atmosphere with medium pressure mercury lamp for 3 h. The resultant photolyte was quenched with aqueous sodium hydrogen carbonate, extracted with dichloromethane, and the combined organic phase was concentrated *in vacuo*. By silica-gel column chromatography with chloroform as eluent, rearrangement product was obtained as a colorless oil almost exclusively (0.21 g, 73%), together with a minor amount of by-product (0.01 g, 1%) in which solvent molecule was inserted. The cyclization product was not detected. **3,3-Dicyano-4-methoxy-2-methyl-4-phenyl-1-pentene**. ^{1}H NMR: 1.88 (3H, dd, *J* = 1.4, 0.7 Hz), 3.38 (3H, s), 4.54 (1H, s), 5.26 (1H, br s), 5.33 (1H, br s), and 7.38-7.46 (5H, m). ^{13}C NMR: 19.8, 51.0, 58.1, 84.3, 112.8, 113.7, 128.1, 128.7, 130.1, 132.8, and 133.5. HRMS (FAB): *m/z* = 249.1006. $C_{14}H_{14}N_2O$+Na requires 249.0999. **3-Aza-1,1-dicyano-2,4-dimethyl-6-methoxy-6-phenyl-1,3-hexadiene.** ^{1}H NMR: 2.09 (3H, s), 2.23 (3H, s), 2.61 (1H, dd, *J* = 14.6, 4.2 Hz), 2.71 (1H, dd, *J* = 14.6, 9.1 Hz), 3.21 (1H, s), 4.51 (1H, dd, *J* = 9.1, 4.2 Hz), and 7.30-7.40 (5H, m). ^{13}C NMR: 21.2, 23.8, 47.7, 56.8, 66.0, 80.7, 112.2, 113.2, 126.5, 128.3, 128.8, 169.8, and 178.5. HRMS (FAB): *m/z* = 290.1266. $C_{16}H_{17}N_3O$+Na requires 290.1264.

Photoreaction of 2b

In a donut-shaped cylindrical Pyrex vessel, **2b** (100 mg, 0.4 mmol) was dissolved in acetonitrile (350 mL, 1.1 mM) and was irradiated under nitrogen atmosphere with high pressure mercury lamp for 3 h. The photolyze was concentrated *in vacuo* and was treated with a short silica-gel column chromatography with *n*-hexane-ethyl acetate (97 : 3) as eluent. The crude product mixtures were separated with normal phase HPLC with *n*-hexane-ethyl acetate (95 : 5) as eluent to give rearrangement product (11 mg, 11%) and an isomer mixture of [2+2]cyclization products (10 mg, 10%). From the latter, one of the isomers was obtained in a pure form by repeated chromatography, which turned out to be the all-*anti* isomer (5 mg, 5%). A minor amount of 1-methyl-3-dicyanomethyl-3-methyl-1*H*-2,3-dihydrophenalene was also isolated (1 mg, 1%). **3,3-Dicyano-2,4-dimethyl-4-(1-naphthyl)-1-butene**. M.p. 88-89 °C. ^{1}H NMR: 1.71 (3H, d, *J* = 7.0 Hz), 1.90 (3H, dd, *J* = 1.4, 0.7 Hz), 4.44 (1H, q, *J* = 7.0 Hz), 5.21 (1H, br s), 5.51 (1H, br s), 7.50-7.59 (3H, m), 7.84 (1H, d, *J* = 6.5 Hz), 7.86 (1H, d, *J* = 8.0 Hz), 7.90 (1H, br d, *J* = 7.8 Hz), and 8.04 (1H, d, J = 8.5 Hz). ^{13}C NMR: 18.1, 19.0, 38.2, 50.3, 113.9, 114.4, 119.6, 122.0, 124.9, 125.4, 125.9, 126.5, 129.1, 129.3, 131.5, 133.9, 133.9, and 134.7. HRMS (EI): *m/z* = 260.1311. $C_{18}H_{16}N_2$ requires 260.1313. **(*ttt*)-10,10-Dicyano-2,3,9,9*a*-tetrahydro-1,3-dimethyl-1,9-methano-1*H*-phenalene**. M.p. = 118-119 °C. ^{1}H NMR: 1.42 (3H, d, *J* = 6.8 Hz), 1.65 (1H, t, *J* = 12.4 Hz), 1.77-1.81 (4H, m), 2.48-2.57 (1H, m), 2.98 (1H, d, *J* = 9.8 Hz), 3.82 (1H, dd, *J* = 9.8, 5.9 Hz) 5.75 (1H, dd, *J* = 9.8, 5.8 Hz), 6.78 (1H, d, *J* = 9.7 Hz), 6.99 (1H, d, *J* = 7.4 Hz) 7.18 (1H, d, *J* = 7.9 Hz), and 7.25 (1H, t, *J* = 7.6 Hz). ^{13}C NMR: 17.1, 25.1, 32.1, 38.5, 40.0, 43.3, 43.9, 47.6, 112.9, 114.0, 118.2, 123.5, 125.4, 127.8, 129.4, 131.0, 134.2, and 144.3. HRMS (EI): *m/z* = 260.1315. $C_{18}H_{16}N_2$ requires 260.1313. Among the remaining isomers, the following isomer was isolated, albeit in low amount. This was tentatively assigned as (ccc)-isomer, judged from the ^{1}H NMR data. ^{1}H NMR: 1.11 (3H, d, *J* = 6.8 Hz), 1.26 (3H, s), 2.37 (1H, dd, *J* = 13.5, 10.6 Hz), 2.47 (1H, dd, *J* = 13.4, 9.3 Hz), 3.07 (1H, tq, *J* = 10.0, 6.8 Hz) 4.28 (1H, br d, *J* = 5.4 Hz), 5.79 (1H, dd, *J* = 9.8, 5.5 Hz), 6.64 (1H, d, *J* = 9.8 Hz), 7.07 (1H, br d, *J* = 7.3 H), 7.12 (1H, d, *J* = 7.2 Hz), 7.20 (1H, br t, *J* = 7.4 Hz), and 7.26 (1H, br t, *J* = 7.4 Hz). **1-Methyl-3-dicyanomethyl-3-methyl-1*H*-2,3-dihydrophenalene**. ^{1}H NMR: 1.57 (3H, d, *J* = 6.5 Hz), 1.87 (3H, s), 1.99 (1H, t, *J* = 13.8 Hz), 2.41 (1H, dd, *J* = 14.1, 4.6 Hz), 3.23 (1H, sept, *J* = 6.0 Hz), 3.89 (1H, s), 7.49-7.56 (3H, m), 7.67 (1H, d, *J* = 6.9 Hz), 7.78 (1H, d, *J* = 7.7 Hz), and 7.85 (1H, d, *J* = 8.2 Hz).

Photoreaction of 2c

The isolation of products from a photolyze of **2c** was done with two independent reactions in different solvents. This facilitated the isolation of minor products. Thus, in the first experiment, **2c** (140 mg, 0.5 mmol) was dissolved in methylcyclohexane (400 mL, 1.3 mM) and the sample solution was placed in a donut-shaped cylindrical Pyrex vessel and

was irradiated under nitrogen atmosphere with high pressure mercury lamp for 4 h. The photolyze was concentrated *in vacuo* and was purified with silica-gel column chromatography with *n*-hexane-ethyl acetate (97 : 3) as eluent to give the rearrangement product (13 mg, 9%). **3,3-Dicyano-2-methyl-4-methoxy-4-(1-naphthyl)-1-butene**. M.p. 115-116 °C. ^{1}H NMR: 1.76 (3H, d, *J* = 7.0 Hz), 1.90 (3H, dd, *J* = 1.4, 0.7 Hz), 4.44 (1H, q, *J* = 7.0 Hz), 5.21 (1H, br s), 5.51 (1H, br s), 7.50-7.59 (3H, m), 7.84 (1H, d, *J* = 6.5 Hz), 7.86 (1H, d, *J* = 8.0 Hz), 7.90 (1H, br d, *J* = 7.8 Hz), and 8.04 (1H, d, *J* = 8.5 Hz). ^{13}C NMR: 20.1, 51.1, 57.8, 77.2, 113.0, 114.0, 120.3, 122.3, 125.4, 126.0, 126.3, 126.6, 129.0, 129.2, 130.6, 132.2, 133.6, and 133.7. HRMS (EI): *m/z* = 275.1182. $C_{18}H_{16}N_2$–H requires 275.1190. The same experiment was performed also in acetonitrile for 18 h. The photolyze was concentrated *in vacuo* and was purified with silica-gel column chromatography with *n*-hexane-ethyl acetate (98 : 2) as eluent to give a pair of meso-cyclization products (*syn* form, 52 mg, 37% and *anti* form, 40 mg, 29%), and the [2+2]addition product (10 mg, 7%), all as colorless oil. ***syn*- and *anti*-1-Methoxy-3-dicyanomethyl-3-methyl-1*H*-2,3-dihydrophenalene**. ^{1}H NMR: 1.89 (3H, s), 2.21 (1H, dd, *J* = 15.0, 3.5 Hz), 2.85 (1H, dd, *J* = 15.0, 2.5 Hz), 3.51 (3H, s), 4.61 (1H, t, *J* = 3.1 Hz) 4.94 (1H, s), 7.48 (1H, d, *J* = 6.8 Hz), 7.54 (1H, t, *J* = 7.9 Hz) 7.56 (1H, d, *J* = 8.0 Hz), 7.79 (1H, d, *J* = 7.4 Hz), 7.88 (1H, d, *J* = 8.3 Hz), and 7.91 (1H, d, *J* = 9.1 Hz). ^{13}C NMR: 25.0, 35.1, 37.5, 39.9, 57.3, 76.7, 112.7, 112.9, 125.5, 125.6, 125.6, 127.1, 128.3, 129.1, 129.7, 130.8, 133.9, and 133.9. HRMS (FAB): *m/z* = 276.1258. $C_{18}H_{16}N_2O$ requires 276.1263. ^{1}H NMR: 1.90 (3H, s), 2.27 (1H, dd, *J* = 13.5, 9.6 Hz), 2.74 (1H, dd, *J* = 13.7, 4.6 Hz), 3.59 (3H, s), 3.93 (1H, s), 4.71 (1H, dd, *J* = 9.4, 4.4 Hz), 7.52 (1H, t, *J* = 8.0 Hz), 7.56 (1H, t, *J* = 7.8 Hz), 7.59 (1H, d, *J* =7.1 Hz), 7.73 (1H, d, *J* = 7.0Hz), 7.84 (1H, d, *J* = 4.7 Hz), and 7.86 (1H, d, *J* = 4.7 Hz). ^{13}C NMR: 25.6, 34.8, 37.2, 41.5, 56.8, 74.1, 111.4, 111.5, 123.7, 124.9, 125.4, 126.1, 127.3, 128.6, 129.2, 133.3, 133.8, and 133.9. HRMS (FAB): *m/z* = 276.1261. $C_{18}H_{16}N_2O$ requires 276.1263. **(*ttt*)-10,10-Dicyano-2,3,3*a*,4-tetrahydro-1-methoxy-3-methyl-3,4-methano-1*H*-phenalene**. ^{1}H NMR: 1.80 (3H, s), 1.80 (1H, dd, *J* = 12.7, 11.4 Hz), 2.22 (1H, dd, *J* = 12.7, 4.0 Hz), 2.92 (1H, d, *J* = 9.3 Hz), 3.63 (3H, s), 3.81 (1H, dd, *J* = 9.8, 6.0 Hz), 4.00 (1H, dd, *J* = 11.4, 3.7 Hz), 5.76 (1H, dd, *J* = 9.6, 6.0 Hz), 6.81 (1H, d, *J* = 9.7 Hz), 7.03 (1H, d, *J* =7.5 Hz), 7.30 (1H, t, *J* = 7.7 Hz), and 7.43 (1H, d, *J* = 7.8 Hz). ^{13}C NMR: 25.3, 37.9, 39.9, 40.6, 43.8, 45.3, 58.0, 76.4, 112.5, 113.7, 118.2, 122.8, 125.9, 126.9, 128.2, 131.0, 134.0, and 141.8. HRMS (FAB): *m/z* = 275.1186. $C_{18}H_{16}N_2O$-H requires 275.1189.

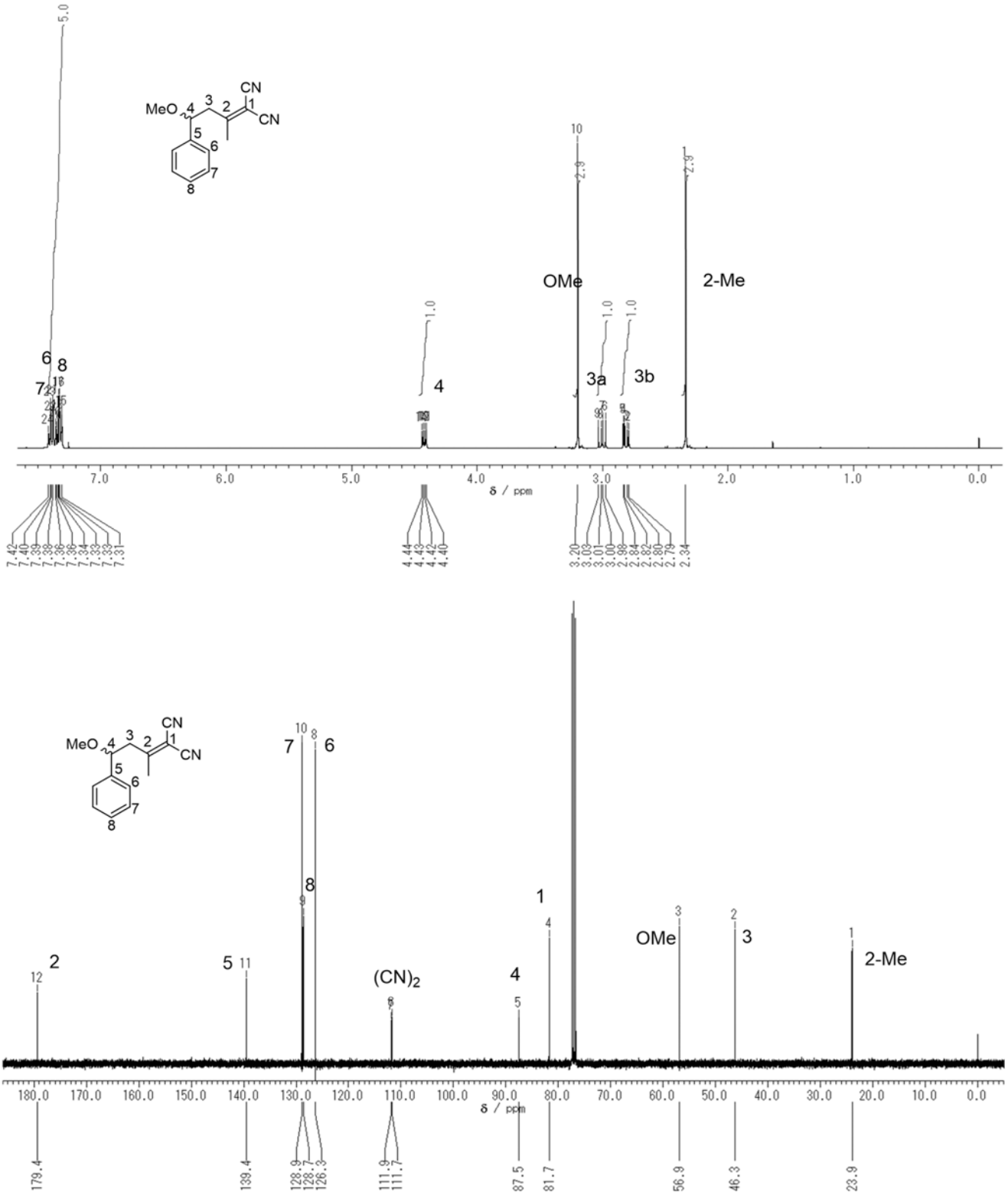


Figure S1. ^{1}H- and ^{13}C-NMR spectra of **1c**.

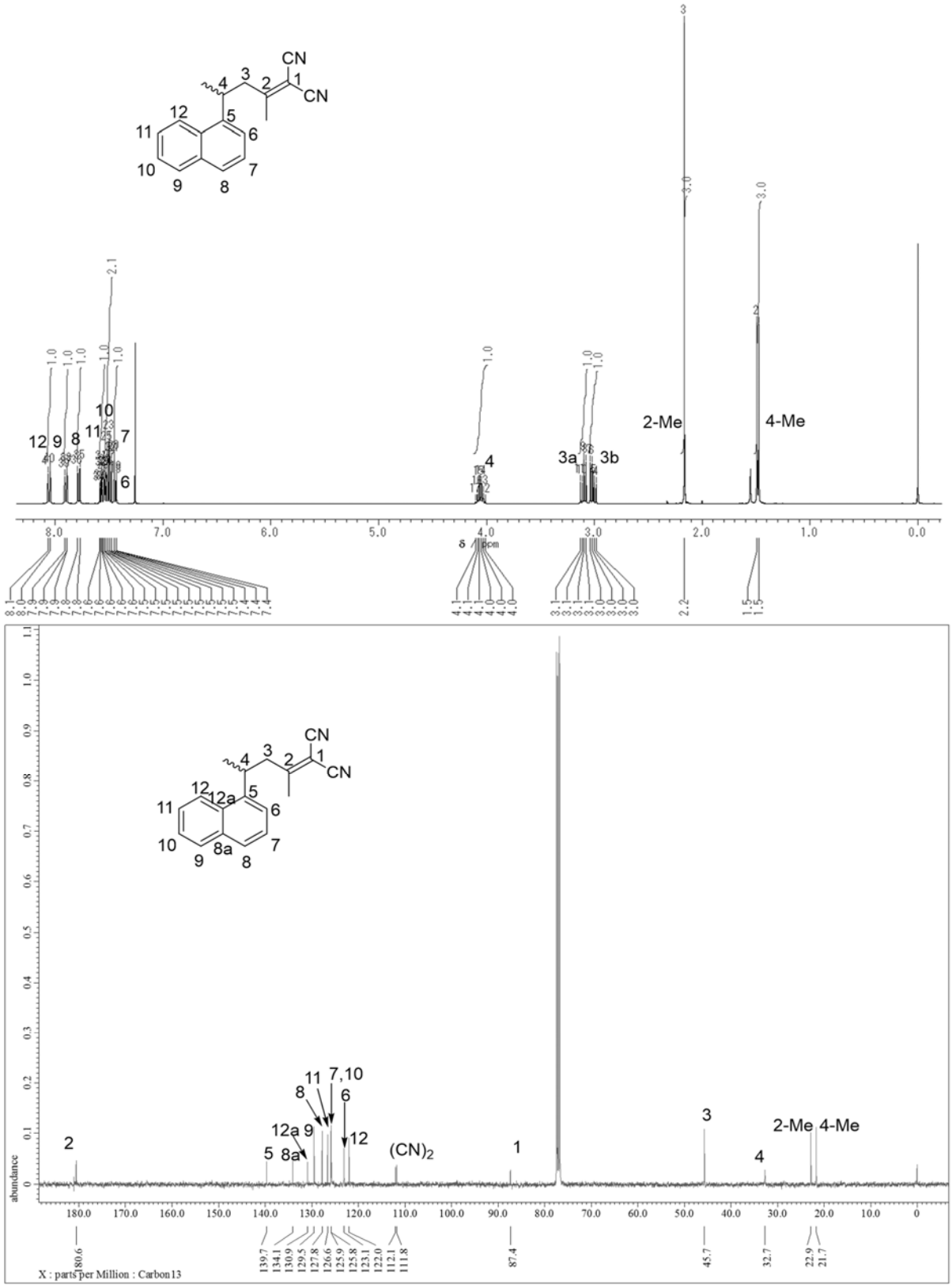


Figure S2. ^{1}H- and ^{13}C-NMR spectra of **2b**.

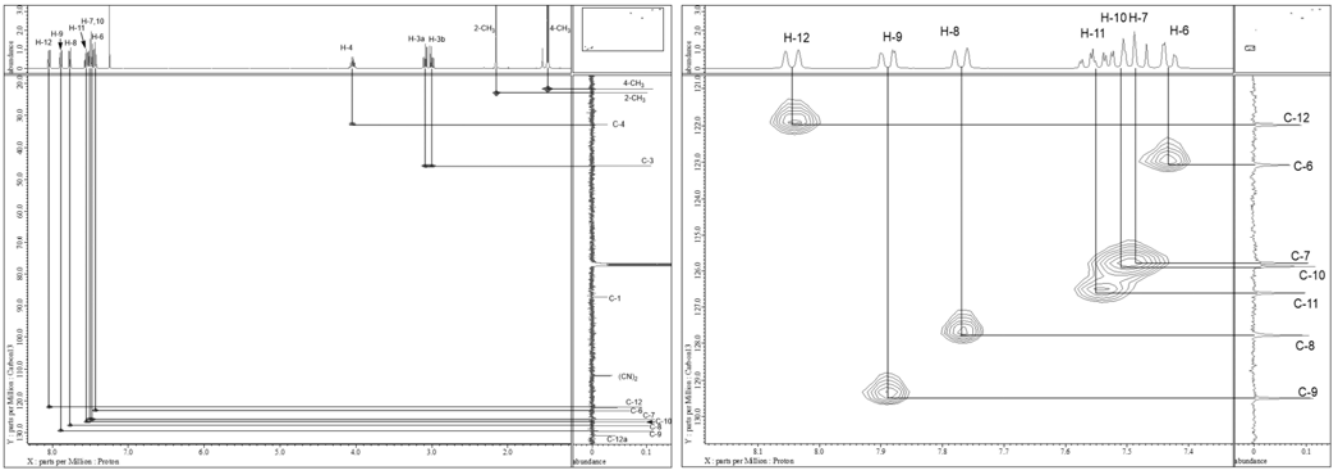


Figure S3. 2D-NMR (HSQC) spectra of **2b**.

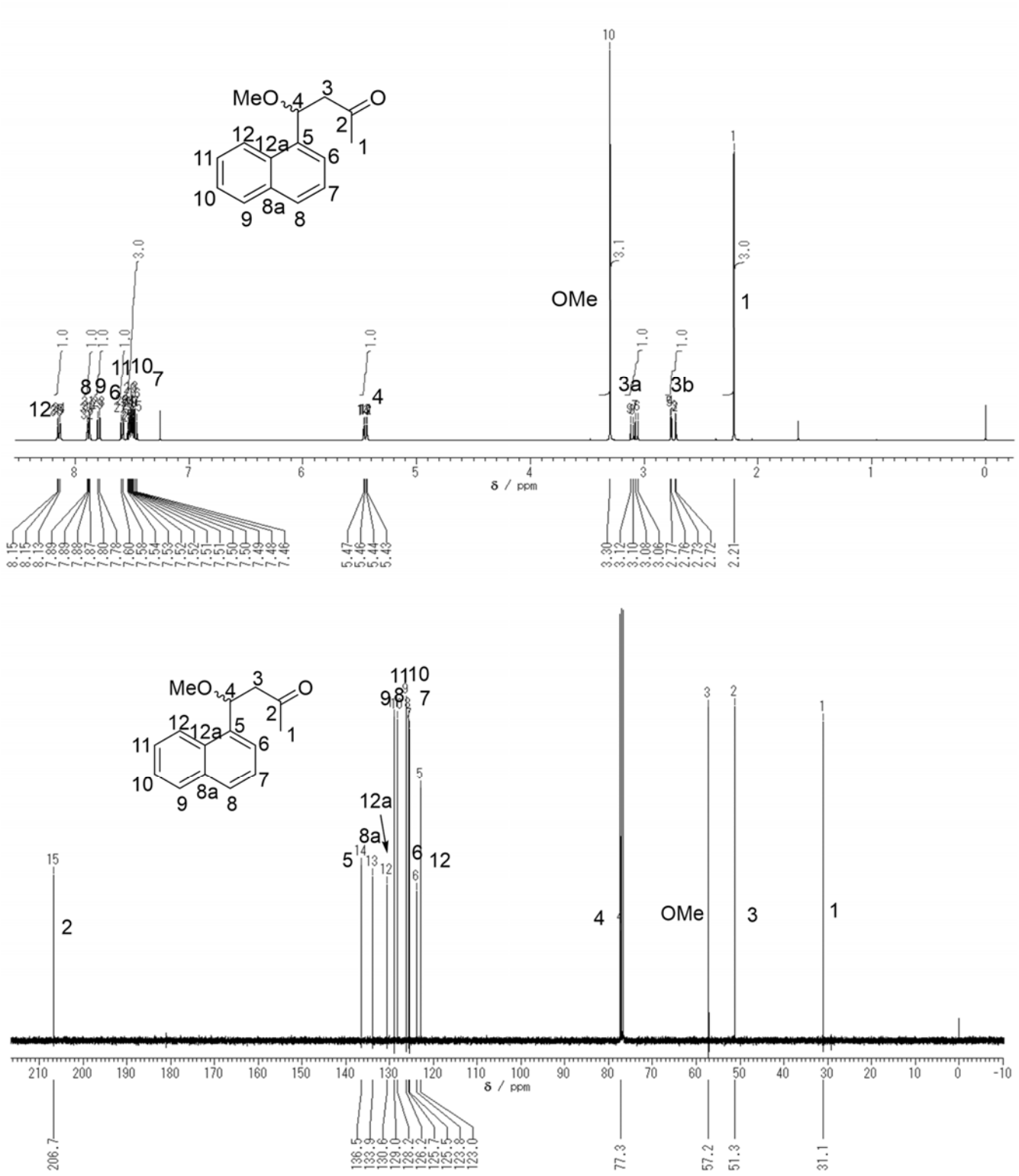


Figure S4. ^{1}H- and ^{13}C-NMR spectra of 4-methoxyl-4-(1-naphthyl)-buene-2-one.

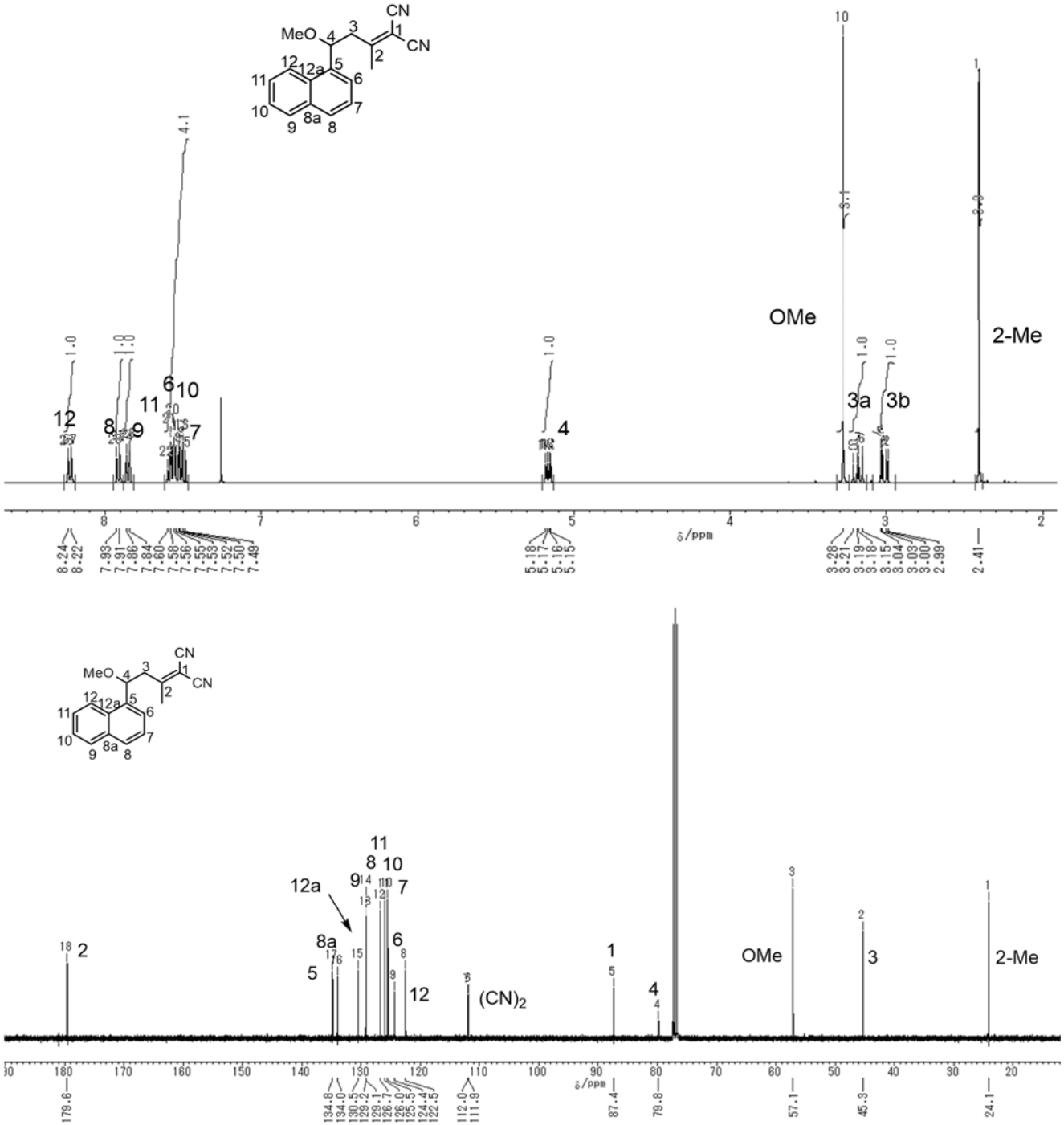


Figure S5. ^{1}H- and ^{13}C-NMR spectra of 4-methoxyl-4-(1-naphthyl)-buene-2-one.

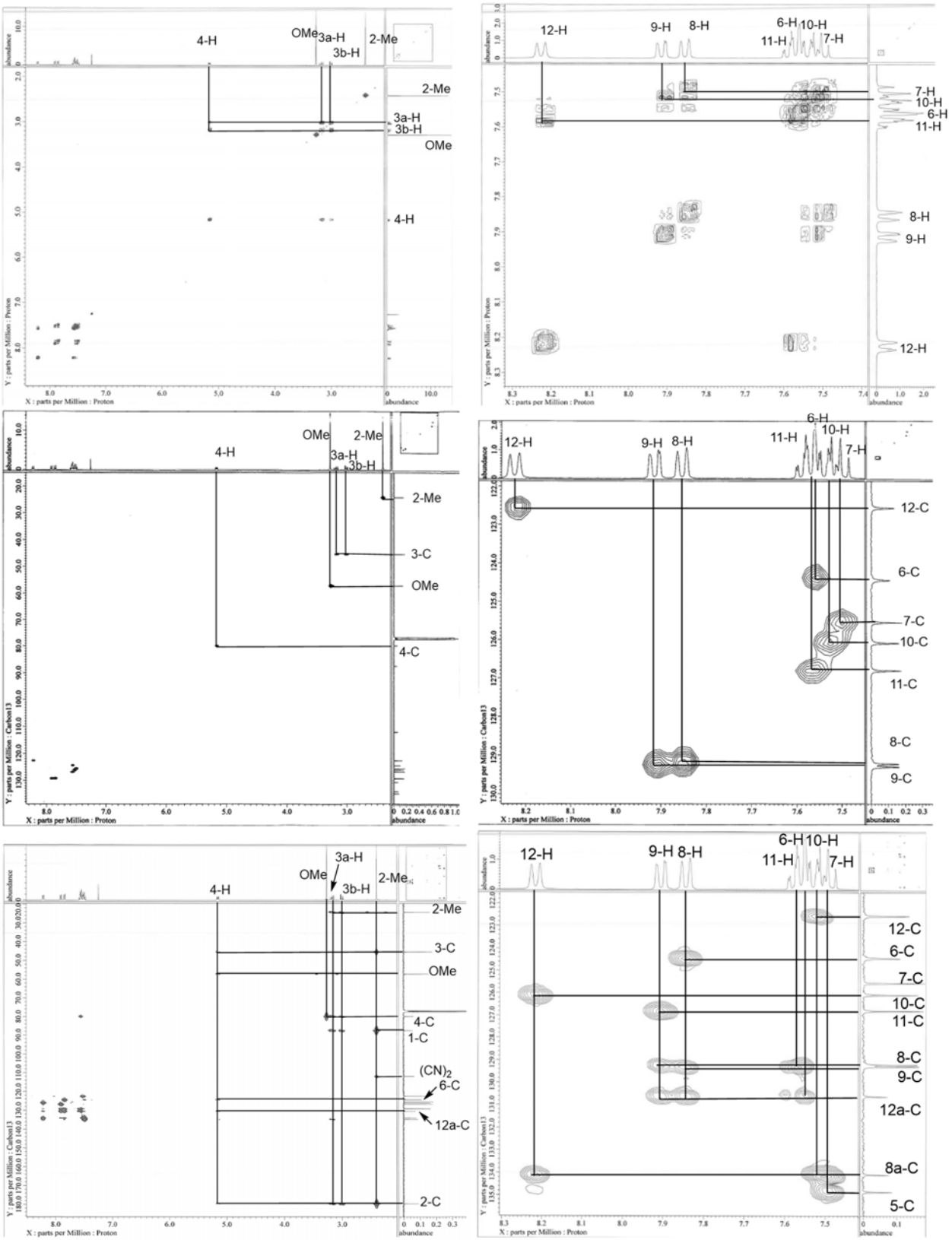


Figure S6. 2D-NMR (^{1}H-^{1}H COSY, top; HSQC, middle; HMBC, bottom) spectra of **2c**.

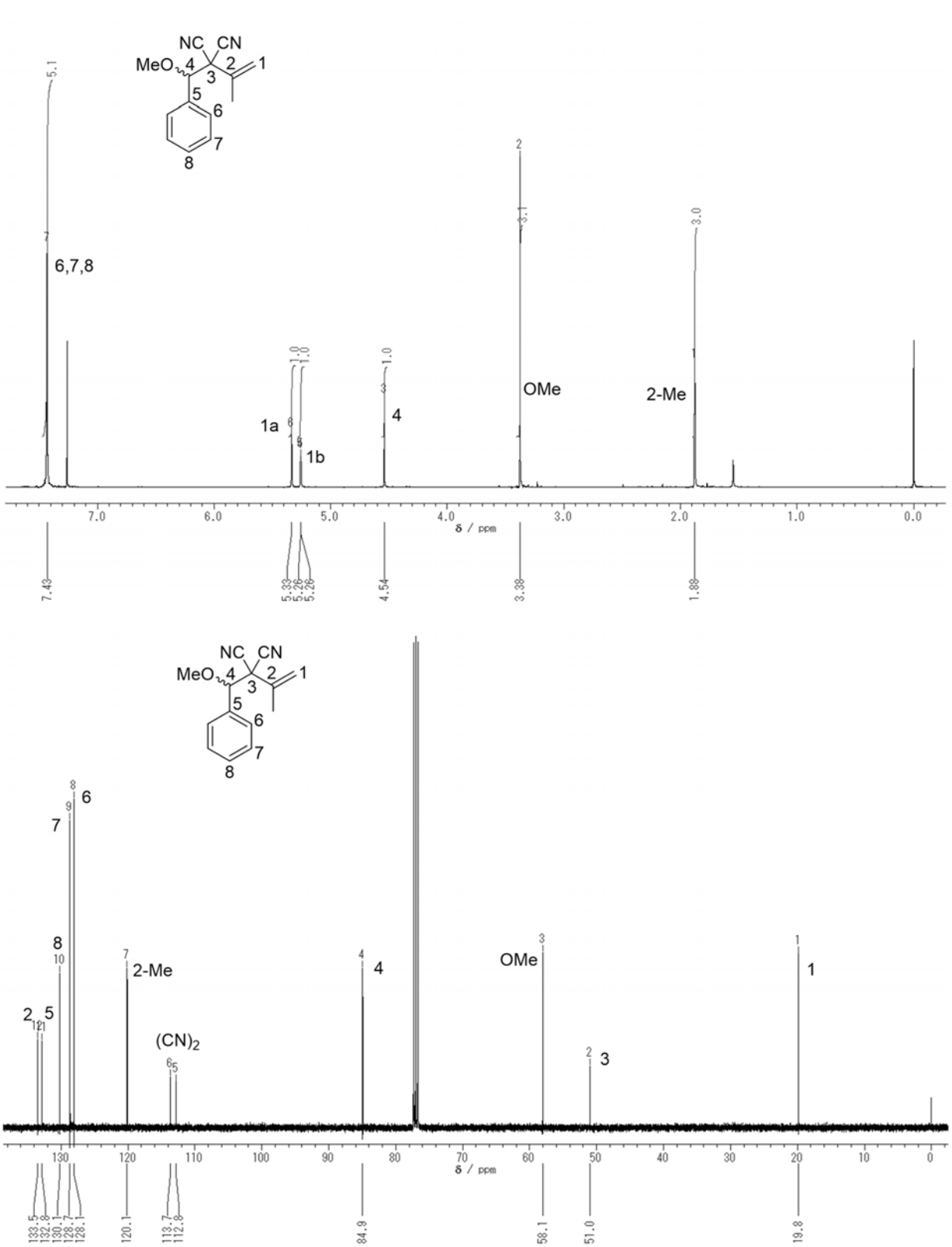


Figure S7. ^{1}H- and ^{13}C-NMR spectra of 3,3-dicyano-4-methoxy-2-methyl-4-phenyl-1-pentene.

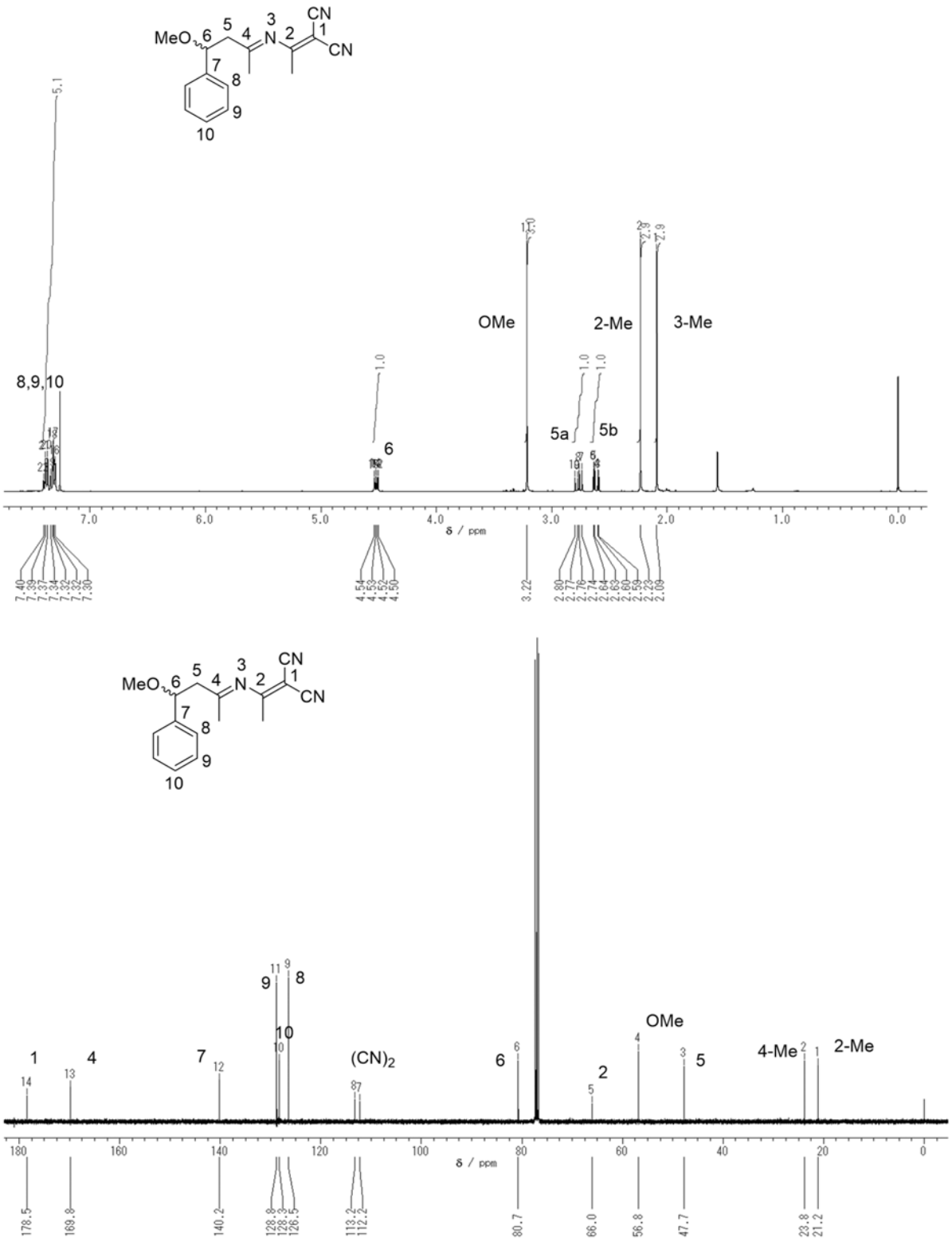


Figure S8. ^{1}H- and ^{13}C-NMR spectra of 3-aza-1,1-dicyano-2,4-dimethyl-6-methoxy-6-phenyl-1,3-hexadiene.

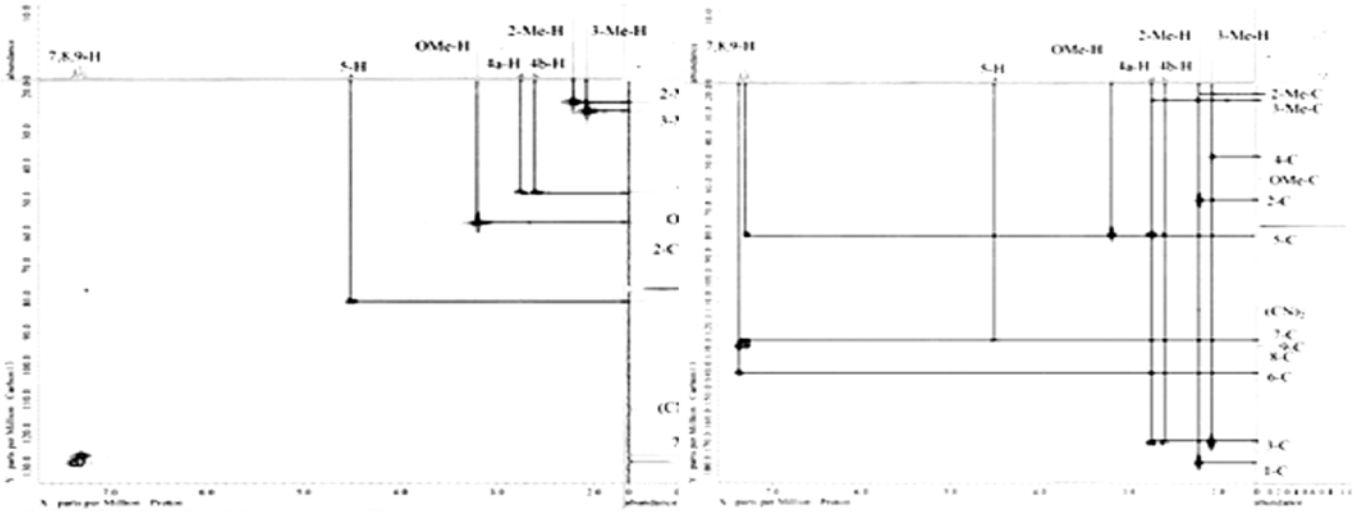


Figure S9. 2D-NMR (HSQC, left; HMBC, right) spectra of 3-aza-1,1-dicyano-2,4-dimethyl-6-methoxy-6-phenyl-1,3-hexadiene.

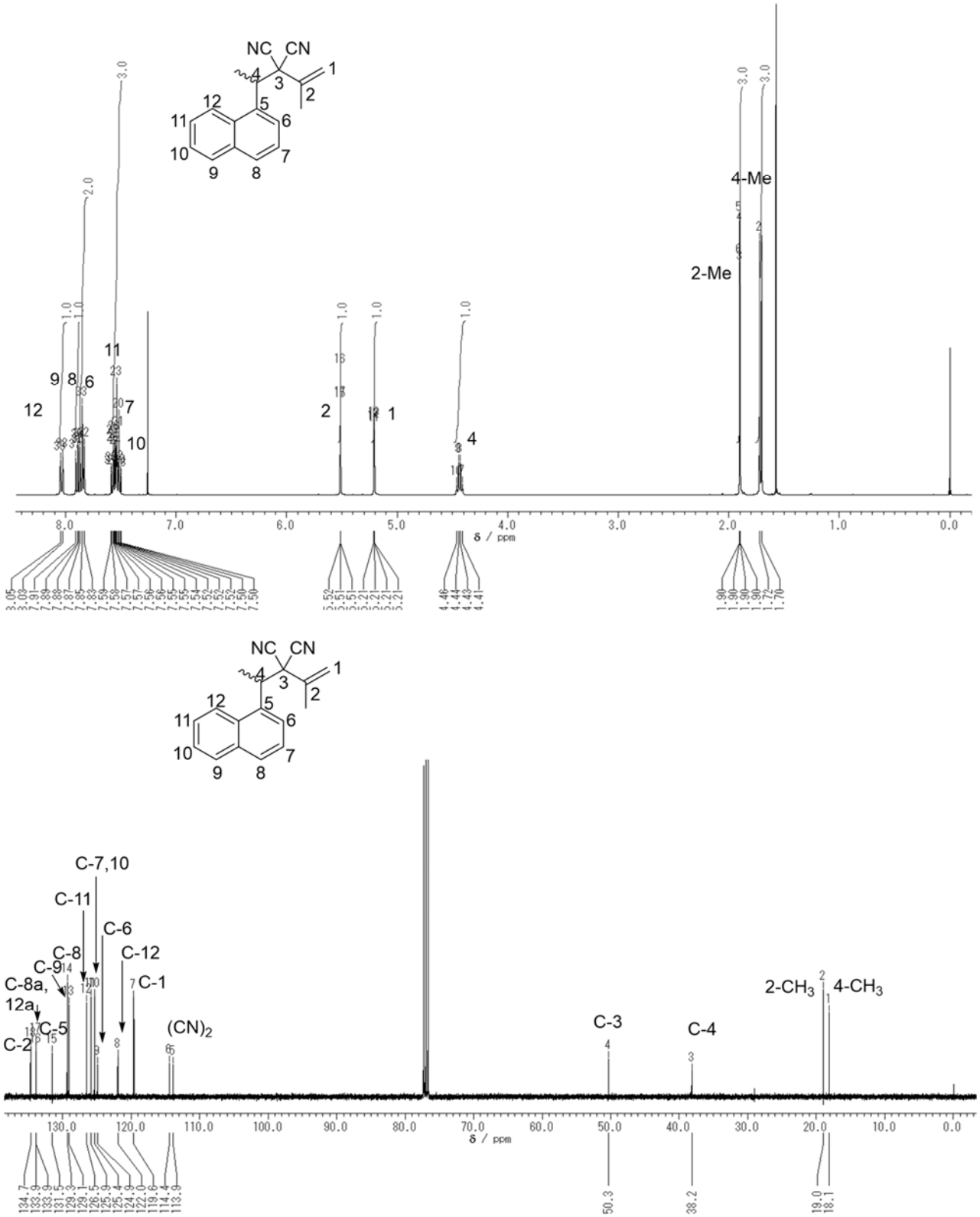


Figure S10. ^{1}H- and ^{13}C-NMR spectra of 3,3-dicyano-2,4-dimethyl-4-(1-naphthyl)-1-butene.

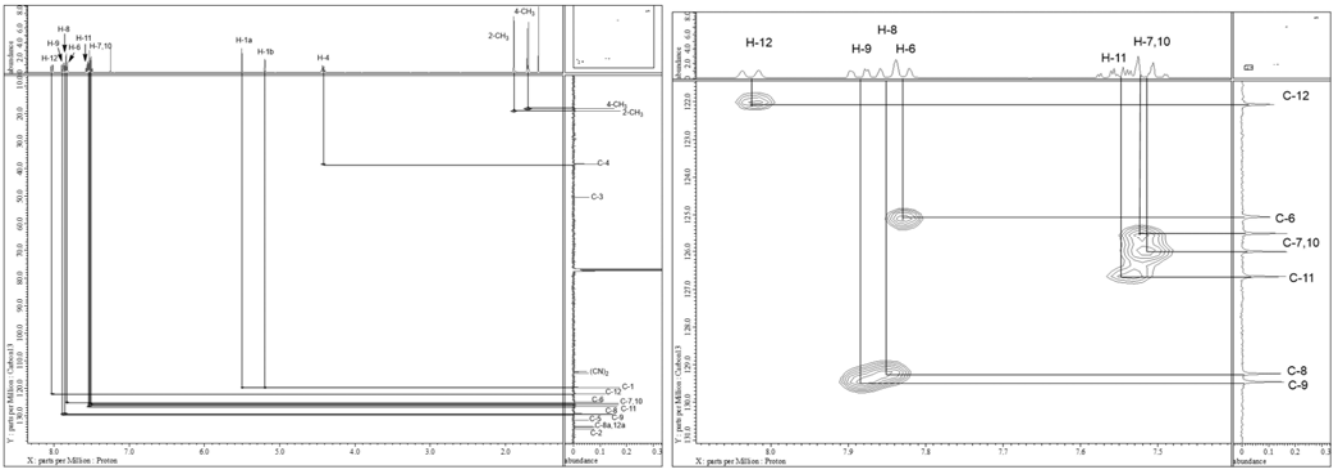


Figure S11. 2D-NMR (HSQC) spectra of 3,3-dicyano-2,4-dimethyl-4-(1-naphthyl)-1-butene.

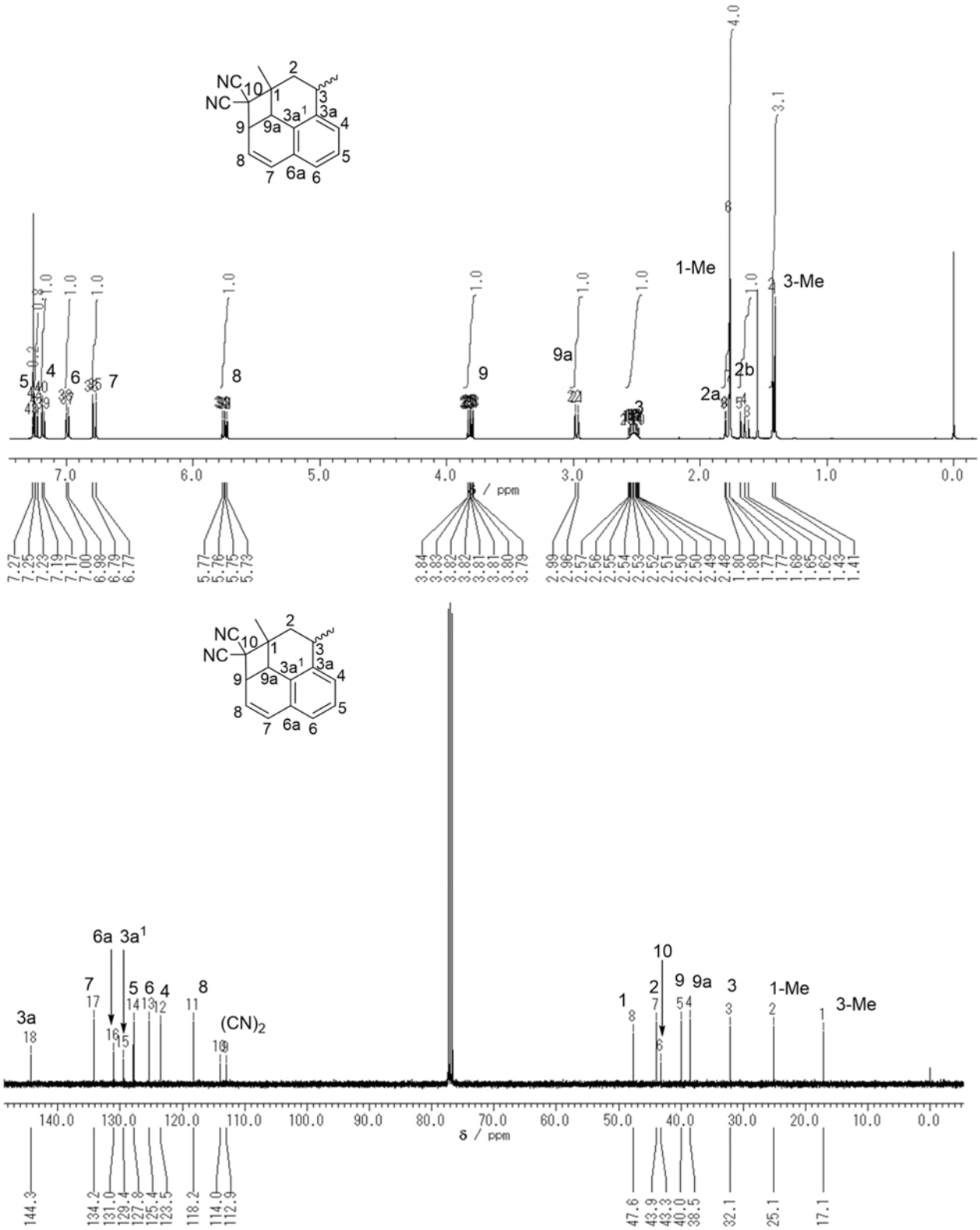


Figure S12. ^{1}H- and ^{13}C-NMR spectra of all *anti*-10,10-dicyano-2,3,9,9*a*-tetrahydro-1,3-dimethyl-1,9-methano-1*H*-phenalene.

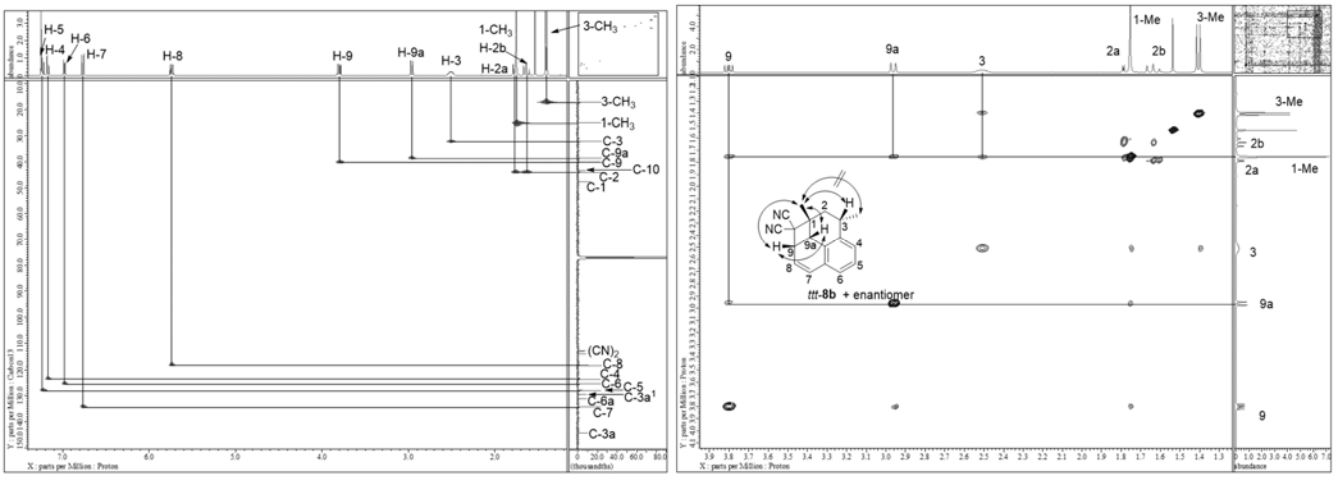


Figure S13. 2D-NMR (HSQC, left; NOESY, right) spectra of (*ttt*)-10,10-dicyano-2,3,9,9*a*-tetrahydro-1,3-dimethyl-1,9-methano-1*H*-phenalene.

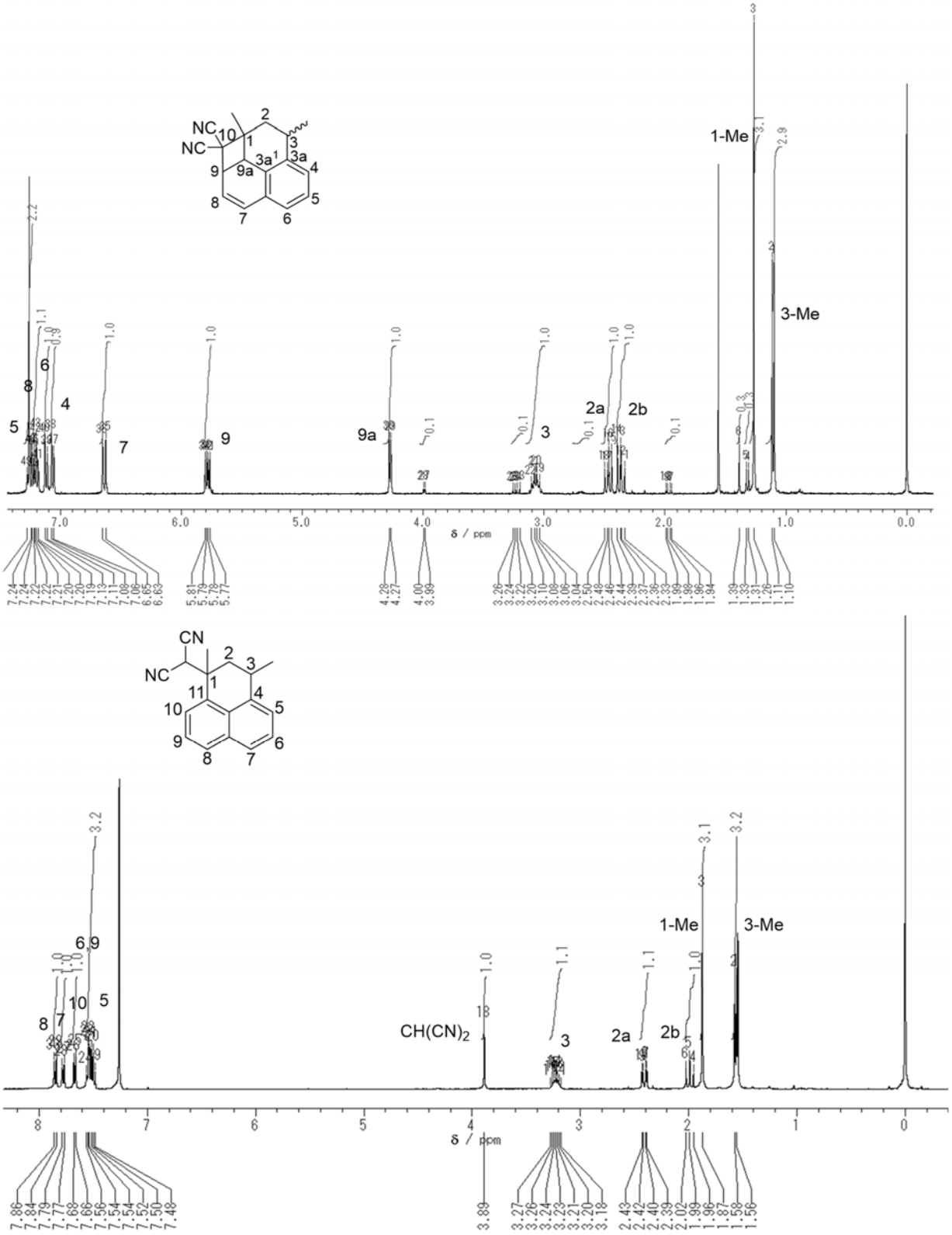


Figure S14. ^{1}H-NMR spectra of (*ccc*)-10,10-dicyano-2,3,9,9*a*-tetrahydro-1,3-dimethyl-1,9-methano-1*H*-phenalene (top) and 1-methyl-3-dicyanomethyl-3-methyl-1*H*-2,3-dihydrophenalene (bottom).

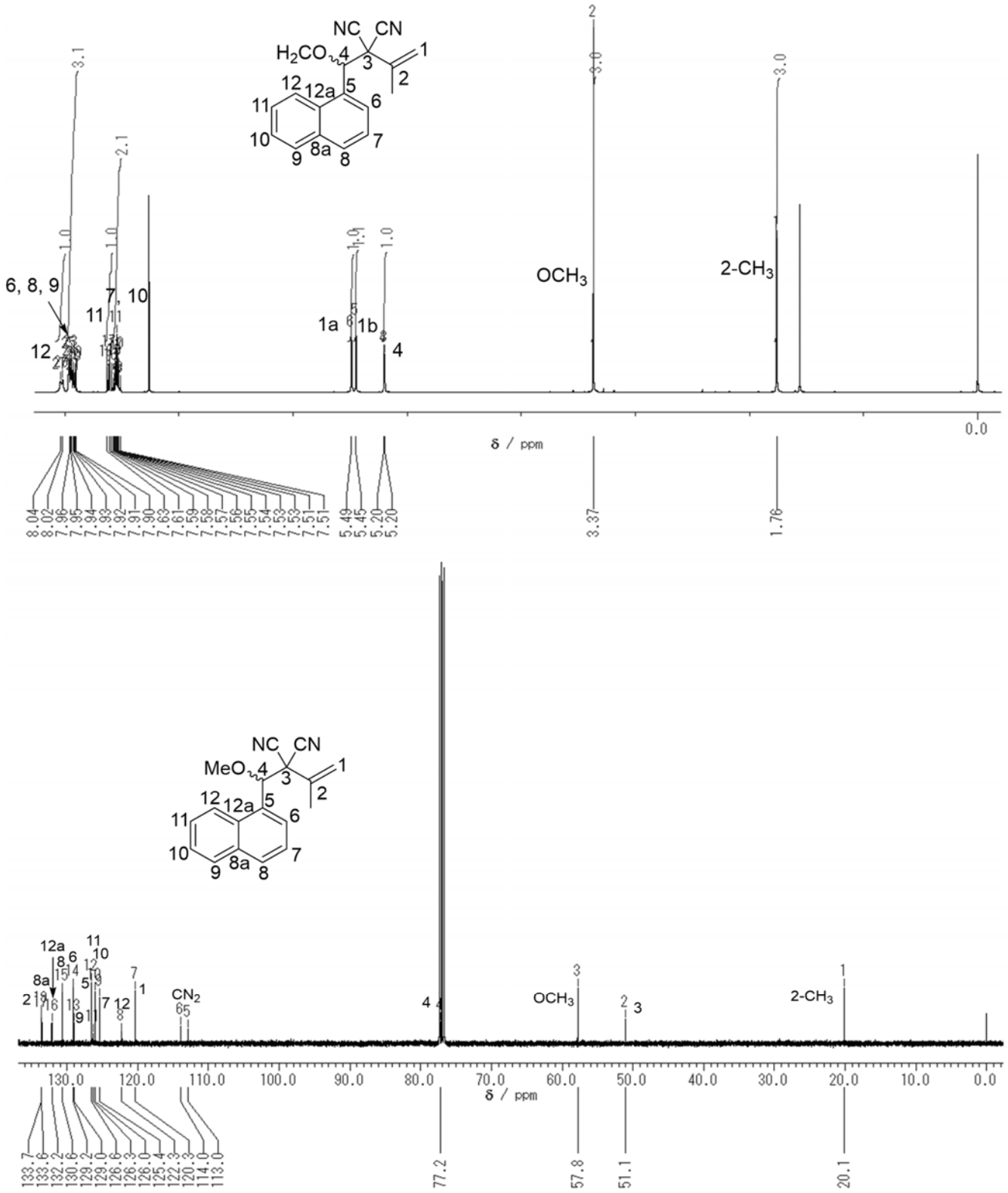


Figure S15. ^{1}H- and ^{13}C-NMR spectra of 3,3-dicyano-2-methyl-4-methoxy-4-(1-naphthyl)-1-butene.

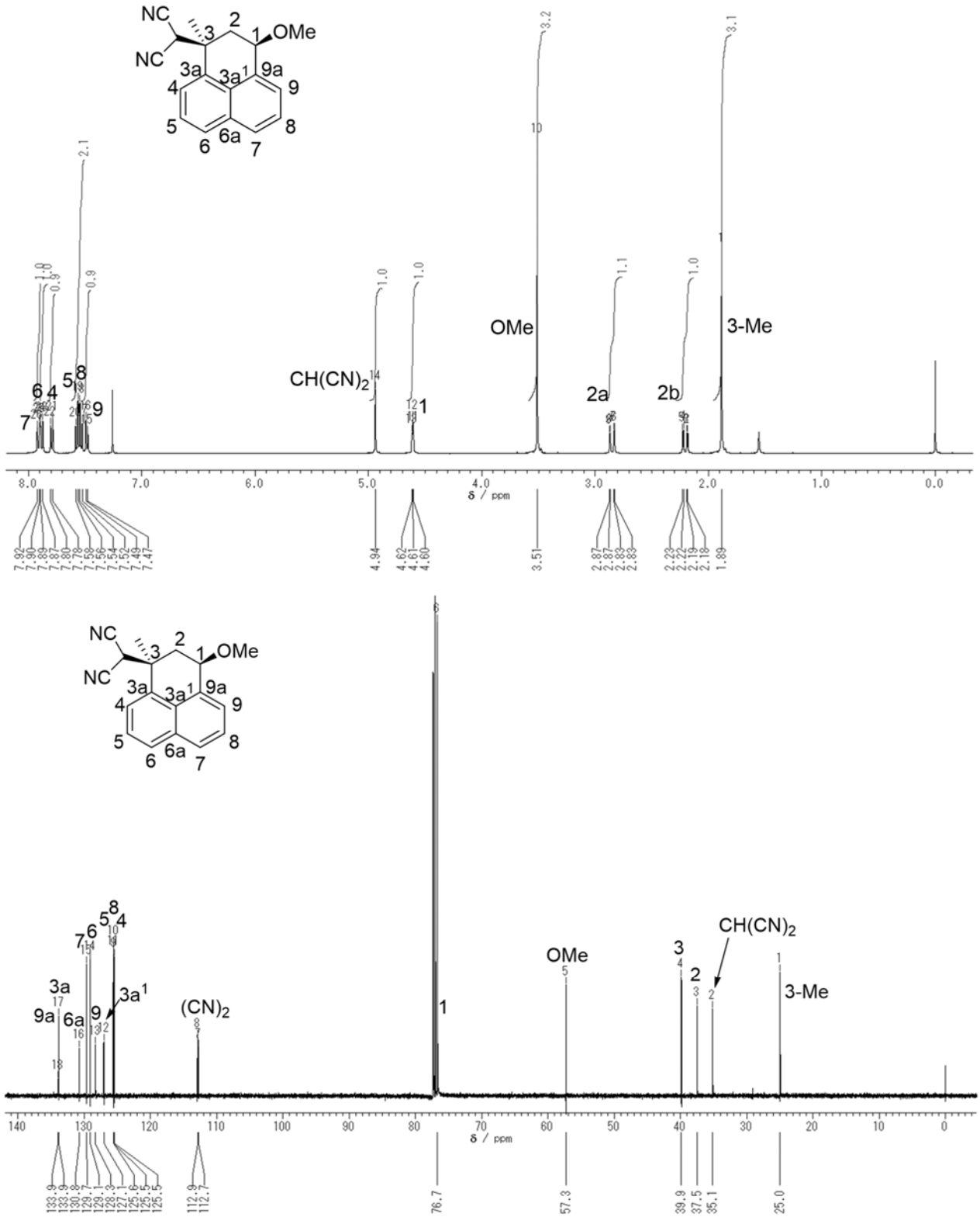


Figure S16. ^{1}H- and ^{13}C-NMR spectra of *syn*-1-Methoxy-3-dicyanomethyl-3-methyl-1*H*-2,3-dihydrophenalene.

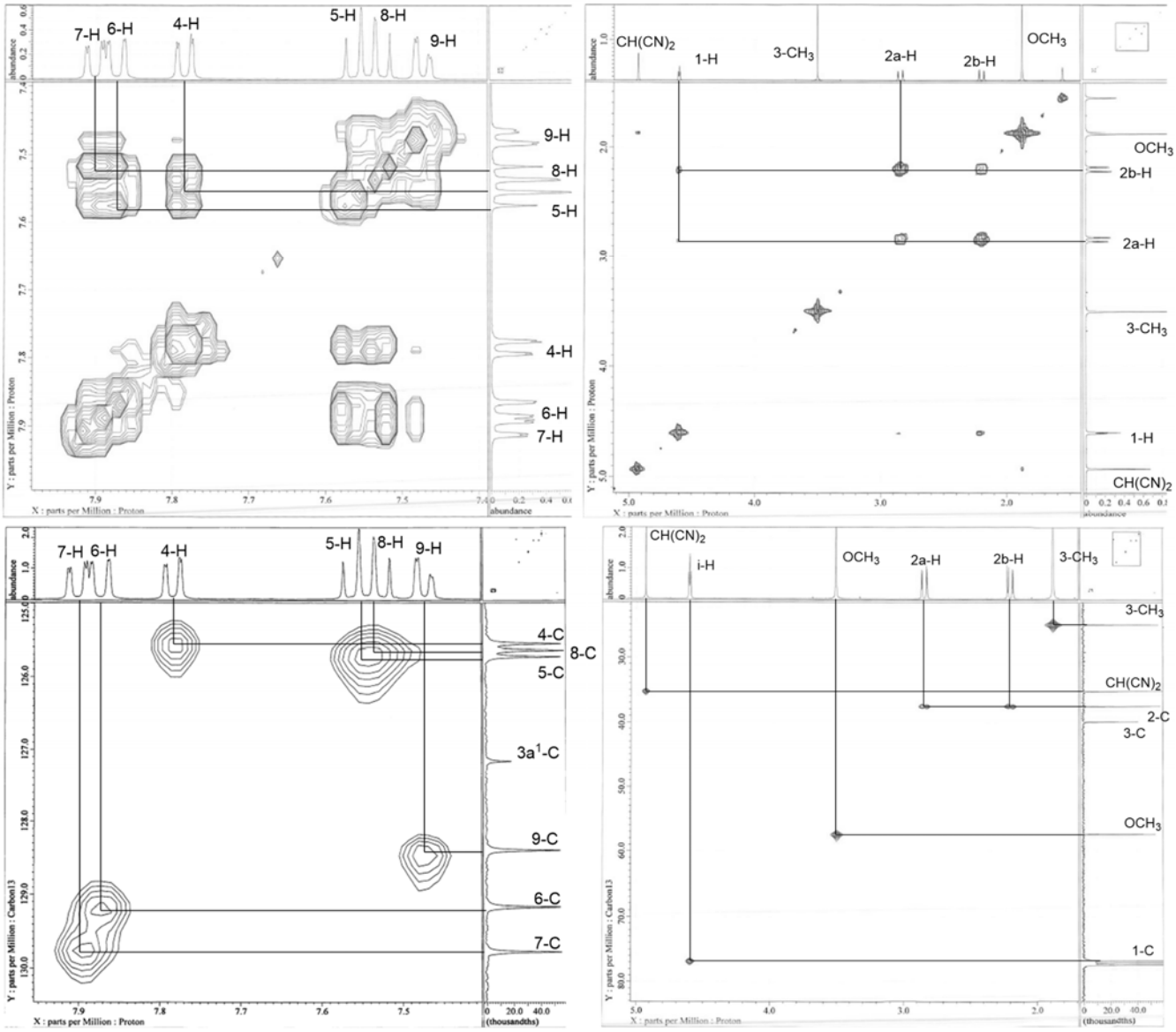


Figure S17. 2D-NMR (^{1}H-^{1}H COSY, top; HSQC, bottom) spectra of *syn*-1-Methoxy-3-dicyanomethyl-3-methyl-1*H*-2,3-dihydrophenalene.

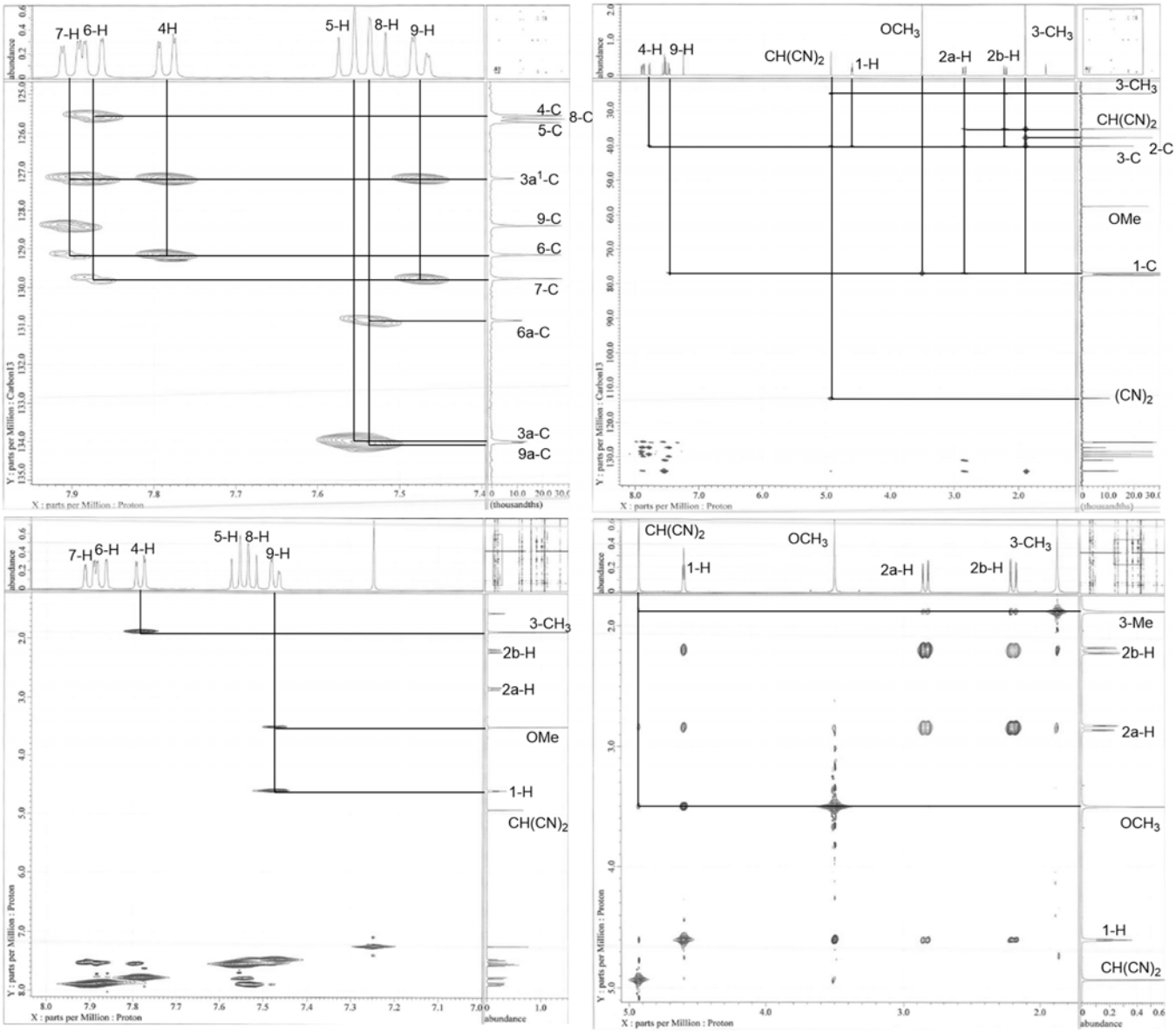


Figure S18. 2D-NMR (HMBC, top; NOESY, bottom) spectra of *syn*-1-Methoxy-3-dicyanomethyl-3-methyl-1*H*-2,3-dihydrophenalene.

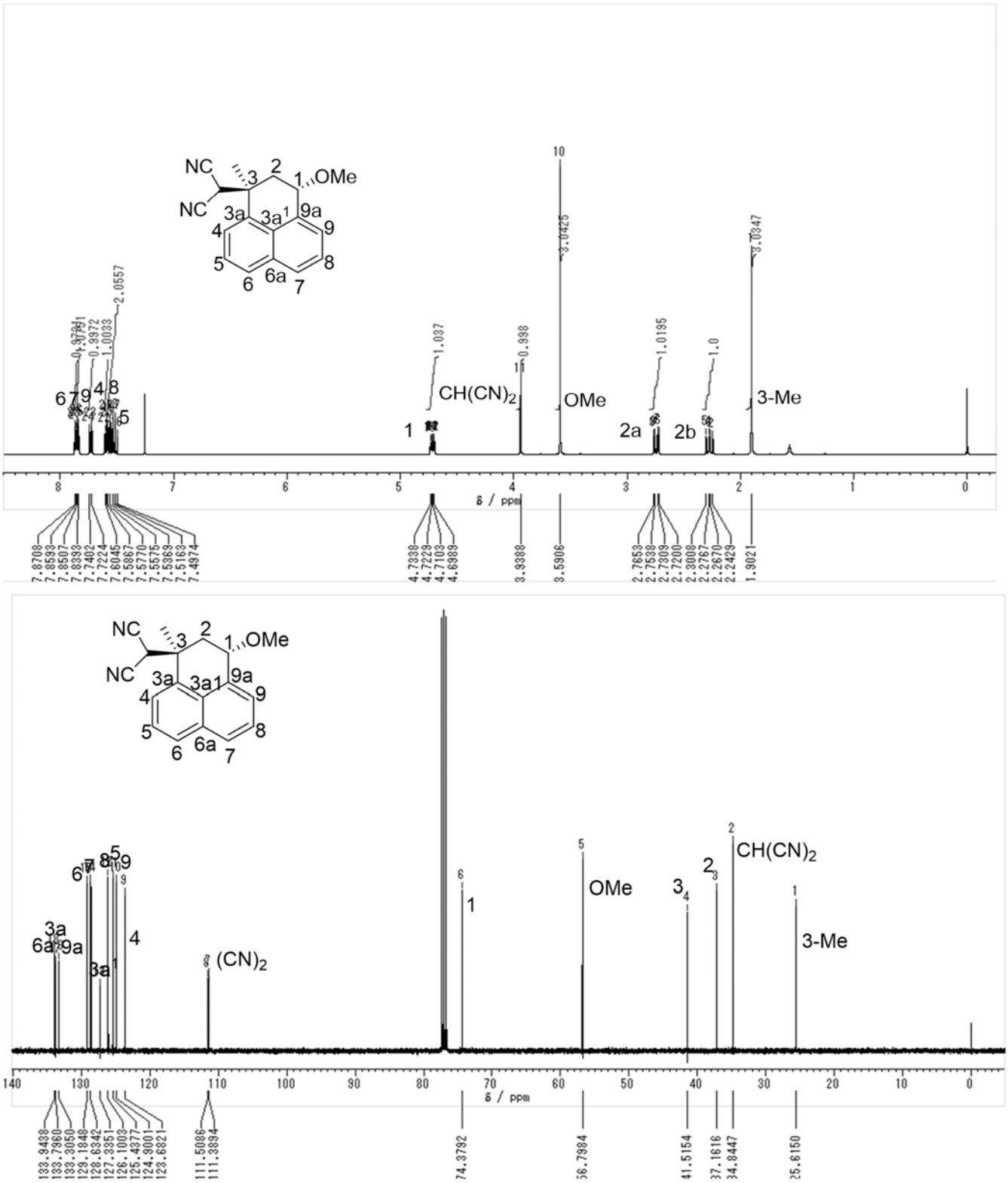


Figure S19. ^{1}H- and ^{13}C-NMR spectra of *anti*-1-Methoxy-3-dicyanomethyl-3-methyl-1*H*-2,3-dihydrophenalene.

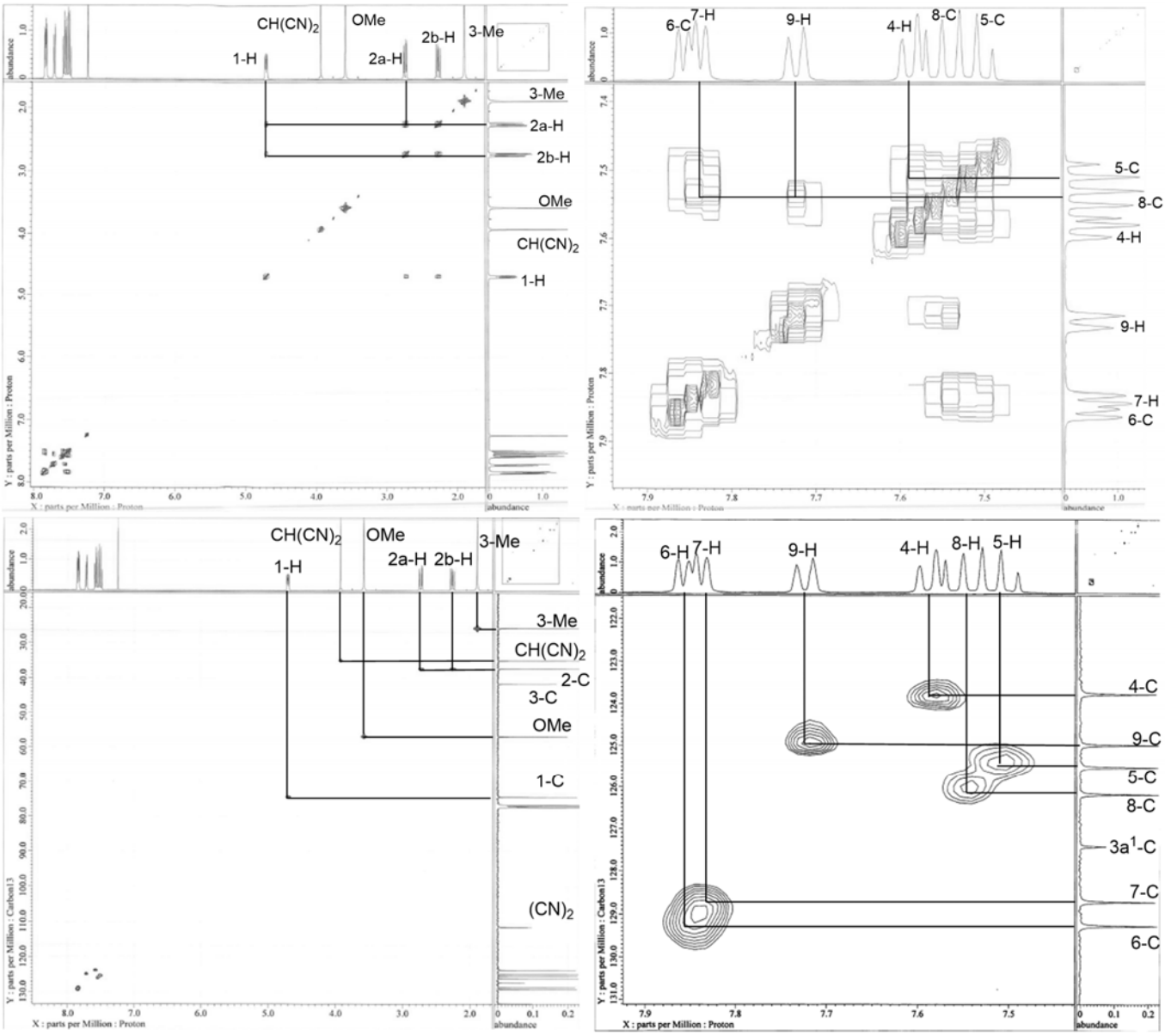


Figure S20. 2D-NMR (^{1}H-^{1}H COSY, top; HSQC, bottom) spectra of *anti*-1-Methoxy-3-dicyanomethyl-3-methyl-1*H*-2,3-dihydrophenalene.

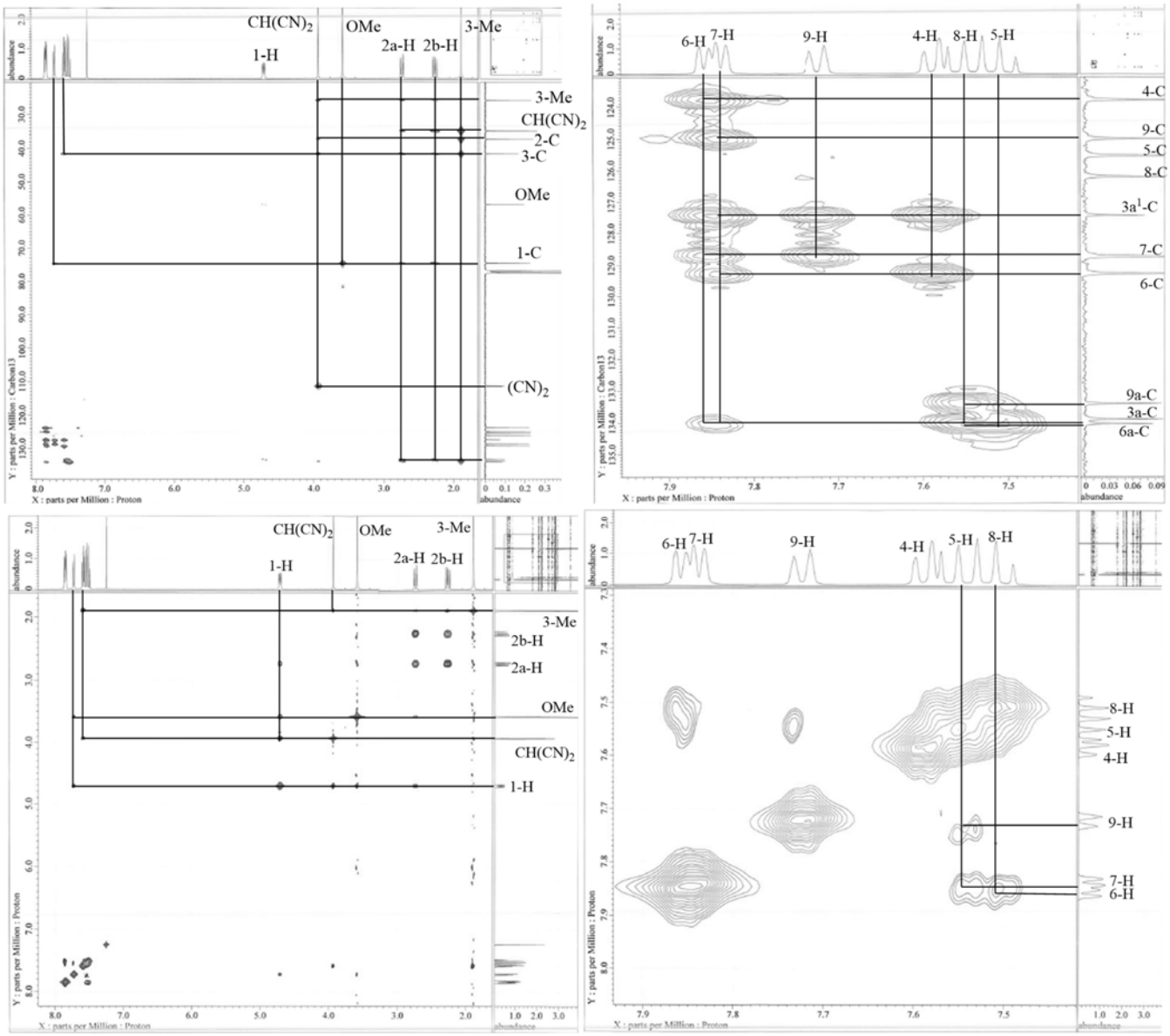


Figure S21. 2D-NMR (HMBC, top; NOESY, bottom) spectra of *anti*-1-Methoxy-3-dicyanomethyl-3-methyl-1*H*-2,3-dihydrophenalene.

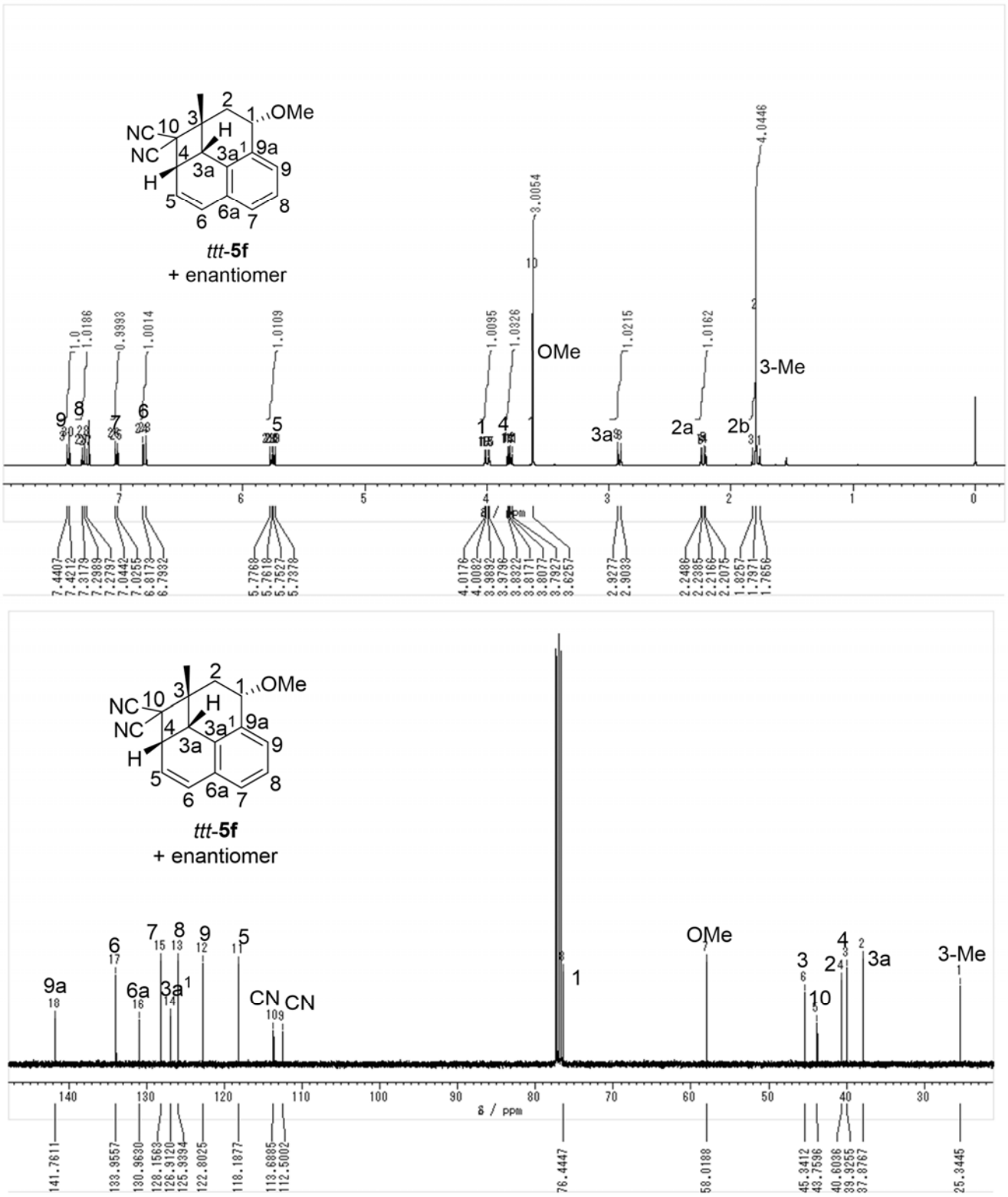


Figure S22. ^{1}H- and ^{13}C-NMR spectra of all-*anti* 10,10-dicyano-2,3,3*a*,4-tetrahydro-1-methoxy-3-methyl-3,4-methano-1*H*-phenalene.

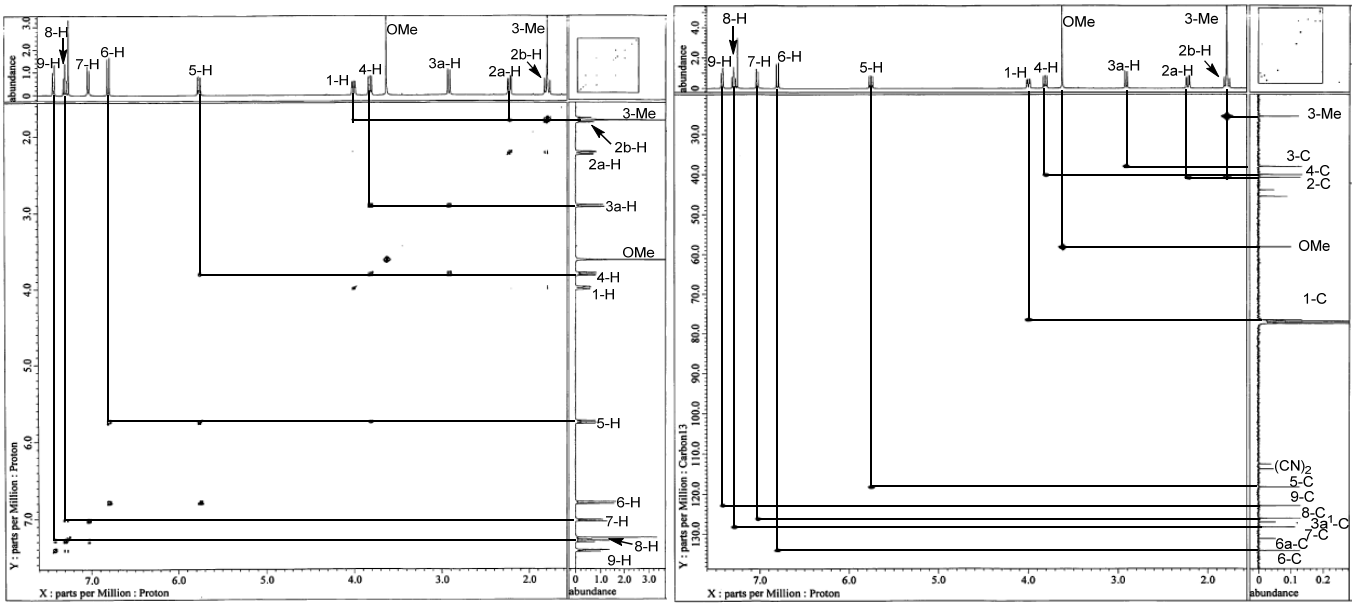


Figure S23. 2D-NMR (^{1}H-^{1}H COSY, left; HSQC, right) spectra of all-*anti* 10,10-dicyano-2,3,3*a*,4-tetrahydro-1-methoxy-3-methyl-3,4-methano-1*H*-phenalene.

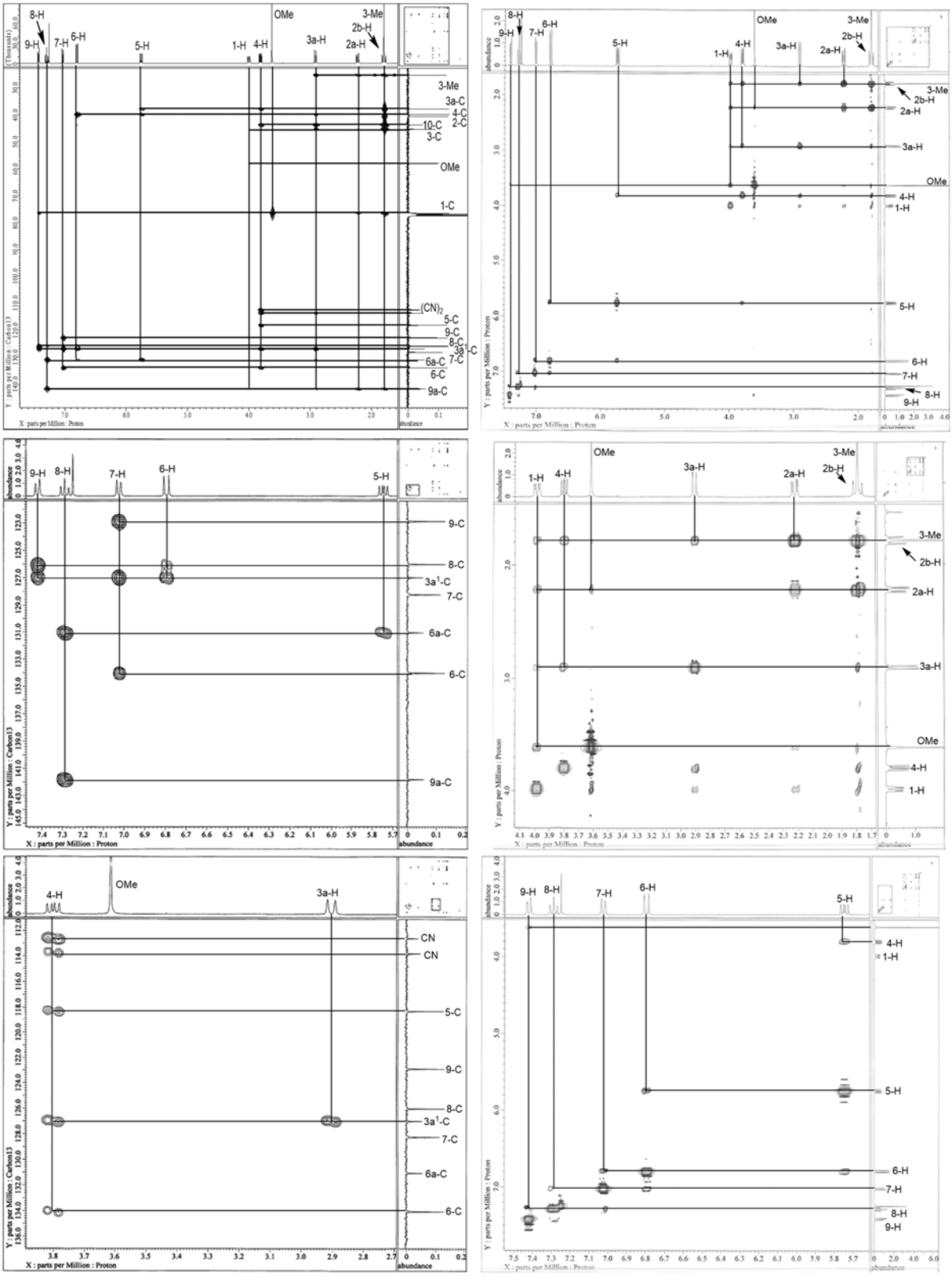


Figure S24. 2D-NMR (HMBC, left; NOESY, right) of all-*anti* 10,10-dicyano-2,3,3*a*,4-tetrahydro-1-methoxy-3-methyl-3,4-methano-1*H*-phenalene.

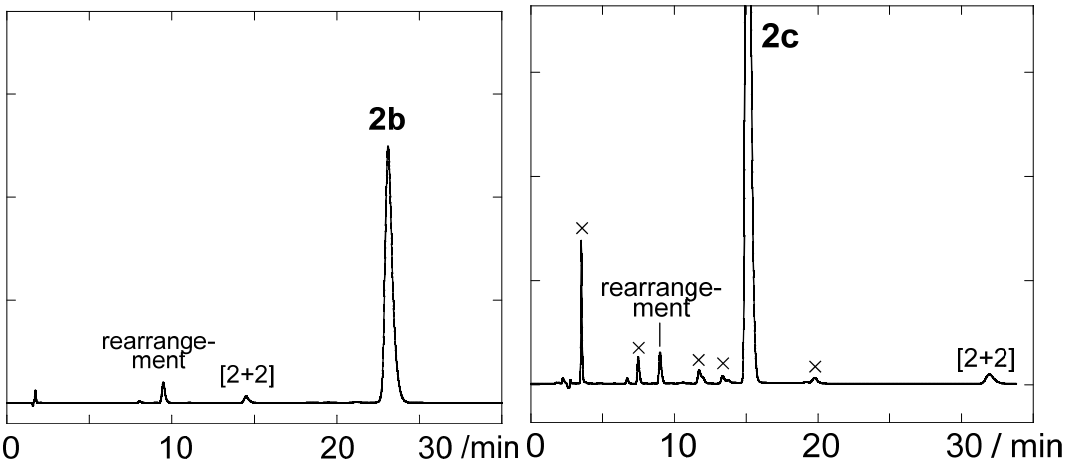


Figure S25. Typical HPLC traces (conditions: column, Kanto Mightysil, 4.6 mm × 250 mm; eluent, *n*-hexane : ethyl acetate = 95 : 5 or 97 : 3; flow rate, 2.0 mL min^{-1}; temperature, 35 °C) of the photoreaction mixtures of **2b** (left) and **2c** (right).

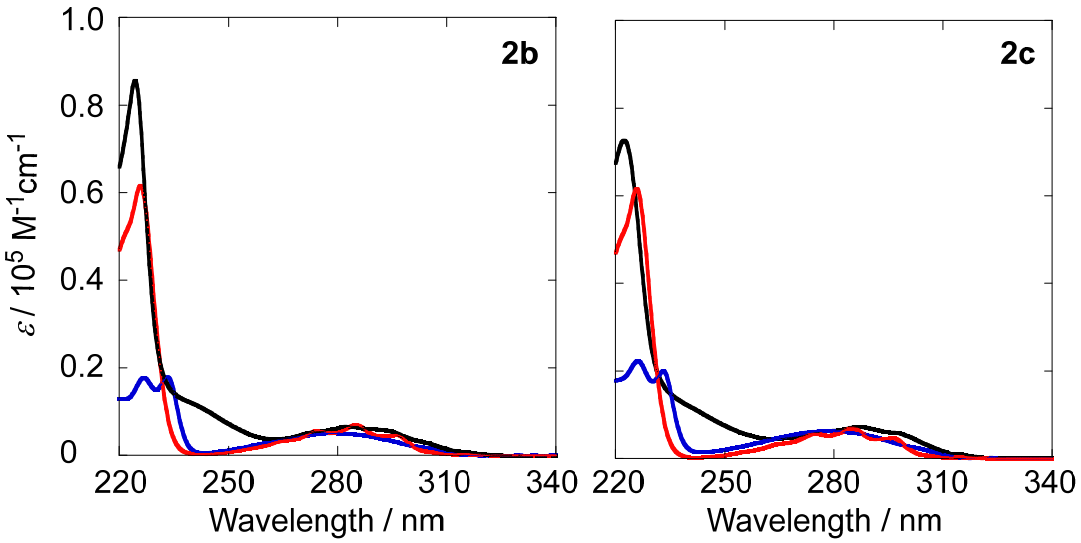


Figure S26. UV-vis spectra of **2b** (left) and **2c** (right) and their photoproducts in methylcyclohexane at 20 °C. Black: starting materials. Red: rearrangement products. Blue: all-*anti*-[2+2]-adducts.

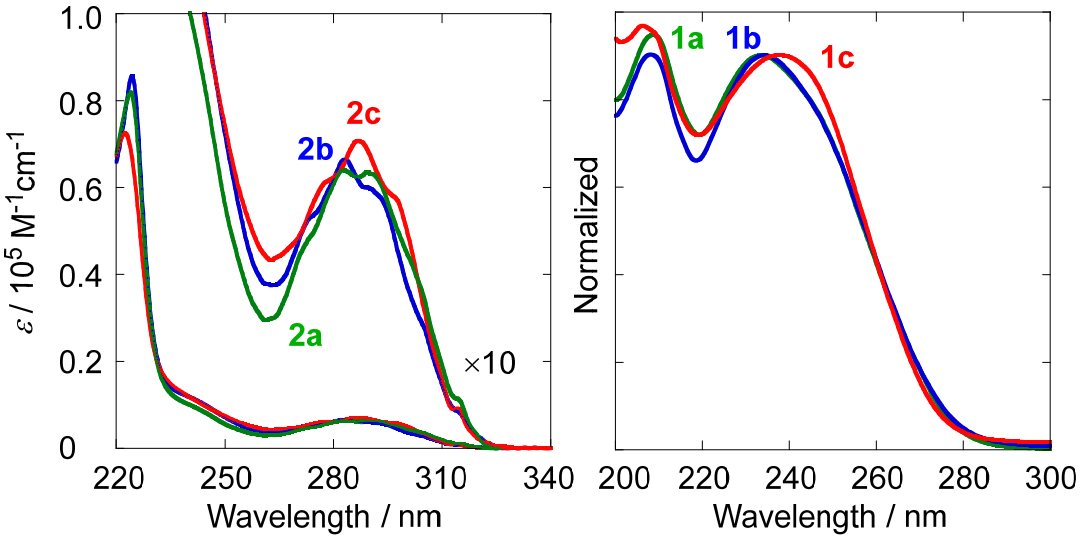


Figure S27. UV-vis spectra of **2a-c** in methylcyclohexane (left) and **1a-c** in acetonitrile (right) at 20 °C.

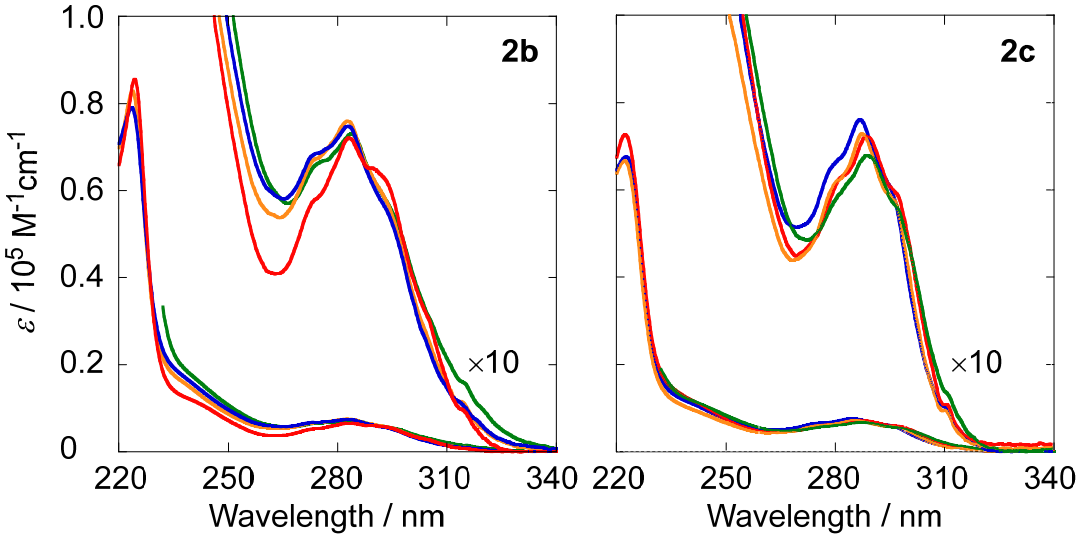


Figure S28. UV-vis spectra of **2b** (left) and **2c** (right) in various solvents at 20 °C. Red: methylcyclohexane, blue: acetonitrile, orange: diethyl ether, green: dichloromethane.

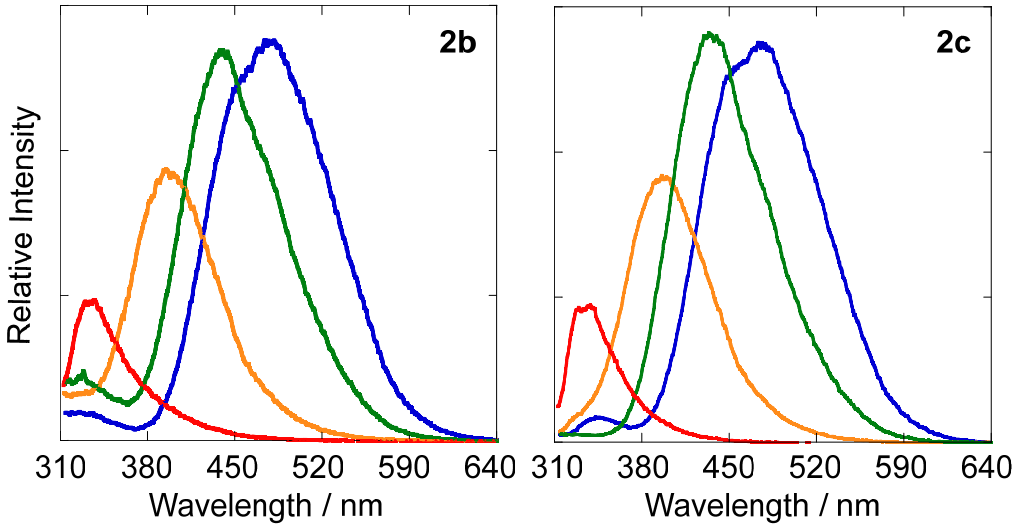


Figure S29. Fluorescence spectra of **2b** (left) and **2c** (right) in various solvents at 20 °C. Red: methylcyclohexane, blue: acetonitrile, orange: diethyl ether, green: dichloromethane.

Table S1. Photoreaction of 1a-c

Substrate	Conc. . mM	Temp. / °C	Irrad. / nm	%Conv.	%Yield	%Distribution (rearrangement : cyclization)
1a	0.1	20	254	7	3	66 : 34
			280	6	2	23 : 77
1b [a]	0.1	0	254	84	36	88 : 12
			280	57	40	69 : 31
1c	1.1	20	254	89	73	>95 : 5
	3.6	10	>280	36	3	>95 : 5

[a] Ref. S10.

Table S2. Effects of Excitation Wavelength, Temperature, and Solvent on the Photoreaction of 2a-c

Substrate	Solvent	Temp. / °C	Irrad. / nm	Time / s	%Conv.	%Yield	%Distribution (rearrangement : cyclization/[2+2]adduct)
2a [a]	methylcyclohexane	20	300	90	10	4.0	3.2 : 96.8 (6.8 [b])
			330	480	3.0	1.1	3.5 : 96.5 (10 [b])
	acetonitrile	20	300	45	16	9.2	<0.1 : >99.9 (29 [b])
			330	180	6.0	4.0	<0.1 : >99.9 (19 [b])
2b	methylcyclohexane	80	300	20	8.9	2.0	48.7 : 51.3
		20	300	10	3.6	2.6	59.1 : 40.9
				20	14	4.3	59.6 : 40.4
				30	11	6.8	60.4 : 39.6
				45	7.6	8.3	58.3 : 41.7
		-40	300	30	4.6	2.6	68.6 : 31.4
		-80	300	30	6.9	3.0	70.6 : 29.4
		80	330	1200	5.4	3.1	18.9 : 81.1
		20	330	1800	11	2.5	14.4 : 85.6
		-40	330	1800	5.5	2.5	18.7 : 81.3
		-80	330	1800	4.2	2.1	21.3 : 78.7
	acetonitrile	20	300	30	12	7.8	5.3 : 94.7
			330	300	9.7	3.4	5.7 : 94.3
2c	methylcyclohexane	20	300	0 [c]	–	–	62.1 : 37.9
				5	0.4	0.4	64.0 : 36.0
				10	3.0	0.9	64.3 : 35.7
				15	7.4	1.1	68.6 : 31.4
				20	3.7	1.6	67.5 : 32.5
				45	10	3.2	69.1 : 30.9
		0	300	0 [c]	–	–	62.8 : 37.2
				5	1.2	0.4	64.5 : 35.5
				10	2.8	0.6	65.4 : 34.6
				15	3.9	1.0	66.9 : 33.1
				20	3.5	1.3	67.6 : 32.4
				45	11	3.2	68.3 : 31.7
		-20	300	0 [c]	–	–	54.1 : 45.9
				10	2.9	0.5	59.2 : 40.8
				20	4.6	1.1	62.8 : 37.2
				30	5.2	1.6	66.4 : 33.6
				45	8.7	2.5	67.2 : 32.8
		-40	300	0 [c]	–	–	53.8 : 46.2
				10	1.3	0.4	56.2 : 43.8
				20	2.6	0.9	59.2 : 40.8
				30	4.5	1.4	60.7 : 39.3
				45	6.7	2.2	62.7 : 37.3
			-50	90	10	3.6	67.3 : 32.7
			-60	45	4.3	1.9	60.0 : 40.0
		20	330	3600	12	2.8	55.7 : 44.3
		0	330	3600	6.2	2.4	51.5 : 48.5
		-20	330	3600	4.4	1.7	47.1 : 52.9
		-40	330	3600	4.3	1.1	41.4 : 58.6
		-50	330	7200	5.5	1.7	37.1 : 62.9
		-60	330	3600	2.6	1.7	26.3 : 73.7
	acetonitrile	20	300	45	30	11	<0.1 : >99.9
		20	330	480	6.0	2.0	<0.1 : >99.9

[a] [**2a-c**] = 0.1 mM. [b] Ref. S11. [c] Ratio of *meso*- and *ortho*-adducts (**mC**/**oC**). [d] Extrapolated value at time = 0 using data of 5-30 s.

(S10) Nishiuchi, E.; Mori, T.; Inoue, Y. *J. Am. Chem. Soc.* **2012**, *134*, 8082-8085.
(S11) Aoki, Y.; Matsuki, N.; Mori, T.; Ikeda, H.; Inoue, Y. *Org. Lett.* **2014**, *16*, 4888-4891.

Table S3. Calculated Conformer Population of 2a-c in Ground and Excited States

Substrate	State	Conformation A	G+	G-
2a	ground state	12 (9/3)	47 (33/14)	41 (10/31)
	excited state	0 (0/0)	77 (57/22)	23 (0/23)
2b	ground state	7 (3/1/0/3)	86 (69/12/4/1)	7 (0/0/1/6)
	excited state	0 (0/0/0/0)	96 (39/57/0/0)	4 (0/0/4/0)
2c	ground state	51 (36/1/10/4)	37 (19/4/2/12)	12 (8/1/2/1)
	excited state	1 (1/0/0/0)	89 (36/45/0/8)	10 (5/0/5/0)

[a] Population was estimated by Boltzmann distribution of the calculated energy at DFT-D3-TPSS/def2-TZVP or TD-DFT-CAM-B3LYP/def2-TZVP level. In parentheses, more detailed distributions are provided (a pair of *peri* and *ortho* for A, or *peri*-pro-*R*, *peri*-pro-*S*, *ortho*-pro-*R*, and *ortho*-pro-*S* for G+ and G-).

Table S4. Details of *E*(2) Stabilization Energy for Hyperconjugation of 2a-c by NBO Analysis [a]

Sub.	Conformation	State	$E(2)_{total}$	$\Delta E(2)^{total}$	$E(2)^{donor}$ (orbital interaction)	$E(2)^{acceptor}$ (orbital interaction)
2a	A	ground state	5.14		2.60 ($\sigma_{C11\text{-}H28} \rightarrow \sigma^*_{C12\text{-}H30}$)	2.54 ($\sigma_{C12\text{-}H30} \rightarrow \sigma^*_{C11\text{-}H28}$)
		excited state	4.70	-0.44	2.36	2.34
	A’	ground state	5.18		2.80 ($\sigma_{C11\text{-}H28} \rightarrow \sigma^*_{C12\text{-}H30}$)	2.38 ($\sigma_{C12\text{-}H30} \rightarrow \sigma^*_{C11\text{-}H28}$)
		excited state	4.97	-0.21	2.62	2.35
	G+-pro-*R*	ground state	5.07		3.99 ($\sigma_{C11\text{-}H28} \rightarrow \sigma^*_{C12\text{-}H13}$)	1.09 ($\sigma_{C12\text{-}H13} \rightarrow \sigma^*_{C11\text{-}H28}$)
		excited state	4.70	-0.37	3.83	0.87
	G+-pro-*S*	ground state	4.80		3.72 ($\sigma_{C11\text{-}H28} \rightarrow \sigma^*_{C12\text{-}H13}$)	1.08 ($\sigma_{C12\text{-}H13} \rightarrow \sigma^*_{C11\text{-}H28}$)
		excited state	4.13	-0.67	3.26	0.87
	G--pro-*R*	ground state	5.10		2.56 ($\sigma_{C11\text{-}H28} \rightarrow \sigma^*_{C12\text{-}H29}$)	2.54 ($\sigma_{C12\text{-}H29} \rightarrow \sigma^*_{C11\text{-}H28}$)
		excited state	4.54	-0.56	2.21	2.33
	G--pro-*S*	ground state	5.06		2.75 ($\sigma_{C11\text{-}H28} \rightarrow \sigma^*_{C12\text{-}H29}$)	2.31 ($\sigma_{C12\text{-}H29} \rightarrow \sigma^*_{C11\text{-}H28}$)
		excited state	4.44	-0.62	2.41	2.03
2b	*peri*-A	ground state	5.13		1.55 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}H33}$)	3.58 ($\sigma_{C13\text{-}H33} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	4.64	-0.49	1.34	3.30
	peri-A’	ground state	5.55		1.60 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}H33}$)	3.95 ($\sigma_{C13\text{-}H33} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	4.99	-0.56	1.28	3.71
	ortho-A	ground state	5.63		1.50 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}H33}$)	4.13 ($\sigma_{C13\text{-}H33} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	5.36	-0.27	1.42	3.94
	ortho-A’	ground state	5.11		1.71 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}H33}$)	3.40 ($\sigma_{C13\text{-}H33} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	4.98	-0.13	1.57	3.41
	peri-G+-pro-*R*	ground state	4.44		2.58 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}C14}$)	1.86 ($\sigma_{C13\text{-}C14} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	3.89	-0.55	2.51	1.38
	peri-G+-pro-*S*	ground state	4.13		2.42 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}C14}$)	1.71 ($\sigma_{C13\text{-}C14} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	3.30	-0.83	1.97	1.33
	ortho- G+-pro-*R*	ground state	4.57		2.39 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}C14}$)	2.18 ($\sigma_{C13\text{-}C14} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	4.20	-0.37	2.44	1.76
	ortho- G+-pro-*S*	ground state	4.26		2.61 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}C14}$)	1.65 ($\sigma_{C13\text{-}C14} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	4.44	+0.18	2.16	2.28
	peri-G--pro-*R*	ground state	5.28		1.29 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}H32}$)	3.99 ($\sigma_{C13\text{-}H32} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	5.12	-0.16	1.41	3.71
	peri-G--pro-*S*	ground state	5.06		1.47 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}H32}$)	3.59 ($\sigma_{C13\text{-}H32} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	2.69	-2.37	0.67	2.02
	ortho-G--pro-*R*	ground state	5.17		1.43 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}H32}$)	3.74 ($\sigma_{C13\text{-}H32} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	4.42	-0.75	1.25	3.17
	ortho-G--pro-*S*	ground state	4.91		1.61 ($\sigma_{C11\text{-}C12} \rightarrow \sigma^*_{C13\text{-}H32}$)	3.30 ($\sigma_{C13\text{-}H32} \rightarrow \sigma^*_{C11\text{-}C12}$)
		excited state	4.82	-0.09	1.49	3.33
2c	*peri*-A	ground state	5.30		1.05 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}H31}$)	4.25 ($\sigma_{C12\text{-}H31} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	4.92	-0.38	0.92	4.00
	peri-A’	ground state	5.35		1.11 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}H31}$)	4.24 ($\sigma_{C12\text{-}H31} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	5.14	-0.21	0.99	4.15
	ortho-A	ground state	5.53		1.06 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}H31}$)	4.47 ($\sigma_{C12\text{-}H31} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	5.17	-0.36	0.95	4.22
	ortho-A’	ground state	5.28		1.13 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}H31}$)	4.15 ($\sigma_{C12\text{-}H31} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	5.49	+0.21	1.02	4.17
	peri-G+-pro-*R*	ground state	3.58		1.71 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}C13}$)	1.87 ($\sigma_{C12\text{-}C13} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	3.07	-0.51	1.53	1.54
	peri-G+-pro-*S*	ground state	3.43		1.57 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}C13}$)	1.86 ($\sigma_{C12\text{-}C13} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	2.79	-0.64	1.17	1.62
	ortho- G+-pro-*R*	ground state	3.75		1.59 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}C13}$)	2.16 ($\sigma_{C12\text{-}C13} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	3.38	-0.37	1.66	1.72
	ortho- G+-pro-*S*	ground state	3.66		1.61 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}C13}$)	2.05 ($\sigma_{C12\text{-}C13} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	3.29	-0.37	1.38	1.91
	peri-G--pro-*R*	ground state	5.44		0.93 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}H30}$)	4.51 ($\sigma_{C12\text{-}H30} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	4.92	-0.52	0.97	3.95
	peri-G--pro-*S*	ground state	5.11		0.99 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}H30}$)	4.12 ($\sigma_{C12\text{-}H30} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	3.51	-1.60	0.54	2.97
	ortho-G--pro-*R*	ground state	5.19		0.99 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}H30}$)	4.20 ($\sigma_{C12\text{-}H30} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	4.65	-0.54	0.74	3.91
	ortho-G--pro-*S*	ground state	4.98		1.05 ($\sigma_{C11\text{-}O16} \rightarrow \sigma^*_{C12\text{-}H30}$)	3.93 ($\sigma_{C12\text{-}H30} \rightarrow \sigma^*_{C11\text{-}O16}$)
		excited state	5.13	+0.15	0.80	4.33

[a] *E*(2) energies were calculated by the Natural Bond Orbital (NBO) analysis at the CAM-B3LYP/def2-TZVP level with geometries optimized at the DFT-D3(BJ)-TPSS/def2-TZVP or TD-DFT-CAM-B3LYP/def2-TZVP level. $E(2)^{total} = E(2)^{donor} + E(2)^{acceptor}$ (all in kcal mol^{-1}).

Table S5. Optimized Geometries of **2a** at DFT-D3(BJ)-TPSS/def2-TZVP or TD-DFT-CAM-B3LYP/def2-TZVP level.

A (GS)				**A (EX)**				**A′ (GS)**			
C	2.213921	2.459203	-0.000811	C	2.156323	2.452278	-0.008754	C	3.068600	-2.427928	0.011933
C	3.590852	2.292258	0.267570	C	3.498686	2.298082	0.276041	C	4.335314	-1.880327	-0.290648
C	4.136854	1.028951	0.301137	C	4.047985	1.026596	0.315752	C	4.500986	-0.514399	-0.329697
C	3.335492	-0.119733	0.074987	C	3.262619	-0.114814	0.072159	C	3.415382	0.363072	-0.075518
C	1.934186	0.046588	-0.192354	C	1.878417	0.043319	-0.225174	C	2.125261	-0.189160	0.228957
C	1.407668	1.364734	-0.226419	C	1.351327	1.336168	-0.259935	C	1.994174	-1.602791	0.264689
C	3.889939	-1.424938	0.105233	C	3.817873	-1.396181	0.134114	C	3.578265	1.771390	-0.115375
C	3.098577	-2.526526	-0.121969	C	3.023093	-2.521662	-0.084517	C	2.513632	2.605210	0.135211
C	1.719765	-2.364619	-0.380741	C	1.686902	-2.379412	-0.368532	C	1.243712	2.063728	0.431960
C	1.130426	-1.115069	-0.417487	C	1.072076	-1.111437	-0.458340	C	1.033876	0.698823	0.483669
C	-0.355623	-1.001240	-0.650532	C	-0.380715	-1.030720	-0.682406	C	-0.352110	0.171738	0.756473
C	-1.128820	-0.756351	0.683214	C	-1.168044	-0.940834	0.686974	C	-1.074197	-0.227605	-0.567675
C	-2.609662	-0.775415	0.455643	C	-2.630138	-0.839194	0.502381	C	-2.428688	-0.801761	-0.286336
C	-3.280081	0.363702	0.110722	C	-3.189670	0.405828	0.134523	C	-3.521151	0.012369	-0.188547
C	-3.309372	-2.091036	0.568869	C	-3.436523	-2.088938	0.456717	C	-2.525114	-2.276193	-0.062569
C	-4.683014	0.369829	-0.162904	C	-4.569304	0.563647	-0.124332	C	-4.821408	-0.491084	0.125559
C	-2.596361	1.613681	-0.007951	C	-2.388911	1.551073	0.007809	C	-3.402774	1.425022	-0.377800
N	-5.824768	0.366602	-0.382174	N	-5.698162	0.665625	-0.335691	N	-5.875659	-0.910114	0.379874
N	-2.018050	2.617251	-0.110002	N	-1.664221	2.448513	-0.103334	N	-3.275792	2.571922	-0.520389
H	1.784282	3.456181	-0.030866	H	1.702740	3.432740	-0.037343	H	2.943438	-3.506463	0.047844
H	4.216034	3.163010	0.443342	H	4.120338	3.160722	0.470446	H	5.175305	-2.539887	-0.488246
H	5.196668	0.890601	0.501439	H	5.098069	0.896760	0.544109	H	5.473181	-0.083534	-0.556641
H	0.355509	1.525993	-0.435361	H	0.306622	1.513268	-0.465384	H	1.031345	-2.044990	0.502207
H	4.952179	-1.537329	0.307814	H	4.869904	-1.509173	0.360729	H	4.559527	2.177858	-0.347199
H	3.527272	-3.524434	-0.105150	H	3.463917	-3.507364	-0.031735	H	2.641200	3.683365	0.105709
H	1.106461	-3.245592	-0.559038	H	1.077446	-3.256085	-0.539996	H	0.409312	2.735265	0.620949
H	-0.589695	-0.184906	-1.341950	H	-0.655676	-0.162238	-1.275379	H	-0.320686	-0.691875	1.430034
H	-0.718513	-1.927892	-1.107502	H	-0.725752	-1.919662	-1.209421	H	-0.946627	0.946156	1.249701
H	-0.857153	-1.546016	1.390985	H	-0.918351	-1.826399	1.275922	H	-1.152549	0.666186	-1.193213
H	-0.809670	0.201845	1.103521	H	-0.773811	-0.073213	1.222267	H	-0.463663	-0.964352	-1.099411
H	-3.255984	-2.442061	1.607709	H	-3.136376	-2.783310	1.245887	H	-1.801780	-2.583229	0.703560
H	-4.356396	-2.041679	0.264854	H	-4.500179	-1.885523	0.574744	H	-3.523992	-2.593517	0.241917
H	-2.790614	-2.841187	-0.040942	H	-3.330671	-2.631135	-0.496435	H	-2.247235	-2.803992	-0.984013

A′ (EX)

C	3.243453	-2.391266	-0.015210
C	4.436470	-1.783257	-0.286703
C	4.511776	-0.376422	-0.316106
C	3.389905	0.423806	-0.060733
C	2.136754	-0.208922	0.237340
C	2.091989	-1.604660	0.242594
C	3.457494	1.820728	-0.099315
C	2.314056	2.621502	0.128473
C	1.121341	2.030952	0.416146
C	1.006827	0.608085	0.501475
C	-0.329713	0.032851	0.770824
C	-1.081710	-0.297372	-0.564847
C	-2.441115	-0.831827	-0.301197
C	-3.508099	0.004302	-0.191250
C	-2.563466	-2.297986	-0.074995
C	-4.817903	-0.467989	0.119158
C	-3.362020	1.412641	-0.366874
N	-5.866735	-0.860789	0.367900
N	-3.206266	2.542181	-0.498709
H	3.164513	-3.469206	0.006814
H	5.323165	-2.369977	-0.483179
H	5.454315	0.104833	-0.543432
H	1.164682	-2.113803	0.460829
H	4.405546	2.293365	-0.321973
H	2.396681	3.698181	0.077730
H	0.238559	2.630880	0.594890
H	-0.264662	-0.873460	1.373846
H	-0.935851	0.752365	1.321763
H	-1.127191	0.615501	-1.157533
H	-0.489794	-1.030003	-1.116361
H	-1.931533	-2.602420	0.765009
H	-3.582944	-2.609884	0.136255
H	-2.202641	-2.842808	-0.950677

G+-pro-R (GS)

C	0.687797	2.348718	-1.045014
C	1.887950	2.833561	-0.479313
C	2.811957	1.950467	0.030426
C	2.574347	0.551589	0.014401
C	1.346657	0.053912	-0.544625
C	0.428573	0.996366	-1.080670
C	3.520006	-0.360499	0.547653
C	3.271350	-1.713293	0.533225
C	2.059084	-2.201820	0.000756
C	1.098572	-1.355680	-0.523451
C	-0.214126	-1.938750	-0.987411
C	-1.247595	-2.122607	0.170156
C	-1.582287	-0.837095	0.870959
C	-2.540178	-0.003879	0.366774
C	-0.820904	-0.497902	2.108766
C	-2.850805	1.253861	0.968198
C	-3.244482	-0.334109	-0.832109
N	-3.096318	2.281009	1.454383
N	-3.790270	-0.616981	-1.819352
H	-0.035256	3.046918	-1.456058
H	2.079450	3.902281	-0.454180
H	3.743377	2.312288	0.459128
H	-0.493894	0.649965	-1.532571
H	4.444773	0.029926	0.964972
H	4.001137	-2.410867	0.933944
H	1.871514	-3.273681	0.007214
H	-0.673092	-1.334168	-1.773274
H	-0.039822	-2.933049	-1.411315
H	-2.153499	-2.563982	-0.258744
H	-0.830489	-2.825751	0.898237
H	0.254318	-0.564159	1.904998
H	-1.059411	0.495856	2.491303
H	-1.040523	-1.244816	2.883351

G+-pro-R (EX)

C	0.197682	2.298027	-0.968347
C	1.235748	2.933145	-0.314030
C	2.288755	2.185876	0.184606
C	2.306542	0.785567	0.065371
C	1.215871	0.123467	-0.563732
C	0.190822	0.909426	-1.111097
C	3.373556	0.036206	0.571640
C	3.373158	-1.347413	0.468603
C	2.297456	-1.992992	-0.101080
C	1.189002	-1.293194	-0.608344
C	-0.005552	-2.052524	-1.031173
C	-0.980959	-2.272797	0.189026
C	-1.398947	-1.050304	0.922859
C	-2.313984	-0.140312	0.309201
C	-1.109131	-0.955877	2.381543
C	-2.707206	1.057767	0.936666
C	-2.784591	-0.350253	-0.995109
N	-2.983145	2.051031	1.458392
N	-3.060731	-0.538642	-2.104650
H	-0.628349	2.868447	-1.366862
H	1.229294	4.007107	-0.195594
H	3.113414	2.677021	0.684928
H	-0.609573	0.456181	-1.669801
H	4.202836	0.547516	1.042868
H	4.206831	-1.917920	0.853211
H	2.283973	-3.073641	-0.145038
H	-0.559944	-1.549714	-1.818618
H	0.290639	-3.032271	-1.407092
H	-1.831970	-2.811637	-0.244964
H	-0.496801	-2.964012	0.880787
H	-0.097867	-1.298761	2.615813
H	-1.209468	0.065446	2.749477
H	-1.791086	-1.570511	2.990533

G+-pro-S (GS)

C	0.520173	2.428201	-1.317847
C	1.544372	2.881423	-0.456628
C	2.337015	1.970862	0.203243
C	2.135051	0.574485	0.049704
C	1.077193	0.108936	-0.803552
C	0.298402	1.079741	-1.487560
C	2.947528	-0.365592	0.730277
C	2.734269	-1.715456	0.575412
C	1.682514	-2.172607	-0.243229
C	0.847773	-1.297832	-0.914247
C	-0.336854	-1.857555	-1.661371
C	-1.595276	-2.008167	-0.741690
C	-2.168209	-0.686174	-0.336950
C	-1.856401	-0.112957	0.861633
C	-3.082785	-0.009649	-1.309278
C	-2.340519	1.184176	1.217646
C	-1.018332	-0.758872	1.823116
N	-2.734851	2.242955	1.491475
N	-0.353688	-1.279691	2.622131
H	-0.096470	3.148986	-1.846915
H	1.704198	3.947049	-0.321985
H	3.133772	2.308398	0.861485
H	-0.487739	0.756551	-2.161431
H	3.738868	0.000537	1.379191
H	3.359062	-2.434087	1.097043
H	1.505916	-3.242655	-0.329681
H	-0.593611	-1.254572	-2.538006
H	-0.092731	-2.860505	-2.025540
H	-2.357342	-2.569768	-1.295289
H	-1.305976	-2.589996	0.138246
H	-4.052477	-0.526003	-1.310202
H	-3.250478	1.041189	-1.066870
H	-2.684822	-0.089867	-2.327207

G+-pro-S (EX)

C	-0.280584	1.883945	-1.452819
C	0.591864	2.774725	-0.857446
C	1.749862	2.306925	-0.267037
C	2.039163	0.927406	-0.216835
C	1.113650	0.003532	-0.777304
C	-0.008045	0.510583	-1.442610
C	3.178018	0.459736	0.432067
C	3.393520	-0.906832	0.572841
C	2.463102	-1.803110	0.101360
C	1.299158	-1.385191	-0.563904
C	0.246680	-2.380320	-0.870672
C	-0.917760	-2.327861	0.193791
C	-1.903911	-1.239463	0.001264
C	-1.913864	-0.078009	0.827009
C	-2.968662	-1.465676	-1.015579
C	-2.892819	0.925949	0.685900
C	-0.905684	0.168321	1.771931
N	-3.689858	1.746467	0.522969
N	-0.022722	0.357148	2.496183
H	-1.185426	2.239348	-1.923622
H	0.368995	3.831979	-0.851883
H	2.440869	2.998595	0.196597
H	-0.678396	-0.155799	-1.955772
H	3.881157	1.168305	0.848993
H	4.277511	-1.262757	1.083180
H	2.614665	-2.862476	0.258417
H	-0.187282	-2.231136	-1.859778
H	0.684161	-3.378432	-0.857837
H	-1.418555	-3.298126	0.110079
H	-0.466070	-2.293539	1.186252
H	-3.616325	-2.311720	-0.749644
H	-3.611968	-0.596040	-1.139266
H	-2.557802	-1.712719	-2.005188

G--pro-R (GS)

C	-3.614610	-1.645633	0.708327
C	-4.415291	-0.493318	0.874084
C	-3.963992	0.727287	0.425567
C	-2.696681	0.854577	-0.199718
C	-1.876347	-0.312969	-0.363396
C	-2.378421	-1.555875	0.106116
C	-2.223230	2.109184	-0.662750
C	-0.994016	2.210149	-1.270960
C	-0.184805	1.063102	-1.427683
C	-0.593925	-0.180353	-0.983114
C	0.350900	-1.351219	-1.086837
C	1.046269	-1.694868	0.268158
C	1.729193	-0.494702	0.862119
C	2.956195	-0.102132	0.409258
C	1.003632	0.264480	1.922077
C	3.617612	1.061111	0.911307
C	3.634265	-0.836728	-0.612883
N	4.151100	2.009859	1.319845
N	4.161658	-1.446797	-1.450570
H	-3.979166	-2.608494	1.054755
H	-5.387638	-0.575877	1.350886
H	-4.576168	1.618245	0.542427
H	-1.783875	-2.455113	-0.022117
H	-2.851382	2.986501	-0.530764
H	-0.635514	3.170441	-1.629774
H	0.788565	1.160497	-1.902314
H	-0.163891	-2.253978	-1.433203
H	1.128642	-1.122863	-1.820910
H	0.299866	-2.063619	0.977627
H	1.772928	-2.492949	0.082325
H	0.831067	-0.392293	2.784775
H	1.544266	1.154095	2.249666
H	0.014400	0.554191	1.547099

G--pro-R (EX)

C	-3.350855	0.906366	-1.009783
C	-3.772725	-0.388842	-0.788486
C	-3.055189	-1.204454	0.073816
C	-1.919801	-0.728908	0.731176
C	-1.479456	0.602730	0.504694
C	-2.215734	1.397389	-0.375184
C	-1.172617	-1.571788	1.575453
C	-0.029885	-1.113182	2.215572
C	0.405587	0.170751	1.996145
C	-0.272899	1.045456	1.113721
C	0.419270	2.289765	0.732955
C	1.361229	2.004574	-0.501679
C	2.268697	0.839509	-0.339637
C	1.928664	-0.404755	-0.934925
C	3.607792	1.069693	0.275124
C	2.705472	-1.562750	-0.717515
C	0.768870	-0.576868	-1.706739
N	3.346222	-2.498041	-0.500781
N	-0.219624	-0.677630	-2.303234
H	-3.894259	1.544074	-1.692555
H	-4.645569	-0.773470	-1.296174
H	-3.363620	-2.229131	0.233608
H	-1.904217	2.410674	-0.575728
H	-1.503256	-2.591612	1.721332
H	0.530697	-1.775713	2.858795
H	1.302941	0.525498	2.478659
H	-0.266310	3.095050	0.475730
H	1.035722	2.630769	1.564513
H	0.717605	1.885606	-1.375456
H	1.930032	2.926092	-0.650523
H	3.544675	1.664509	1.193390
H	4.106214	0.133903	0.525561
H	4.285704	1.620036	-0.393975

G--pro-S (GS)

C	3.298908	1.358818	0.960229
C	3.953978	0.108329	0.999276
C	3.435936	-0.959609	0.303320
C	2.244190	-0.829880	-0.453989
C	1.574410	0.438688	-0.494764
C	2.140648	1.518248	0.231782
C	1.696123	-1.931379	-1.158904
C	0.535204	-1.792022	-1.882141
C	-0.125521	-0.544886	-1.920394
C	0.362977	0.557554	-1.244854
C	-0.426494	1.841386	-1.245505
C	-1.295111	2.002369	0.044769
C	-2.377362	0.968856	0.102418
C	-2.234454	-0.162474	0.851028
C	-3.595613	1.199358	-0.734306
C	-3.227733	-1.191993	0.856413
C	-1.089813	-0.391087	1.678177
N	-4.035767	-2.027811	0.850816
N	-0.175144	-0.579785	2.369941
H	3.710910	2.199196	1.511607
H	4.863701	-0.006466	1.581317
H	3.930820	-1.927306	0.328828
H	1.654793	2.489013	0.217819
H	2.209277	-2.888531	-1.112693
H	0.116603	-2.637302	-2.420350
H	-1.047219	-0.451923	-2.491100
H	0.230625	2.714215	-1.311353
H	-1.079407	1.869135	-2.124058
H	-0.643548	1.927464	0.920096
H	-1.751192	2.999524	0.034042
H	-3.306957	1.418097	-1.769538
H	-4.277166	0.347081	-0.727264
H	-4.130680	2.083823	-0.364807

G--pro-S (EX)

C	-4.108969	-1.380779	0.499049
C	-4.768368	-0.165554	0.449174
C	-4.075223	0.973290	0.068371
C	-2.723333	0.909474	-0.267229
C	-2.039933	-0.337103	-0.222712
C	-2.764058	-1.467870	0.166910
C	-2.014746	2.078336	-0.637393
C	-0.674978	2.027486	-0.970219
C	-0.001004	0.825412	-0.936537
C	-0.651452	-0.382053	-0.553157
C	0.193984	-1.564609	-0.405490
C	1.072905	-1.457744	0.916168
C	1.939310	-0.258646	1.018767
C	3.073808	-0.145542	0.174201
C	1.740198	0.670965	2.168115
C	3.918256	0.983059	0.215445
C	3.371714	-1.137144	-0.778259
N	4.574907	1.930891	0.265266
N	3.540284	-1.977008	-1.555589
H	-4.641263	-2.273794	0.795628
H	-5.816234	-0.101835	0.706163
H	-4.580973	1.929492	0.033319
H	-2.278658	-2.430427	0.207303
H	-2.546265	3.020929	-0.660808
H	-0.152649	2.929078	-1.256313
H	1.036342	0.776834	-1.222845
H	-0.365768	-2.494347	-0.369932
H	0.901585	-1.622867	-1.233150
H	0.393354	-1.505482	1.768272
H	1.648881	-2.388042	0.910939
H	2.126045	0.258775	3.112166
H	2.253178	1.619903	2.013885
H	0.681324	0.885316	2.339437

Table S6. Optimized Geometries of **2b** at DFT-D3(BJ)-TPSS/def2-TZVP or TD-DFT-CAM-B3LYP/def2-TZVP level.

peri-A (GS)

C	-1.6038186	-3.1958124	0.0769501
C	-2.9770829	-3.2380740	0.4031169
C	-3.7021567	-2.0697756	0.4632783
C	-3.0911002	-0.8150090	0.2083955
C	-1.6929282	-0.7664276	-0.1198759
C	-0.9805534	-1.9935118	-0.1788856
C	-3.8373832	0.3889526	0.2706788
C	-3.2316288	1.5961151	0.0180952
C	-1.8564605	1.6471533	-0.3000891
C	-1.0807407	0.5050911	-0.3733411
C	0.4082766	0.5973213	-0.6634759
C	0.8092340	1.8399900	-1.4661837
C	1.1804895	0.5096140	0.7005413
C	2.6653244	0.6816959	0.5623738
C	3.4549370	-0.3318811	0.0964074
C	3.2513623	2.0020333	0.9463434
C	4.8652804	-0.1783351	-0.0784311
C	2.9096447	-1.6093745	-0.2383424
N	6.0118031	-0.0472414	-0.2205601
N	2.4581172	-2.6474442	-0.5041364
H	-1.0300747	-4.1164154	0.0233155
H	-3.4573759	-4.1919999	0.6013492
H	-4.7615815	-2.0886907	0.7078233
H	0.0729661	-2.0033210	-0.4344274
H	-4.8946704	0.3375097	0.5187036
H	-3.8036560	2.5186209	0.0608390
H	-1.4081568	2.6167991	-0.4934273
H	0.7043452	-0.2785465	-1.2509864
H	1.8635141	1.7814214	-1.7557640
H	0.2114367	1.9130867	-2.3790874
H	0.6692614	2.7644002	-0.8952649
H	0.7892801	1.2878882	1.3633662
H	0.9513168	-0.4622047	1.1512169
H	3.0826869	2.1697159	2.0184063
H	4.3213201	2.0674391	0.7408338
H	2.7287717	2.8092169	0.4202442

peri-A (EX)

C	-2.224981	2.527017	0.113827
C	-3.551573	2.383194	-0.241815
C	-4.082489	1.113093	-0.388545
C	-3.295014	-0.035673	-0.186094
C	-1.924418	0.109279	0.177007
C	-1.419383	1.403345	0.324695
C	-3.841246	-1.310896	-0.349154
C	-3.048878	-2.442563	-0.166170
C	-1.725635	-2.314815	0.180343
C	-1.114285	-1.055530	0.366284
C	0.340315	-0.963962	0.634450
C	0.926045	-2.143510	1.400297
C	1.086150	-0.766028	-0.758280
C	2.553372	-0.621244	-0.659399
C	3.099660	0.593300	-0.183290
C	3.445734	-1.780511	-0.945260
C	4.492506	0.774780	-0.031074
C	2.284601	1.685172	0.150059
N	5.632675	0.896645	0.090584
N	1.557339	2.542911	0.429629
H	-1.783401	3.506367	0.231508
H	-4.173514	3.251954	-0.405546
H	-5.120313	0.987920	-0.669474
H	-0.390816	1.580765	0.596072
H	-4.883097	-1.412629	-0.623140
H	-3.479676	-3.425460	-0.297403
H	-1.131891	-3.204695	0.320005
H	0.543733	-0.062686	1.208570
H	1.949909	-1.906640	1.678506
H	0.367160	-2.349713	2.313848
H	0.960113	-3.054153	0.800841
H	0.837339	-1.625835	-1.385091
H	0.635604	0.116557	-1.223960
H	2.966465	-2.483125	-1.629127
H	4.384866	-1.457982	-1.398794
H	3.727538	-2.349470	-0.047511

peri-A′ (GS)

C	1.5175702	-3.0185330	0.2872903
C	2.9050440	-3.1100060	0.5306897
C	3.6765570	-1.9713937	0.5058226
C	3.1029444	-0.7006133	0.2416824
C	1.6892648	-0.5985690	-0.0080947
C	0.9301605	-1.8004494	0.0239653
C	3.9098641	0.4650730	0.2229763
C	3.3517720	1.6947710	-0.0287130
C	1.9652447	1.7986508	-0.2694365
C	1.1291599	0.6961318	-0.2687424
C	-0.3469250	0.9397217	-0.5434486
C	-0.8727146	0.2578607	-1.8196308
C	-1.2047045	0.6212739	0.7280106
C	-2.6601016	0.9043451	0.5243033
C	-3.5484659	-0.1133425	0.3194396
C	-3.0996406	2.3332386	0.5207967
C	-4.9395968	0.1243403	0.0912051
C	-3.1224316	-1.4787378	0.3023036
N	-6.0694737	0.3257093	-0.0946505
N	-2.7587242	-2.5829146	0.2791137
H	0.9020751	-3.9131113	0.3069682
H	3.3573616	-4.0759260	0.7360358
H	4.7468247	-2.0248844	0.6905953
H	-0.1360171	-1.7798675	-0.1602418
H	4.9757580	0.3648894	0.4120499
H	3.9679341	2.5891667	-0.0439760
H	1.5379269	2.7797385	-0.4665042
H	-0.4365745	2.0206326	-0.7082251
H	-1.8706565	0.6331275	-2.0702872
H	-0.2054380	0.4830623	-2.6564711
H	-0.9389327	-0.8275896	-1.7250838
H	-1.0590572	-0.4195008	1.0224454
H	-0.8286438	1.2529357	1.5412567
H	-2.5371402	2.8939113	-0.2362503
H	-4.1671534	2.4449107	0.3236940
H	-2.8630699	2.7919477	1.4891114

peri-A′ (EX)

C	1.979706	2.480791	0.035223
C	3.338423	2.461174	-0.205902
C	3.993726	1.244398	-0.290806
C	3.303433	0.027406	-0.135235
C	1.902334	0.041147	0.132282
C	1.270846	1.286686	0.205191
C	3.980095	-1.187050	-0.269985
C	3.289666	-2.391156	-0.158706
C	1.941467	-2.387739	0.105286
C	1.201755	-1.197566	0.278353
C	-0.260265	-1.316599	0.531216
C	-0.739168	-0.668567	1.835105
C	-1.079095	-0.865867	-0.750659
C	-2.543612	-0.800849	-0.571353
C	-3.157833	0.438122	-0.254616
C	-3.326824	-2.065861	-0.595938
C	-4.550853	0.556985	-0.062199
C	-2.399653	1.608931	-0.114188
N	-5.691136	0.625439	0.098850
N	-1.697557	2.522349	0.017030
H	1.432300	3.410965	0.090828
H	3.887871	3.382866	-0.335310
H	5.057110	1.214110	-0.490621
H	0.212693	1.374821	0.372507
H	5.042548	-1.183528	-0.474920
H	3.817054	-3.327674	-0.274556
H	1.417159	-3.328422	0.198798
H	-0.461930	-2.383460	0.640655
H	-1.770394	-0.966368	2.008992
H	-0.137917	-1.014276	2.676973
H	-0.722124	0.416752	1.823004
H	-0.698655	0.098693	-1.084069
H	-0.828364	-1.588240	-1.534951
H	-3.257234	-2.638683	0.341978
H	-4.387854	-1.880195	-0.760120
H	-2.974847	-2.731644	-1.390238

ortho-A (GS)

C	2.5521474	2.4456795	-0.5708948
C	3.8681254	1.9988886	-0.8195487
C	4.1688377	0.6633444	-0.6852206
C	3.1800435	-0.2791290	-0.3005795
C	1.8373718	0.1680260	-0.0401247
C	1.5703477	1.5561420	-0.1923598
C	3.5015413	-1.6541586	-0.1755192
C	2.5377699	-2.5638381	0.1865479
C	1.2201249	-2.1283548	0.4416090
C	0.8515656	-0.7978723	0.3464731
C	-0.6001997	-0.4598706	0.6481659
C	-0.8045575	0.4917515	1.8402351
C	-1.3486957	-0.0137390	-0.6525091
C	-2.8200648	0.1769136	-0.4273742
C	-3.6511724	-0.9038115	-0.3342831
C	-3.3376411	1.5726572	-0.2976304
C	-5.0523262	-0.7686989	-0.0876887
C	-3.1479270	-2.2347918	-0.4766547
N	-6.1911709	-0.6501178	0.1143532
N	-2.7148788	-3.3080219	-0.5894455
H	2.3117197	3.4997725	-0.6776178
H	4.6351703	2.7084603	-1.1157378
H	5.1771166	0.3032027	-0.8750410
H	0.5726834	1.9335081	-0.0062106
H	4.5216003	-1.9720263	-0.3761652
H	2.7795046	-3.6187861	0.2769911
H	0.4662868	-2.8622783	0.7167476
H	-1.0642996	-1.4099506	0.9338777
H	-1.8603336	0.5111992	2.1320824
H	-0.2273595	0.1347684	2.6979320
H	-0.4885903	1.5172921	1.6331664
H	-0.9183101	0.9129983	-1.0396609
H	-1.1845185	-0.7970727	-1.4000304
H	-3.1793374	2.1036049	-1.2458100
H	-4.3986561	1.6096713	-0.0438576
H	-2.7619177	2.1146374	0.4617829

ortho-A (EX)

C	-3.282505	-2.335438	-0.305387
C	-4.468500	-1.696297	-0.522511
C	-4.520417	-0.290180	-0.439845
C	-3.387074	0.473674	-0.129139
C	-2.137851	-0.191550	0.128548
C	-2.120641	-1.585066	0.012000
C	-3.448322	1.870036	-0.085125
C	-2.298280	2.647255	0.177546
C	-1.114731	2.027533	0.436346
C	-1.003947	0.598962	0.462031
C	0.357568	0.053816	0.766094
C	0.437615	-0.933475	1.933066
C	1.034399	-0.471252	-0.551601
C	2.463536	-0.847988	-0.369395
C	3.430407	0.106898	-0.328975
C	2.790545	-2.295637	-0.235469
C	4.807807	-0.208808	-0.130855
C	3.110342	1.489080	-0.482443
N	5.912248	-0.473686	0.030374
N	2.816184	2.592570	-0.597230
H	-3.213397	-3.412511	-0.368339
H	-5.364581	-2.253093	-0.759156
H	-5.456030	0.222378	-0.623173
H	-1.204348	-2.128069	0.169442
H	-4.393039	2.359001	-0.285467
H	-2.365509	3.726148	0.174868
H	-0.227021	2.612737	0.636439
H	0.957442	0.913697	1.064564
H	1.478343	-1.077004	2.224771
H	-0.092299	-0.532175	2.796408
H	0.013971	-1.910312	1.713176
H	0.473470	-1.325677	-0.930125
H	0.953459	0.328679	-1.288492
H	2.551704	-2.808704	-1.171616
H	3.837718	-2.473526	-0.004201
H	2.175013	-2.757885	0.537585

ortho-A′ (GS)

C	-2.4114335	2.6546811	-0.3239144
C	-3.7345928	2.2995390	-0.6658165
C	-4.1162239	0.9775746	-0.6361428
C	-3.2001575	-0.0429836	-0.2726495
C	-1.8518498	0.3111001	0.0736050
C	-1.4981536	1.6868008	0.0356460
C	-3.5931593	-1.4052031	-0.2459452
C	-2.6932081	-2.3810970	0.1083339
C	-1.3658060	-2.0358076	0.4462128
C	-0.9300252	-0.7247402	0.4374773
C	0.5137105	-0.3788220	0.7529895
C	1.2371371	-1.4104215	1.6253355
C	1.2726067	-0.1655090	-0.6014785
C	2.6578844	0.3678064	-0.4168955
C	3.7546567	-0.4208229	-0.6208026
C	2.7971052	1.7920803	0.0191274
C	5.0852215	0.0678634	-0.4305095
C	3.6338342	-1.7877595	-1.0249491
N	6.1639570	0.4716301	-0.2721706
N	3.5316665	-2.9007962	-1.3446066
H	-2.1125702	3.6990014	-0.3418234
H	-4.4462150	3.0701540	-0.9474093
H	-5.1333919	0.6915056	-0.8927178
H	-0.4908844	1.9912881	0.3010003
H	-4.6162623	-1.6602437	-0.5103881
H	-2.9935937	-3.4246553	0.1294105
H	-0.6767415	-2.8294902	0.7168188
H	0.5203369	0.5743868	1.2946174
H	2.2231019	-1.0357252	1.9178481
H	0.6659020	-1.6132289	2.5358876
H	1.3918159	-2.3547836	1.0945406
H	1.2895685	-1.1202510	-1.1348761
H	0.6986912	0.5481847	-1.2044807
H	2.2887137	1.9409056	0.9801690
H	3.8390313	2.0991176	0.1238025
H	2.2993276	2.4487210	-0.7052460

ortho-A′ (EX)

C	3.098529	-2.489294	-0.120446
C	4.300019	-1.980264	-0.522962
C	4.479306	-0.584477	-0.580373
C	3.454606	0.303407	-0.220835
C	2.189322	-0.222455	0.208506
C	2.042775	-1.612183	0.242138
C	3.635377	1.687785	-0.280247
C	2.590698	2.579668	0.053152
C	1.386705	2.092169	0.462182
C	1.153207	0.685596	0.565070
C	-0.200035	0.182615	0.940585
C	-1.015355	1.129267	1.814988
C	-0.974582	-0.168781	-0.383559
C	-2.303931	-0.784270	-0.146264
C	-3.459306	-0.114420	-0.400924
C	-2.313171	-2.164679	0.413542
C	-4.740091	-0.695974	-0.158500
C	-3.461639	1.215495	-0.918975
N	-5.763784	-1.173677	0.041536
N	-3.446616	2.288906	-1.324031
H	2.938181	-3.557287	-0.071738
H	5.113266	-2.636302	-0.801121
H	5.426069	-0.178496	-0.912574
H	1.115434	-2.052778	0.575470
H	4.593625	2.078981	-0.597172
H	2.755417	3.645869	-0.016268
H	0.593182	2.776967	0.719185
H	-0.074749	-0.749145	1.495183
H	-1.909684	0.626115	2.181144
H	-0.438260	1.454237	2.680362
H	-1.346392	2.013045	1.270043
H	-1.063670	0.742506	-0.973572
H	-0.353601	-0.872740	-0.944960
H	-1.871989	-2.171208	1.414560
H	-3.312913	-2.584679	0.484175
H	-1.696923	-2.821977	-0.204772

peri-G+-pro-R (GS)

C	-0.0042083	-2.6199804	-1.6144176
C	-1.0864562	-3.3841044	-1.1249698
C	-2.0859543	-2.7705000	-0.4065475
C	-2.0444633	-1.3783424	-0.1340853
C	-0.9388504	-0.5953860	-0.6192450
C	0.0641370	-1.2661098	-1.3715655
C	-3.0704003	-0.7525900	0.6173533
C	-3.0149461	0.5948331	0.8855653
C	-1.9245351	1.3621777	0.4238538
C	-0.8930522	0.8037010	-0.3096683
C	0.3046669	1.6562254	-0.6907128
C	-0.0696365	3.0495737	-1.2149664
C	1.2783534	1.8086420	0.5248603
C	1.7442045	0.4879438	1.0670567
C	2.7657056	-0.1827848	0.4567526
C	1.0383384	-0.0748165	2.2551318
C	3.2079189	-1.4679414	0.8956540
C	3.4119296	0.3604786	-0.6963400
N	3.5638308	-2.5163199	1.2503825
N	3.9066207	0.8174478	-1.6445495
H	0.7818203	-3.1032647	-2.1870330
H	-1.1265829	-4.4516792	-1.3201275
H	-2.9281502	-3.3454792	-0.0292401
H	0.9050631	-0.7099003	-1.7697175
H	-3.8993351	-1.3578056	0.9756133
H	-3.8034883	1.0750541	1.4578432
H	-1.8957434	2.4212952	0.6648541
H	0.8661037	1.1542742	-1.4819735
H	0.8275910	3.5743113	-1.5583276
H	-0.7658386	2.9658035	-2.0545085
H	-0.5412721	3.6634913	-0.4407510
H	2.1370634	2.4021933	0.1916289
H	0.7599121	2.3625062	1.3148908
H	-0.0387107	-0.1138968	2.0528558
H	1.3954551	-1.0701848	2.5244670
H	1.1729095	0.6011340	3.1099829

peri-G+-pro-R (EX)

C	-0.196245	2.198689	-1.342508
C	0.711786	3.101373	-0.822108
C	1.857868	2.634472	-0.205492
C	2.101377	1.255398	-0.065501
C	1.140926	0.321530	-0.545545
C	0.020973	0.824590	-1.225654
C	3.268404	0.796080	0.550434
C	3.491559	-0.564230	0.701169
C	2.539056	-1.470083	0.285348
C	1.336003	-1.067948	-0.318019
C	0.246455	-2.046948	-0.553205
C	0.696595	-3.470003	-0.857611
C	-0.701694	-2.049355	0.719522
C	-1.250584	-0.746802	1.166302
C	-2.302579	-0.131718	0.418657
C	-0.877636	-0.232109	2.512967
C	-2.840711	1.119378	0.775293
C	-2.779187	-0.710819	-0.767283
N	-3.235405	2.164336	1.071495
N	-3.061394	-1.202957	-1.777303
H	-1.092747	2.545944	-1.834467
H	0.531402	4.163689	-0.901447
H	2.584785	3.332817	0.189011
H	-0.681084	0.159826	-1.697602
H	3.998293	1.512370	0.904550
H	4.402065	-0.913763	1.167483
H	2.711312	-2.523202	0.448763
H	-0.374996	-1.712612	-1.380609
H	-0.174950	-4.064678	-1.127479
H	1.397580	-3.509634	-1.691825
H	1.157802	-3.953219	0.005000
H	-1.495153	-2.754075	0.443147
H	-0.140745	-2.513972	1.533636
H	0.196642	-0.323368	2.699722
H	-1.149716	0.816030	2.636565
H	-1.375677	-0.779662	3.328144

peri-G+-pro-S (GS)

C	-0.1443755	-2.6382144	-1.4540939
C	-0.9897867	-3.4531105	-0.6694418
C	-1.8458493	-2.8725495	0.2371006
C	-1.8850611	-1.4649672	0.4146701
C	-1.0088695	-0.6310904	-0.3622900
C	-0.1591454	-1.2690619	-1.3057637
C	-2.7629776	-0.8727149	1.3550002
C	-2.7807387	0.4904990	1.5274985
C	-1.9055260	1.3077399	0.7847180
C	-1.0187644	0.7837195	-0.1379026
C	-0.0125850	1.6943882	-0.8185606
C	-0.5589688	3.0918640	-1.1452285
C	1.2653753	1.8505296	0.0816890
C	2.0555139	0.5856601	0.1879498
C	1.9188791	-0.2558859	1.2535479
C	2.9952187	0.2717004	-0.9341001
C	2.6168700	-1.5019995	1.3152686
C	1.0697209	0.0451840	2.3634646
N	3.1848373	-2.5157853	1.3503104
N	0.4016046	0.2849046	3.2840863
H	0.5233565	-3.0953930	-2.1786291
H	-0.9628344	-4.5322629	-0.7871748
H	-2.5081412	-3.4868189	0.8421723
H	0.4959931	-0.6718868	-1.9300429
H	-3.4139150	-1.5165997	1.9406555
H	-3.4497750	0.9447902	2.2519881
H	-1.9174023	2.3775792	0.9695618
H	0.2997841	1.2407834	-1.7647136
H	0.1698514	3.6501044	-1.7421204
H	-1.4903350	3.0170261	-1.7138507
H	-0.7574688	3.6722659	-0.2387747
H	1.8995711	2.6251146	-0.3672699
H	0.9418749	2.1956993	1.0685331
H	3.8816944	0.9153625	-0.8506866
H	3.3225815	-0.7694280	-0.9288921
H	2.5297927	0.5028540	-1.8986785

peri-G+-pro-S (EX)

C	0.901559	-1.611811	-1.586062
C	0.409739	-2.789926	-1.059011
C	-0.821731	-2.798260	-0.435258
C	-1.572293	-1.610593	-0.277457
C	-1.028050	-0.378709	-0.738745
C	0.170935	-0.418837	-1.463203
C	-2.794987	-1.620632	0.382661
C	-3.461388	-0.427109	0.636365
C	-2.887340	0.775444	0.290569
C	-1.651720	0.841117	-0.370441
C	-0.918031	2.131089	-0.506969
C	-1.780799	3.376143	-0.353542
C	0.254879	2.142230	0.562717
C	1.504475	1.453608	0.164910
C	1.967307	0.274270	0.807293
C	2.380813	2.176479	-0.800336
C	3.245362	-0.260904	0.536383
C	1.159027	-0.473985	1.678464
N	4.285435	-0.688232	0.274850
N	0.446821	-1.099285	2.341784
H	1.852282	-1.598408	-2.098772
H	0.985429	-3.701125	-1.135802
H	-1.219178	-3.718196	-0.027487
H	0.534383	0.462525	-1.961325
H	-3.211991	-2.561120	0.717195
H	-4.415251	-0.441528	1.145416
H	-3.394606	1.690515	0.555128
H	-0.443909	2.176978	-1.489120
H	-1.188419	4.258844	-0.591206
H	-2.642975	3.362730	-1.021222
H	-2.140009	3.497369	0.669335
H	0.468772	3.204326	0.728999
H	-0.139619	1.754524	1.502855
H	2.824889	3.075811	-0.353406
H	3.203381	1.559284	-1.157993
H	1.820711	2.527299	-1.676248

ortho-G+-pro-R (GS)

C	2.7777082	1.5598010	-1.3920956
C	3.7486988	0.5421582	-1.5142935
C	3.5785254	-0.6445687	-0.8396900
C	2.4411222	-0.8692856	-0.0213425
C	1.4492662	0.1646099	0.1132211
C	1.6645851	1.3747272	-0.6013826
C	2.2684891	-2.1039973	0.6542333
C	1.1576979	-2.3209606	1.4325651
C	0.1820163	-1.3093596	1.5621842
C	0.2983250	-0.0826114	0.9322361
C	-0.8372312	0.9093818	1.1299410
C	-0.4388209	2.2266092	1.8185866
C	-1.6516677	1.1855516	-0.1757774
C	-2.1494903	-0.0880652	-0.7972777
C	-3.2566112	-0.7100400	-0.2935075
C	-1.3784032	-0.6644197	-1.9370494
C	-3.7405030	-1.9489349	-0.8159774
C	-3.9802378	-0.1482011	0.8042132
N	-4.1306680	-2.9576921	-1.2424836
N	-4.5469252	0.3267607	1.7017925
H	2.9104295	2.4980049	-1.9233831
H	4.6235082	0.6992568	-2.1384047
H	4.3167014	-1.4383425	-0.9248364
H	0.9421188	2.1772428	-0.5250732
H	3.0286024	-2.8726211	0.5399482
H	1.0199737	-3.2670534	1.9476614
H	-0.6946591	-1.4994208	2.1768911
H	-1.5422940	0.4130536	1.8060761
H	-1.3390435	2.7949872	2.0747345
H	0.1067847	2.0119702	2.7422129
H	0.1965503	2.8593833	1.1944787
H	-2.4975751	1.8248343	0.1005985
H	-1.0395387	1.7253729	-0.9025660
H	-0.3373162	-0.8197303	-1.6289487
H	-1.7965460	-1.6068310	-2.2948136
H	-1.3535721	0.0584296	-2.7626715

ortho-G+-pro-R (EX)

C	3.399754	1.300075	-1.577368
C	4.317772	0.300307	-1.455926
C	4.079057	-0.745668	-0.536893
C	2.925204	-0.783663	0.256251
C	1.946773	0.265245	0.134334
C	2.218907	1.284556	-0.786006
C	2.706176	-1.827943	1.161404
C	1.550819	-1.868553	1.975435
C	0.617331	-0.885863	1.861986
C	0.771417	0.192904	0.929528
C	-0.365930	1.170202	0.859059
C	0.001439	2.595913	1.295081
C	-1.113054	1.204265	-0.514172
C	-1.856016	-0.051160	-0.822652
C	-3.158120	-0.192903	-0.473669
C	-1.101956	-1.135286	-1.503643
C	-3.892728	-1.388229	-0.740821
C	-3.865043	0.849362	0.200863
N	-4.474946	-2.352046	-0.957385
N	-4.406899	1.697761	0.750354
H	3.555861	2.115475	-2.270052
H	5.221242	0.298231	-2.049542
H	4.800526	-1.546714	-0.439626
H	1.533095	2.106296	-0.903134
H	3.449364	-2.610300	1.246664
H	1.417771	-2.678478	2.679058
H	-0.270804	-0.906723	2.478970
H	-1.107019	0.825120	1.581810
H	-0.906905	3.189322	1.401973
H	0.508231	2.576152	2.259390
H	0.654253	3.102947	0.588563
H	-1.804912	2.044741	-0.473462
H	-0.396757	1.396903	-1.313052
H	-0.228441	-1.405638	-0.903520
H	-1.700507	-2.024676	-1.681345
H	-0.713075	-0.769500	-2.457193

ortho-G+-pro-S (GS)

C	1.9502864	0.9275896	-2.1967581
C	2.7915878	-0.1758324	-2.4550671
C	2.8790803	-1.1964668	-1.5366228
C	2.1284105	-1.1673816	-0.3331954
C	1.2563496	-0.0531292	-0.0701014
C	1.2119500	0.9869252	-1.0357645
C	2.2297560	-2.2217405	0.6089324
C	1.5003195	-2.1876722	1.7725321
C	0.6294754	-1.1054555	2.0211971
C	0.4821212	-0.0516425	1.1353406
C	-0.5017479	1.0451790	1.5203341
C	0.1865695	2.3703934	1.8966606
C	-1.6385893	1.3219435	0.4853742
C	-2.2259174	0.0894191	-0.1315697
C	-2.2964826	-0.0523559	-1.4878981
C	-2.7386724	-0.9753702	0.7838067
C	-2.8468033	-1.2243588	-2.0957269
C	-1.8469431	0.9667311	-2.3851570
N	-3.2934860	-2.1792757	-2.5857158
N	-1.4998364	1.8011589	-3.1163620
H	1.8725584	1.7322312	-2.9213640
H	3.3662522	-0.2147540	-3.3757866
H	3.5269435	-2.0503181	-1.7195035
H	0.5825324	1.8507490	-0.8690100
H	2.8952046	-3.0535455	0.3922402
H	1.5795959	-2.9911042	2.4990836
H	0.0494405	-1.0990256	2.9422672
H	-0.9981367	0.6770873	2.4265311
H	-0.5535429	3.0997536	2.2446692
H	0.9113701	2.2029884	2.6985163
H	0.7194925	2.8037631	1.0462096
H	-2.4393957	1.8410190	1.0321237
H	-1.3001789	2.0069652	-0.2948502
H	-3.3831135	-0.5298547	1.5510285
H	-3.2920881	-1.7497369	0.2498304
H	-1.8943622	-1.4448763	1.3037756

ortho-G+-pro-S (EX)

C	1.871410	-1.649514	-1.516439
C	2.640114	-2.129006	-0.476437
C	2.743597	-1.387547	0.684649
C	2.080150	-0.152974	0.828485
C	1.263483	0.336055	-0.233117
C	1.197089	-0.428200	-1.395907
C	2.212794	0.582338	2.003432
C	1.568321	1.809851	2.141029
C	0.757433	2.274185	1.135049
C	0.530880	1.548827	-0.049048
C	-0.464754	2.118584	-1.032336
C	0.158514	2.646205	-2.328323
C	-1.631940	1.135179	-1.257397
C	-2.030458	0.439323	0.007794
C	-1.982766	-0.979455	0.091120
C	-2.775508	1.236712	1.021635
C	-2.356964	-1.662931	1.268584
C	-1.509214	-1.778521	-0.957229
N	-2.651701	-2.193476	2.250050
N	-1.070642	-2.389276	-1.841105
H	1.750138	-2.221130	-2.423354
H	3.144670	-3.080584	-0.561409
H	3.339224	-1.752591	1.511317
H	0.599100	-0.103855	-2.226608
H	2.829583	0.197494	2.804722
H	1.690941	2.384399	3.048351
H	0.237491	3.212581	1.265942
H	-0.887814	2.988065	-0.526841
H	-0.614577	3.133513	-2.922293
H	0.939891	3.380506	-2.129702
H	0.590411	1.855222	-2.939487
H	-2.465430	1.716865	-1.675520
H	-1.374158	0.412124	-2.029979
H	-3.753908	1.569817	0.642887
H	-2.963089	0.664806	1.928954
H	-2.244194	2.148281	1.318139

peri-G--pro-R (GS)

C	0.0809712	-2.4221279	1.3534939
C	-0.8910115	-3.3011455	0.8287560
C	-1.9249396	-2.7965207	0.0760099
C	-2.0321825	-1.4068641	-0.1926710
C	-1.0419505	-0.5032469	0.3312792
C	0.0009612	-1.0686782	1.1137975
C	-3.0950669	-0.9088148	-0.9849649
C	-3.1892891	0.4341936	-1.2569975
C	-2.2148600	1.3182882	-0.7548410
C	-1.1473048	0.8918414	0.0174489
C	-0.1380555	1.9595886	0.4175656
C	0.1658818	2.0963909	1.9193280
C	1.1338928	1.9601323	-0.5114037
C	1.9906951	0.7332061	-0.4995157
C	1.8159952	-0.2498434	-1.4318810
C	3.0715098	0.6346779	0.5316481
C	2.5929823	-1.4488213	-1.4102489
C	0.8332857	-0.1547167	-2.4654544
N	3.2252074	-2.4239482	-1.3754950
N	0.0505846	-0.0802423	-3.3218591
H	0.9027716	-2.8164195	1.9440233
H	-0.8162356	-4.3678785	1.0175873
H	-2.6806856	-3.4592773	-0.3383301
H	0.7672809	-0.4272323	1.5260896
H	-3.8273547	-1.6102605	-1.3762534
H	-4.0008039	0.8197293	-1.8668185
H	-2.2939413	2.3759513	-0.9971231
H	-0.6181191	2.9065682	0.1425097
H	0.7671331	2.9959068	2.0937371
H	-0.7732085	2.2036082	2.4707619
H	0.6979981	1.2488567	2.3528109
H	0.7722068	2.1367811	-1.5289546
H	1.7485775	2.8187982	-0.2133298
H	2.6857602	0.8932746	1.5230300
H	3.5300392	-0.3552266	0.5649907
H	3.8512748	1.3734713	0.3012741

peri-G--pro-R (EX)

C	-0.195010	1.968776	-1.627777
C	-1.297327	2.694437	-1.226243
C	-2.318603	2.051858	-0.551770
C	-2.245754	0.680754	-0.244872
C	-1.106828	-0.074372	-0.646436
C	-0.107166	0.599373	-1.360748
C	-3.256454	0.084339	0.508434
C	-3.142382	-1.239517	0.899271
C	-2.027527	-1.962160	0.544999
C	-0.982998	-1.428217	-0.231825
C	0.189910	-2.330747	-0.483918
C	0.616405	-2.493010	-1.944657
C	1.405165	-2.002005	0.464763
C	2.168450	-0.752328	0.212087
C	1.837312	0.439568	0.932302
C	3.480284	-0.838313	-0.498718
C	2.503280	1.657140	0.691975
C	0.787520	0.472730	1.861077
N	3.040535	2.649325	0.441933
N	-0.131287	0.448861	2.565968
H	0.623765	2.456172	-2.136575
H	-1.357387	3.754951	-1.423997
H	-3.185697	2.609137	-0.221997
H	0.765733	0.068571	-1.686073
H	-4.113462	0.672923	0.807539
H	-3.916194	-1.697523	1.498850
H	-1.939561	-2.986655	0.878753
H	-0.146383	-3.318143	-0.161006
H	1.212372	-3.401202	-2.035972
H	-0.243976	-2.592889	-2.607088
H	1.233978	-1.674756	-2.303735
H	1.021905	-2.034331	1.488868
H	2.069790	-2.865009	0.360292
H	3.468226	-1.594875	-1.284867
H	3.766227	0.111417	-0.953878
H	4.304528	-1.107748	0.180642

peri-G--pro-S (GS)

C	-0.1631667	-2.5866066	1.0614399
C	-1.3693854	-3.2584011	0.7681080
C	-2.4504994	-2.5431358	0.3078654
C	-2.3766184	-1.1388946	0.1156436
C	-1.1527658	-0.4441982	0.4201219
C	-0.0642015	-1.2223732	0.8980164
C	-3.4900011	-0.4220914	-0.3897804
C	-3.4059491	0.9328927	-0.5996423
C	-2.2065137	1.6138571	-0.3048297
C	-1.0857323	0.9713365	0.1957177
C	0.1332362	1.8469758	0.4621790
C	0.7767269	1.7173815	1.8537235
C	1.1990464	1.8381012	-0.6980390
C	1.8186469	0.5156250	-1.0241902
C	3.0023978	0.1284912	-0.4571296
C	1.1326576	-0.3395416	-2.0417163
C	3.5804653	-1.1507919	-0.7254939
C	3.7325099	0.9808708	0.4277989
N	4.0364151	-2.1996375	-0.9355372
N	4.3282444	1.6839208	1.1370711
H	0.6962153	-3.1475943	1.4168678
H	-1.4385801	-4.3337066	0.9035948
H	-3.3857424	-3.0458194	0.0734992
H	0.8748181	-0.7401377	1.1279769
H	-4.4052428	-0.9657133	-0.6100297
H	-4.2563090	1.4867366	-0.9867115
H	-2.1608373	2.6883840	-0.4701161
H	-0.2549452	2.8712552	0.4127450
H	1.3922039	2.5993536	2.0542809
H	-0.0007833	1.6525816	2.6206066
H	1.4253445	0.8468221	1.9605948
H	0.6975435	2.2097694	-1.5983854
H	1.9757836	2.5565737	-0.4145996
H	1.3210646	0.0929199	-3.0349815
H	1.4933615	-1.3693865	-2.0390499
H	0.0505915	-0.3258187	-1.8876190

peri-G--pro-S (EX)

C	0.231791	1.861334	-1.476892
C	-0.688563	2.823736	-1.104801
C	-1.867074	2.436284	-0.496108
C	-2.140879	1.081582	-0.213726
C	-1.172013	0.089797	-0.541771
C	-0.011684	0.511504	-1.211309
C	-3.337179	0.712552	0.403817
C	-3.579549	-0.614890	0.719605
C	-2.611636	-1.565100	0.466099
C	-1.388274	-1.256436	-0.149338
C	-0.356095	-2.329993	-0.236843
C	0.168408	-2.658709	-1.643270
C	0.845098	-2.079115	0.796453
C	1.177443	-0.692538	1.204559
C	2.230225	0.043899	0.579706
C	0.515192	-0.166132	2.428825
C	2.572628	1.346102	0.992082
C	2.931573	-0.470007	-0.523241
N	2.805555	2.425704	1.332202
N	3.417096	-0.918145	-1.473300
H	1.154531	2.139066	-1.964227
H	-0.491211	3.869571	-1.290714
H	-2.600073	3.180946	-0.213260
H	0.703790	-0.204437	-1.563984
H	-4.071466	1.473377	0.634677
H	-4.509640	-0.900979	1.190219
H	-2.788347	-2.590173	0.762942
H	-0.849904	-3.237815	0.109802
H	0.574649	-3.669708	-1.627552
H	-0.630208	-2.634095	-2.385614
H	0.979286	-2.015950	-1.974311
H	0.582390	-2.648279	1.692178
H	1.708547	-2.575536	0.349689
H	0.809123	-0.730288	3.325620
H	0.758464	0.878853	2.613578
H	-0.577158	-0.248038	2.375025

ortho-G--pro-R (GS)

C	3.0494541	1.2363888	1.9437771
C	3.8717848	0.0914870	2.0147330
C	3.6074680	-0.9892994	1.2055407
C	2.5173464	-0.9766537	0.2995027
C	1.6813139	0.1873649	0.2165594
C	1.9858171	1.2816718	1.0684683
C	2.2308631	-2.1032177	-0.5116113
C	1.1659224	-2.0850356	-1.3785387
C	0.3444558	-0.9400894	-1.4651286
C	0.5741631	0.1840586	-0.6938336
C	-0.3641890	1.3732284	-0.7530608
C	-0.9863465	1.6078855	-2.1341004
C	-1.4335361	1.2917363	0.4026125
C	-2.4540552	0.2108739	0.2206048
C	-2.2482470	-1.0467788	0.7123817
C	-3.7246914	0.5539923	-0.4940695
C	-3.1892005	-2.1014607	0.4897861
C	-1.1172401	-1.3905537	1.5172888
N	-3.9507186	-2.9588417	0.2975623
N	-0.2368402	-1.6889362	2.2151577
H	3.2557962	2.0881996	2.5857066
H	4.7059830	0.0663480	2.7097623
H	4.2277952	-1.8807700	1.2548703
H	1.3728559	2.1768351	1.0407089
H	2.8651934	-2.9818697	-0.4280074
H	0.9425719	-2.9500509	-1.9960429
H	-0.4936566	-0.9584395	-2.1548637
H	0.2140998	2.2725040	-0.5168381
H	-1.6179195	2.5031218	-2.1224189
H	-0.1966969	1.7569093	-2.8763315
H	-1.6001477	0.7674096	-2.4696553
H	-0.8878042	1.1407856	1.3397696
H	-1.9475386	2.2587667	0.4528625
H	-3.5188880	1.1076954	-1.4144444
H	-4.3269789	-0.3268215	-0.7246427
H	-4.3181893	1.2215559	0.1459325

ortho-G--pro-R (EX)

C	-3.370657	0.609305	-1.320796
C	-3.901195	-0.482885	-0.665645
C	-3.239396	-1.004513	0.434793
C	-2.050887	-0.434516	0.893300
C	-1.494174	0.685847	0.219477
C	-2.182737	1.185949	-0.887402
C	-1.370646	-0.993213	1.990468
C	-0.179582	-0.447017	2.443176
C	0.368896	0.632932	1.794897
C	-0.236389	1.203201	0.649199
C	0.532763	2.193653	-0.144965
C	1.376074	3.152372	0.690603
C	1.418049	1.394440	-1.186408
C	2.252728	0.288917	-0.638576
C	1.780668	-1.050150	-0.739367
C	3.701195	0.543023	-0.363838
C	2.497482	-2.124304	-0.168435
C	0.568368	-1.385525	-1.361113
N	3.090458	-2.980355	0.329005
N	-0.455953	-1.613143	-1.853280
H	-3.870856	1.016499	-2.188080
H	-4.816095	-0.939706	-1.014685
H	-3.633378	-1.874392	0.943450
H	-1.794753	2.033703	-1.428758
H	-1.792088	-1.860509	2.481153
H	0.330962	-0.889177	3.286301
H	1.302378	1.038213	2.145124
H	-0.155271	2.799392	-0.733300
H	1.795474	3.917212	0.037485
H	0.781667	3.654466	1.455226
H	2.211155	2.652767	1.176243
H	0.738827	1.023680	-1.958320
H	2.046148	2.152537	-1.662636
H	3.870561	1.519229	0.093042
H	4.127279	-0.211170	0.298186
H	4.305892	0.521997	-1.283757

ortho-G--pro-S (GS)

C	2.9869441	1.9562266	1.1870955
C	3.9705770	0.9745087	1.4384161
C	3.8198916	-0.2918454	0.9214895
C	2.6841922	-0.6358378	0.1435468
C	1.6725795	0.3538526	-0.1034416
C	1.8706744	1.6525763	0.4378804
C	2.5335630	-1.9387698	-0.3960150
C	1.4343985	-2.2513390	-1.1591330
C	0.4333291	-1.2825957	-1.3940838
C	0.5182321	-0.0036033	-0.8758117
C	-0.6088588	0.9942388	-1.0706890
C	-1.5215649	0.6844770	-2.2612185
C	-1.4451487	1.2014514	0.2476389
C	-2.1084767	-0.0366702	0.7722092
C	-3.4123772	-0.3173972	0.4709531
C	-1.3118878	-0.9376638	1.6597063
C	-4.0616409	-1.5006832	0.9445535
C	-4.2151201	0.5662793	-0.3163627
N	-4.5870868	-2.4654139	1.3252930
N	-4.8665427	1.2927371	-0.9485580
H	3.1139424	2.9595878	1.5835112
H	4.8452825	1.2244661	2.0316590
H	4.5751332	-1.0537057	1.0987216
H	1.1391087	2.4313353	0.2484824
H	3.3047098	-2.6793824	-0.1999359
H	1.3224666	-3.2459861	-1.5807614
H	-0.4309259	-1.5649919	-1.9862741
H	-0.1581116	1.9766845	-1.2579254
H	-2.2350535	1.4988056	-2.4108969
H	-0.9289679	0.5673053	-3.1735257
H	-2.0998107	-0.2327320	-2.1124321
H	-0.7700402	1.5789775	1.0224479
H	-2.1956393	1.9704457	0.0377429
H	-1.0073609	-0.3778905	2.5536357
H	-1.8710495	-1.8233161	1.9664927
H	-0.3893607	-1.2441316	1.1555891

ortho-G--pro-S (EX)

C	3.525991	-1.765433	-1.149326
C	4.429771	-0.752888	-1.291770
C	4.177032	0.490033	-0.675273
C	3.021144	0.712220	0.083380
C	2.057626	-0.343449	0.227354
C	2.344626	-1.565047	-0.388511
C	2.782115	1.942736	0.706828
C	1.625086	2.158697	1.487870
C	0.696789	1.170512	1.617904
C	0.866735	-0.092765	0.964866
C	-0.224357	-1.110920	1.019476
C	-1.184383	-0.965555	2.194926
C	-1.013674	-1.238023	-0.343217
C	-1.786664	-0.044603	-0.777381
C	-3.127536	0.051745	-0.569541
C	-1.038417	1.011910	-1.512093
C	-3.879485	1.186401	-0.998707
C	-3.868519	-0.983447	0.075224
N	-4.475231	2.104311	-1.343231
N	-4.447162	-1.826658	0.595259
H	3.698201	-2.728972	-1.608690
H	5.332988	-0.892483	-1.869110
H	4.885420	1.300222	-0.791349
H	1.675971	-2.404121	-0.267829
H	3.515693	2.732368	0.606570
H	1.483520	3.111622	1.978865
H	-0.183415	1.339618	2.218082
H	0.247917	-2.090677	1.117733
H	-1.855013	-1.822372	2.235496
H	-0.638487	-0.916926	3.137012
H	-1.807386	-0.075178	2.119041
H	-0.280123	-1.474516	-1.117418
H	-1.674899	-2.096569	-0.231658
H	-0.708771	0.612494	-2.476078
H	-1.631553	1.904347	-1.693697
H	-0.131220	1.285793	-0.970828

Table S7. Optimized Geometries of **2c** at DFT-D3(BJ)-TPSS/def2-TZVP or TD-DFT-CAM-B3LYP/def2-TZVP level.

peri-A (GS)				**peri-A (EX)**				**peri-A′ (GS)**			
C	3.1454808	-0.4062354	0.5152634	C	-3.383748	0.022408	-0.243460	C	1.1075342	-1.3163750	-0.3527366
C	3.2990578	-1.7822896	0.8211570	C	-3.850683	-1.256694	-0.560664	C	1.4403531	-2.6949013	-0.3919396
C	2.2271797	-2.6409843	0.7447433	C	-2.973548	-2.365961	-0.589903	C	0.4886364	-3.6549958	-0.1421085
C	0.9588564	-2.1575829	0.3575108	C	-1.656437	-2.205010	-0.279883	C	-0.8371691	-3.2673919	0.1487351
C	0.7639206	-0.8275491	0.0406525	C	-1.141366	-0.923247	0.084492	C	-1.2154809	-1.9390112	0.1870560
C	1.8567994	0.0902714	0.1174511	C	-1.997905	0.208765	0.082175	C	-0.2405353	-0.9177883	-0.0529541
C	1.7311280	1.4754597	-0.1719307	C	-1.564694	1.505418	0.368074	C	-0.5342239	0.4718479	-0.0060699
C	2.8140076	2.3223793	-0.0774858	C	-2.448780	2.614494	0.354196	C	0.4400022	1.4118951	-0.2628859
C	4.0804763	1.8302756	0.3090072	C	-3.768928	2.430677	0.056662	C	1.7611006	1.0165700	-0.5678299
C	4.2390100	0.4938300	0.5975209	C	-4.235121	1.136468	-0.244743	C	2.0855613	-0.3203836	-0.6059921
C	-0.6279849	-0.3567932	-0.3445626	C	0.323967	-0.798569	0.337600	C	-2.6789641	-1.6299731	0.4392684
C	-1.3923574	0.1637371	0.8994273	C	1.068885	-0.436104	-0.985252	C	-3.3792685	-1.0898006	-0.8334956
C	-2.8062746	0.5420935	0.5602722	C	2.542947	-0.355685	-0.801197	C	-4.7974828	-0.6956305	-0.5513399
C	-3.0845224	1.7498209	-0.0145680	C	3.119936	0.761151	-0.278923	C	-5.1635821	0.6180223	-0.5182076
C	-3.8756651	-0.4592514	0.8402540	C	3.344779	-1.554649	-1.165680	C	-5.7817188	-1.7870436	-0.2790283
O	-1.4294250	-1.4037251	-0.8993968	O	0.903215	-1.993968	0.811758	O	-2.9231695	-0.6585224	1.4601412
C	-1.0449762	-1.7348282	-2.2376880	C	0.600517	-2.279722	2.160898	C	-2.3855157	-1.0334341	2.7297308
C	-4.4104951	2.1274354	-0.3914387	C	4.523090	0.855334	-0.038674	C	-6.5049547	1.0220572	-0.2308328
C	-2.0500380	2.6993582	-0.2806709	C	2.345250	1.909318	0.058126	C	-4.2212999	1.6695096	-0.7463762
N	-5.4900058	2.4325942	-0.6967272	N	5.652240	0.926678	0.151481	N	-7.5975221	1.3443419	0.0018852
N	-1.1943070	3.4577886	-0.4931132	N	1.693496	2.815616	0.327937	N	-3.4548628	2.5241817	-0.9295811
H	4.2800826	-2.1445121	1.1185192	H	-4.897049	-1.391152	-0.802006	H	2.4654521	-2.9768148	-0.6195852
H	2.3491235	-3.6942010	0.9809953	H	-3.357477	-3.341029	-0.856885	H	0.7485380	-4.7092322	-0.1653760
H	0.1154619	-2.8390192	0.2935346	H	-0.977110	-3.044713	-0.289960	H	-1.5842481	-4.0339897	0.3450972
H	0.7736418	1.8905705	-0.4671667	H	-0.531852	1.703183	0.612034	H	-1.5332437	0.7994829	0.2518292
H	2.6878485	3.3776083	-0.3011662	H	-2.056680	3.595934	0.580449	H	0.1836517	2.4666531	-0.2301361
H	4.9256069	2.5091308	0.3782406	H	-4.456974	3.264472	0.044840	H	2.5183715	1.7693408	-0.7674712
H	5.2089626	0.1045589	0.8976575	H	-5.279107	0.989418	-0.491338	H	3.1007908	-0.6371965	-0.8324793
H	-0.5634345	0.4588268	-1.0788649	H	0.523845	0.000138	1.059606	H	-3.1648613	-2.5755323	0.7339752
H	-1.3903381	-0.6268374	1.6552243	H	0.827048	-1.204937	-1.719349	H	-2.8096004	-0.2451649	-1.2260770
H	-0.8367007	1.0208451	1.2935114	H	0.658155	0.512950	-1.333994	H	-3.3607411	-1.8908567	-1.5814194
H	-3.6120655	-1.3974302	0.3385562	H	2.968477	-2.417720	-0.614610	H	-5.7976197	-2.4946185	-1.1170446
H	-3.9043926	-0.6699298	1.9174293	H	3.215921	-1.774334	-2.229051	H	-5.4679279	-2.3519495	0.6079398
H	-4.8626022	-0.1264822	0.5141275	H	4.405343	-1.431876	-0.961920	H	-6.7904460	-1.4065914	-0.1103696
H	-1.7245874	-2.5222975	-2.5676425	H	1.144139	-3.184045	2.424555	H	-2.6899961	-0.2546528	3.4304203
H	-1.1464528	-0.8589561	-2.8936833	H	0.924116	-1.463590	2.814845	H	-2.7921434	-2.0031692	3.0531104
H	-0.0100191	-2.0976797	-2.2749503	H	-0.470239	-2.448082	2.308153	H	-1.2906131	-1.0958943	2.6950026

peri-A′ (EX)

C	3.344431	0.025416	-0.315369
C	3.941130	-1.205259	-0.607537
C	3.192203	-2.405615	-0.555928
C	1.875115	-2.369787	-0.210135
C	1.223236	-1.138103	0.108412
C	1.958780	0.076011	0.059916
C	1.409153	1.330692	0.343127
C	2.164088	2.530086	0.238849
C	3.478064	2.477896	-0.121661
C	4.065927	1.225655	-0.398225
C	-0.252097	-1.195139	0.352044
C	-1.036462	-0.707835	-0.899540
C	-2.508298	-0.691704	-0.679463
C	-3.172527	0.463650	-0.441356
C	-3.208293	-2.006034	-0.700605
O	-0.721092	-0.429443	1.439946
C	-0.234975	-0.846630	2.696170
C	-4.579971	0.493462	-0.198671
C	-2.501494	1.724020	-0.401817
N	-5.710707	0.508672	-0.008179
N	-1.948437	2.728155	-0.368568
H	4.988052	-1.233686	-0.879373
H	3.674667	-3.346313	-0.783182
H	1.302874	-3.287170	-0.157120
H	0.382528	1.403584	0.665205
H	1.676141	3.471071	0.450146
H	4.071033	3.378155	-0.202774
H	5.103986	1.182109	-0.703665
H	-0.515785	-2.246856	0.529712
H	-0.667672	0.280654	-1.166883
H	-0.794419	-1.391368	-1.715758
H	-3.031224	-2.507264	-1.655086
H	-2.801762	-2.657503	0.076992
H	-4.279785	-1.916377	-0.544295
H	-0.741484	-0.243986	3.446296
H	-0.461700	-1.904071	2.872877
H	0.844849	-0.699449	2.782179

ortho-A (GS)

C	2.8602299	-1.3002342	-0.3882870
C	2.6910286	-2.7007561	-0.2395291
C	1.4778106	-3.2245523	0.1395188
C	0.3858608	-2.3634886	0.3804952
C	0.4976796	-0.9929143	0.2423400
C	1.7511378	-0.4196193	-0.1428502
C	1.9619597	0.9785855	-0.2916813
C	3.1893312	1.4758217	-0.6735195
C	4.2742215	0.6063894	-0.9229800
C	4.1094556	-0.7520405	-0.7783348
C	-0.7598420	-0.1696994	0.4511007
C	-1.3401072	0.3382065	-0.8923397
C	-2.6297395	1.0782451	-0.6806605
C	-3.7962343	0.3845450	-0.5230156
C	-2.5796845	2.5670908	-0.6090188
O	-0.5970090	0.9828242	1.2872614
C	-0.2037122	0.6425337	2.6194511
C	-5.0446446	1.0360324	-0.2799805
C	-3.8131203	-1.0445580	-0.5750321
N	-6.0581950	1.5704803	-0.0830833
N	-3.7938086	-2.2067810	-0.6116399
H	3.5411288	-3.3511888	-0.4299525
H	1.3514421	-4.2968615	0.2554265
H	-0.5731916	-2.7874559	0.6699018
H	1.1482557	1.6589833	-0.0712052
H	3.3260415	2.5485704	-0.7784562
H	5.2357882	1.0129371	-1.2228139
H	4.9383551	-1.4316238	-0.9610247
H	-1.5109748	-0.8295138	0.9116965
H	-0.6066619	0.9877528	-1.3767704
H	-1.4974156	-0.5398020	-1.5258955
H	-1.8731795	2.8529553	0.1790746
H	-2.1843775	2.9658311	-1.5523586
H	-3.5559959	3.0134839	-0.4119375
H	-0.1661502	1.5795963	3.1772550
H	-0.9391574	-0.0331498	3.0788476
H	0.7834750	0.1633746	2.6299976

ortho-A (EX)

C	-3.378255	0.582949	-0.257111
C	-3.406354	1.976415	-0.138159
C	-2.245383	2.706114	0.211695
C	-1.082723	2.044641	0.461402
C	-1.010594	0.616671	0.382528
C	-2.157528	-0.129692	0.008571
C	-2.175390	-1.522038	-0.131058
C	-3.342978	-2.225609	-0.530663
C	-4.497247	-1.544313	-0.781901
C	-4.513460	-0.138914	-0.648384
C	0.350100	0.021404	0.576158
C	1.034186	-0.230235	-0.795467
C	2.441484	-0.701043	-0.647465
C	3.444375	0.188879	-0.450550
C	2.685023	-2.167627	-0.690254
O	0.396690	-1.196037	1.290209
C	0.024815	-1.077146	2.647221
C	4.801948	-0.216167	-0.268760
C	3.188101	1.593603	-0.402454
N	5.890374	-0.546571	-0.124717
N	2.947439	2.714278	-0.356007
H	-4.333351	2.501069	-0.330035
H	-2.290613	3.783927	0.282431
H	-0.188282	2.593354	0.727122
H	-1.284492	-2.084294	0.099230
H	-3.302804	-3.302127	-0.622152
H	-5.397123	-2.063684	-1.080920
H	-5.423828	0.405864	-0.864470
H	0.959128	0.760199	1.111293
H	0.442954	-0.971160	-1.334229
H	0.996519	0.706879	-1.350595
H	2.070724	-2.651297	0.070261
H	2.365264	-2.562966	-1.657907
H	3.728362	-2.428517	-0.533387
H	0.178714	-2.051259	3.105685
H	0.648639	-0.337583	3.159571
H	-1.024648	-0.789793	2.752793

ortho-A′ (GS)

C	-2.9877385	-1.1478110	-0.4963026
C	-2.7616784	-2.5390973	-0.6500190
C	-1.5098617	-3.0718997	-0.4466744
C	-0.4347076	-2.2355002	-0.0778221
C	-0.6106649	-0.8769662	0.0955782
C	-1.8966801	-0.2926455	-0.1179500
C	-2.1541708	1.0989277	0.0138276
C	-3.4114366	1.6176999	-0.2077846
C	-4.4818470	0.7720240	-0.5746186
C	-4.2699344	-0.5806459	-0.7136592
C	0.5868763	-0.0196350	0.4627026
C	1.2886902	0.4955924	-0.8162659
C	2.4968900	1.3205532	-0.4946685
C	3.7488149	0.8816135	-0.8114849
C	2.2827392	2.6240372	0.2064389
O	1.5852081	-0.7333107	1.1901141
C	1.1891548	-1.0279718	2.5317125
C	4.9166492	1.6463443	-0.4993658
C	3.9704679	-0.3724808	-1.4631249
N	5.8610859	2.2737922	-0.2423504
N	4.1550416	-1.3883912	-1.9968693
H	-3.5960076	-3.1749161	-0.9353164
H	-1.3397189	-4.1373758	-0.5705926
H	0.5531589	-2.6584876	0.0803975
H	-1.3505480	1.7727193	0.2945701
H	-3.5820664	2.6850433	-0.0994082
H	-5.4682540	1.1929074	-0.7459783
H	-5.0864243	-1.2403642	-0.9970365
H	0.2574476	0.8360101	1.0714427
H	1.5539822	-0.3688275	-1.4301492
H	0.5646001	1.1017659	-1.3746487
H	1.5477455	3.2282865	-0.3389964
H	1.8676678	2.4419923	1.2060425
H	3.2069011	3.1938020	0.3166888
H	2.0344440	-1.5385591	2.9954272
H	0.9696551	-0.1009696	3.0819311
H	0.3045188	-1.6772561	2.5542130

ortho-A′ (EX)

C	-3.499025	-0.331632	-0.348151
C	-3.563340	-1.724306	-0.457052
C	-2.433943	-2.541346	-0.201889
C	-1.261434	-1.971867	0.186810
C	-1.161008	-0.554069	0.348151
C	-2.265389	0.282905	0.059526
C	-2.226654	1.679293	0.137847
C	-3.363451	2.481494	-0.155014
C	-4.533954	1.890332	-0.528988
C	-4.603672	0.482248	-0.630853
C	0.169716	0.016858	0.728570
C	0.978318	0.354973	-0.547501
C	2.340267	0.873976	-0.238639
C	3.451217	0.189768	-0.587728
C	2.420621	2.172527	0.486967
O	0.965017	-0.870654	1.477599
C	0.525049	-1.063111	2.804509
C	4.762156	0.676552	-0.288544
C	3.391506	-1.064460	-1.271985
N	5.808877	1.076057	-0.046028
N	3.343254	-2.067069	-1.825230
H	-4.496231	-2.182455	-0.759824
H	-2.512113	-3.612825	-0.322659
H	-0.385049	-2.572841	0.381571
H	-1.321570	2.181975	0.445857
H	-3.286063	3.556792	-0.075142
H	-5.408682	2.485491	-0.751865
H	-5.530586	0.013899	-0.936023
H	0.025185	0.934199	1.311828
H	1.028920	-0.540308	-1.164444
H	0.415677	1.113060	-1.099520
H	1.791387	2.917638	-0.004094
H	2.040691	2.052887	1.504630
H	3.435696	2.554807	0.551099
H	1.254929	-1.706422	3.289953
H	0.472898	-0.109730	3.341989
H	-0.457764	-1.541465	2.841421

peri-G+-pro-R (GS)

C	-1.5079409	-0.2087414	-0.3827535
C	-0.7694376	-1.3446427	-1.1956253
C	0.5312416	-2.3201486	-1.3414126
C	1.1502915	-2.1846870	-0.6970724
C	0.4730782	-1.0917468	0.0995620
C	-0.8895893	-0.0772753	0.2948006
C	-1.6674558	1.0678460	1.1140487
C	-2.9625283	2.0342158	1.2402923
C	-3.5578100	1.9085791	0.5582193
C	-2.8447827	0.8059429	-0.2289848
C	1.2382358	-0.9657176	0.6784380
C	1.9833796	-0.3912527	-0.3585278
C	1.0414596	0.9160992	-0.9450162
C	0.6254895	2.0824485	-0.2653884
C	0.5616977	0.8913264	-2.2661767
O	2.2677998	-2.2291891	1.0461740
C	1.7433492	-2.7644755	2.2236192
C	-0.3291301	3.3441221	-0.7584790
C	1.0986939	2.0877659	1.0130165
N	-1.1125327	4.3701440	-1.1556868
N	1.4856118	2.0666601	2.0619908
H	-1.2483966	-1.4309223	-1.6988932
H	1.0955058	-3.1925886	-1.9590325
H	2.1870630	-2.9505397	-0.8196502
H	-1.2395196	1.1901765	1.6567279
H	-3.5304696	2.9005343	1.8694338
H	-4.5763745	2.6814292	0.6620846
H	-3.2942339	0.6941610	-0.7517537
H	0.5553150	-0.3109318	1.5592816
H	2.6552340	-0.2791007	0.1508162
H	2.5814826	-1.1363336	-1.1529561
H	0.2874146	0.1924823	-2.2208990
H	1.3829281	1.8758820	-2.5727284
H	-0.2860698	0.5025800	-3.0282001
H	2.6052650	-3.7120962	2.4259827
H	1.1261045	-2.0832088	3.0750155
H	1.1396307	-2.9387972	2.0697331

peri-G+-pro-R (EX)

C	1.270914	2.186056	-0.093846
C	2.463151	2.312405	0.627875
C	3.188935	1.187881	0.989944
C	2.713596	-0.069372	0.679754
C	1.513000	-0.249197	-0.021546
C	0.805232	0.893371	-0.462036
C	-0.353245	0.807333	-1.251619
C	-1.083345	1.950533	-1.582930
C	-0.657410	3.198834	-1.173456
C	0.518388	3.317742	-0.450993
C	0.943577	-1.627272	-0.131253
C	-0.023158	-1.888923	1.072740
C	-1.116057	-0.906809	1.292737
C	-2.232892	-0.887021	0.399645
C	-1.185222	-0.195217	2.599775
O	1.942033	-2.615592	-0.075794
C	2.526227	-2.920068	-1.323914
C	-3.284968	0.038086	0.540676
C	-2.270241	-1.717836	-0.729474
N	-4.113670	0.834726	0.657479
N	-2.183848	-2.364479	-1.687207
H	2.815276	3.299532	0.897992
H	4.113504	1.296383	1.539466
H	3.246250	-0.953958	0.997363
H	-0.684004	-0.139607	-1.641865
H	-1.993856	1.842301	-2.153531
H	-1.233087	4.079218	-1.420247
H	0.868693	4.294731	-0.143609
H	0.365468	-1.743194	-1.049922
H	-0.396306	-2.900355	0.875205
H	0.608383	-1.957282	1.959853
H	-0.201898	0.161275	2.917831
H	-1.856404	0.662911	2.559971
H	-1.555769	-0.838876	3.413065
H	3.233750	-3.729077	-1.156607
H	1.768717	-3.248805	-2.040928
H	3.062050	-2.061131	-1.744130

peri-G+-pro-S (GS)

C	-2.3940305	-0.2087414	-0.3827535
C	-2.6355312	-1.3446427	-1.1956253
C	-1.6758015	-2.3201486	-1.3414126
C	-0.4283703	-2.1846870	-0.6970724
C	-0.1434303	-1.0917468	0.0995620
C	-1.1318071	-0.0772753	0.2948006
C	-0.9328359	1.0678460	1.1140487
C	-1.9056039	2.0342158	1.2402923
C	-3.1365224	1.9085791	0.5582193
C	-3.3742646	0.8059429	-0.2289848
C	1.2562362	-0.9657176	0.6784380
C	2.2584009	-0.3912527	-0.3585278
C	1.8071965	0.9160992	-0.9450162
C	2.0113217	2.0824485	-0.2653884
C	1.1138995	0.8913264	-2.2661767
O	1.8102676	-2.2291891	1.0461740
C	1.1989804	-2.7644755	2.2236192
C	1.5571813	3.3441221	-0.7584790
C	2.6507523	2.0877659	1.0130165
N	1.1818926	4.3701440	-1.1556868
N	3.1522907	2.0666601	2.0619908
H	-3.5953203	-1.4309223	-1.6988932
H	-1.8688151	-3.1925886	-1.9590325
H	0.3324991	-2.9505397	-0.8196502
H	-0.0022739	1.1901765	1.6567279
H	-1.7242128	2.9005343	1.8694338
H	-3.8923412	2.6814292	0.6620846
H	-4.3210239	0.6941610	-0.7517537
H	1.2522198	-0.3109318	1.5592816
H	3.2205812	-0.2791007	0.1508162
H	2.3647571	-1.1363336	-1.1529561
H	0.2699992	0.1924823	-2.2208990
H	0.7570711	1.8758820	-2.5727284
H	1.8023539	0.5025800	-3.0282001
H	1.7007586	-3.7120962	2.4259827
H	1.3378972	-2.0832088	3.0750155
H	0.1256279	-2.9387972	2.0697331

peri-G+-pro-S (EX)

C	0.491232	2.261599	-0.301592
C	1.516043	2.831431	0.447071
C	2.588353	2.055928	0.874979
C	2.620281	0.707800	0.601193
C	1.615433	0.094390	-0.158959
C	0.570090	0.891755	-0.678817
C	-0.458542	0.361114	-1.470032
C	-1.606952	1.112924	-1.755889
C	-1.711940	2.420163	-1.323368
C	-0.667219	2.998406	-0.627235
C	1.555546	-1.398549	-0.225534
C	0.476181	-1.909402	0.793293
C	-0.918840	-1.884622	0.291377
C	-1.895084	-0.986367	0.805020
C	-1.316195	-2.985849	-0.631362
O	2.783321	-1.997124	0.108503
C	3.713243	-2.037050	-0.949194
C	-3.248542	-1.064628	0.414901
C	-1.560606	0.082518	1.651392
N	-4.343167	-1.134916	0.053546
N	-1.240144	0.988315	2.296270
H	1.455833	3.876464	0.720311
H	3.375571	2.505724	1.463906
H	3.409499	0.087484	0.999276
H	-0.374915	-0.630078	-1.879621
H	-2.410813	0.657012	-2.315087
H	-2.607249	2.989389	-1.528087
H	-0.739814	4.024489	-0.291863
H	1.259531	-1.736421	-1.224683
H	0.790406	-2.937947	0.996803
H	0.589518	-1.351947	1.723186
H	-0.605941	-3.105907	-1.459717
H	-1.340473	-3.958378	-0.121844
H	-2.303130	-2.827927	-1.063482
H	4.593853	-2.560060	-0.583286
H	3.306896	-2.581333	-1.808405
H	4.006040	-1.033942	-1.278056

ortho-G+-pro-R (GS)

C	1.5642480	-1.7122151	0.7202365
C	0.8154595	-2.2733470	1.7861860
C	-0.2111475	-1.5701649	2.3698302
C	-0.5395946	-0.2846416	1.8885181
C	0.1425079	0.2968476	0.8363951
C	1.2398532	-0.3988737	0.2361212
C	2.0298493	0.1429886	-0.8130237
C	3.0595271	-0.5815294	-1.3710773
C	3.3610488	-1.8807244	-0.9085734
C	2.6310186	-2.4288408	0.1205338
C	-0.3829207	1.6177653	0.3022822
C	-1.0576675	1.4518226	-1.0839709
C	-2.2136351	0.4996148	-1.0374595
C	-2.1552565	-0.7097615	-1.6652142
C	-3.4255858	0.9069877	-0.2601435
O	0.5983221	2.6415489	0.1200259
C	1.2766321	2.9721646	1.3339676
C	-3.2404004	-1.6403105	-1.6020038
C	-1.0196666	-1.1285859	-2.4273925
N	-4.1241156	-2.3934667	-1.5433314
N	-0.1151959	-1.4802516	-3.0670566
H	1.0743476	-3.2694294	2.1365128
H	-0.7763110	-1.9980310	3.1925792
H	-1.3572229	0.2622817	2.3538326
H	1.8233724	1.1472835	-1.1631774
H	3.6438736	-0.1504203	-2.1787586
H	4.1701797	-2.4427905	-1.3657473
H	2.8597452	-3.4247395	0.4921435
H	-1.1348617	1.9830677	1.0213254
H	-1.4128786	2.4437742	-1.3897745
H	-0.3072440	1.1162540	-1.8028202
H	-3.7346661	1.9176335	-0.5509080
H	-4.2595804	0.2168131	-0.3998544
H	-3.1864081	0.9432085	0.8102023
H	1.9494433	3.7966930	1.0924098
H	0.5607247	3.2926561	2.1053801
H	1.8542060	2.1187182	1.7118047

ortho-G+-pro-R (EX)

C	2.729838	-1.071408	0.448327
C	2.273854	-1.928241	1.458730
C	1.044658	-1.695994	2.119052
C	0.272168	-0.635432	1.755182
C	0.680734	0.252654	0.708689
C	1.926781	0.057070	0.061716
C	2.420435	0.884265	-0.954837
C	3.656527	0.622688	-1.605298
C	4.411830	-0.450503	-1.237124
C	3.944435	-1.300191	-0.208643
C	-0.324240	1.282036	0.286329
C	-1.086221	0.901858	-1.015181
C	-1.877249	-0.360072	-0.930842
C	-3.141449	-0.356162	-0.444275
C	-1.219201	-1.605566	-1.406701
O	0.202317	2.564704	0.025020
C	0.687254	3.227555	1.172720
C	-3.923154	-1.547761	-0.347246
C	-3.760204	0.847097	0.014393
N	-4.542521	-2.509426	-0.268431
N	-4.235257	1.822809	0.385125
H	2.886856	-2.772094	1.747556
H	0.729783	-2.360381	2.911822
H	-0.665121	-0.443731	2.260385
H	1.861746	1.763660	-1.234076
H	3.988033	1.291785	-2.387333
H	5.356851	-0.660040	-1.718270
H	4.530383	-2.165703	0.073934
H	-1.071181	1.367895	1.085423
H	-1.734751	1.750683	-1.228373
H	-0.349676	0.822904	-1.815643
H	-0.985069	-1.509063	-2.470112
H	-0.264199	-1.737160	-0.891502
H	-1.829380	-2.492796	-1.260448
H	0.993185	4.222339	0.857588
H	-0.096881	3.318522	1.931490
H	1.544922	2.706910	1.608364

ortho-G+-pro-S (GS)

C	1.9696244	-0.2087414	-0.3827535
C	1.2943494	-1.3446427	-1.1956253
C	0.0877663	-2.3201486	-1.3414126
C	-0.4934677	-2.1846870	-0.6970724
C	0.1149818	-1.0917468	0.0995620
C	1.3815738	-0.0772753	0.2948006
C	2.0878999	1.0678460	1.1140487
C	3.2956247	2.0342158	1.2402923
C	3.8658243	1.9085791	0.5582193
C	3.2154688	0.8059429	-0.2289848
C	-0.6582992	-0.9657176	0.6784380
C	-1.2344940	-0.3912527	-0.3585278
C	-2.0474660	0.9160992	-0.9450162
C	-3.3255087	2.0824485	-0.2653884
C	-1.4021144	0.8913264	-2.2661767
O	0.0940569	-2.2291891	1.0461740
C	0.5441694	-2.7644755	2.2236192
C	-4.1177475	3.3441221	-0.7584790
C	-3.9322940	2.0877659	1.0130165
N	-4.7582320	4.3701440	-1.1556868
N	-4.4068540	2.0666601	2.0619908
H	1.7524477	-1.4309223	-1.6988932
H	-0.4247584	-3.1925886	-1.9590325
H	-1.4523416	-2.9505397	-0.8196502
H	1.6773608	1.1901765	1.6567279
H	3.8189888	2.9005343	1.8694338
H	4.8189798	2.6814292	0.6620846
H	3.6480216	0.6941610	-0.7517537
H	-1.5079640	-0.3109318	1.5592816
H	-1.8465133	-0.2791007	0.1508162
H	-0.4063033	-1.1363336	-1.1529561
H	-1.1205738	0.1924823	-2.2208990
H	-0.4702618	1.8758820	-2.5727284
H	-2.0485519	0.5025800	-3.0282001
H	1.0594861	-3.7120962	2.4259827
H	-0.3081822	-2.0832088	3.0750155
H	1.2353030	-2.9387972	2.0697331

ortho-G+-pro-S (EX)

C	1.671532	-1.235085	0.892291
C	0.868031	-1.687529	1.953731
C	-0.155178	-0.900468	2.458131
C	-0.400028	0.331932	1.901139
C	0.353325	0.822169	0.811900
C	1.421513	0.038628	0.308604
C	2.188621	0.412201	-0.802855
C	3.179965	-0.426498	-1.305851
C	3.426940	-1.651789	-0.726378
C	2.667300	-2.057611	0.363100
C	-0.186828	2.060458	0.160510
C	-1.183423	1.641750	-0.960546
C	-2.249472	0.698187	-0.526605
C	-2.121651	-0.689498	-0.806019
C	-3.522155	1.270792	0.000111
O	0.772873	2.920732	-0.401452
C	1.483996	3.690377	0.541180
C	-3.042821	-1.629635	-0.296453
C	-1.049501	-1.217333	-1.541190
N	-3.797557	-2.376689	0.155965
N	-0.124916	-1.611716	-2.118155
H	1.054921	-2.668579	2.370148
H	-0.770127	-1.264538	3.268134
H	-1.201223	0.943313	2.287247
H	2.001431	1.364008	-1.272191
H	3.745579	-0.111949	-2.171384
H	4.187545	-2.305508	-1.128537
H	2.829428	-3.032760	0.802999
H	-0.750457	2.613396	0.921772
H	-1.606167	2.582254	-1.322790
H	-0.581319	1.231268	-1.774276
H	-4.126707	1.741628	-0.789370
H	-4.148639	0.508565	0.462050
H	-3.348058	2.051062	0.749636
H	2.129097	4.366502	-0.015364
H	0.800804	4.280289	1.160876
H	2.102312	3.066752	1.196007

peri-G--pro-R (GS)

C	-2.4948101	-0.0223258	0.4740729
C	-3.0545552	-1.2189420	0.9897410
C	-2.3556680	-2.4011129	0.9305165
C	-1.0653981	-2.4223831	0.3603753
C	-0.4659209	-1.2821659	-0.1426186
C	-1.1830627	-0.0420881	-0.1164319
C	-0.6627605	1.1803057	-0.6239595
C	-1.3789687	2.3535690	-0.5281293
C	-2.6606388	2.3705928	0.0642889
C	-3.2065216	1.2031315	0.5461560
C	0.9638624	-1.4298218	-0.6456769
C	2.0611996	-1.0723433	0.4016805
C	2.0086380	0.3301148	0.9271920
C	2.7253538	1.3291141	0.3323212
C	1.1873191	0.5835401	2.1514233
O	1.2759206	-0.6865591	-1.8177033
C	0.5191557	-1.0982635	-2.9578406
C	2.6410292	2.6805593	0.7915344
C	3.6017207	1.0972164	-0.7734927
N	2.5548952	3.7805105	1.1585525
N	4.3433201	0.9243152	-1.6516157
H	-4.0477341	-1.1821770	1.4303623
H	-2.7883995	-3.3189797	1.3174078
H	-0.5209601	-3.3638996	0.3182988
H	0.3084000	1.1766853	-1.1001310
H	-0.9516513	3.2743992	-0.9142896
H	-3.2129589	3.3032438	0.1332142
H	-4.1956872	1.2002832	0.9975800
H	1.1120121	-2.5017352	-0.8599910
H	1.9482984	-1.7715893	1.2368624
H	3.0199544	-1.2609874	-0.0912564
H	0.2265423	0.0659635	2.0823661
H	1.7163844	0.1619860	3.0181655
H	1.0190997	1.6466403	2.3307292
H	0.8891132	-0.5079106	-3.7970327
H	0.6765519	-2.1678102	-3.1591349
H	-0.5530752	-0.9110763	-2.8135367

peri-G--pro-R (EX)

C	-3.132373	-0.649778	0.406771
C	-2.855199	-1.404856	1.551743
C	-1.616644	-1.294758	2.231359
C	-0.661275	-0.445362	1.765745
C	-0.895709	0.339284	0.591622
C	-2.135186	0.258420	-0.090283
C	-2.448297	1.007783	-1.229041
C	-3.700501	0.883476	-1.891886
C	-4.640054	0.017974	-1.416265
C	-4.356982	-0.752293	-0.264709
C	0.208591	1.219854	0.086685
C	0.969918	0.654907	-1.150189
C	1.791534	-0.558151	-0.871794
C	3.108581	-0.460215	-0.588429
C	1.104376	-1.876187	-0.962192
O	1.180664	1.492940	1.061944
C	0.822573	2.507194	1.974605
C	3.908083	-1.614649	-0.317642
C	3.795764	0.793934	-0.559975
N	4.542631	-2.544066	-0.099562
N	4.358225	1.792321	-0.561610
H	-3.612656	-2.080219	1.928585
H	-1.439381	-1.890569	3.116006
H	0.292459	-0.349236	2.262577
H	-1.740825	1.723900	-1.620951
H	-3.893193	1.483374	-2.770406
H	-5.596957	-0.087315	-1.908273
H	-5.100537	-1.442566	0.112573
H	-0.226553	2.166770	-0.258017
H	0.228702	0.421317	-1.916330
H	1.601262	1.463986	-1.514031
H	0.180812	-1.861659	-0.381946
H	0.814900	-2.056590	-2.001261
H	1.725707	-2.702608	-0.627718
H	1.670753	2.648871	2.639689
H	0.617853	3.447380	1.451991
H	-0.057127	2.230025	2.563906

peri-G--pro-S (GS)

C	-1.4571858	-1.0633163	1.5811448
C	-0.9784142	-2.2602376	2.1691395
C	0.0475496	-2.9653222	1.5866993
C	0.6469378	-2.4793808	0.4083789
C	0.2391736	-1.3013002	-0.1902442
C	-0.8578080	-0.5722660	0.3701379
C	-1.3867897	0.6192516	-0.1970967
C	-2.4147681	1.3048581	0.4111775
C	-2.9818128	0.8335430	1.6157798
C	-2.5151453	-0.3308511	2.1797864
C	1.0818136	-0.8171862	-1.3590895
C	2.1716632	0.2119531	-0.9357439
C	1.6473408	1.5078716	-0.3973100
C	1.5113488	1.7022816	0.9475339
C	1.2990234	2.5767166	-1.3827964
O	0.3641560	-0.2513328	-2.4585785
C	-0.5344614	-1.1871355	-3.0606346
C	0.9644808	2.9113267	1.4779465
C	1.8794538	0.7044841	1.9025544
N	0.5103365	3.8945831	1.9004554
N	2.1915088	-0.0964728	2.6854661
H	-1.4386080	-2.6086016	3.0901466
H	0.4105410	-3.8848463	2.0354244
H	1.4753404	-3.0322326	-0.0300925
H	-0.9727512	0.9826923	-1.1285492
H	-2.7909566	2.2194446	-0.0381003
H	-3.7850465	1.3897052	2.0899441
H	-2.9475682	-0.7099707	3.1024035
H	1.6402735	-1.6929353	-1.7289195
H	2.7972256	-0.2861032	-0.1891331
H	2.7770718	0.4129793	-1.8265896
H	0.7072121	2.1460300	-2.1965861
H	0.7647367	3.4104925	-0.9240635
H	2.2244140	2.9595676	-1.8351670
H	-0.9849090	-0.6763201	-3.9131567
H	0.0107898	-2.0768239	-3.4074617
H	-1.3161670	-1.4951455	-2.3548060

peri-G--pro-S (EX)

C	1.884822	-1.487484	-0.353278
C	3.093284	-1.483489	0.346571
C	3.540663	-0.328159	0.966300
C	2.759677	0.813785	0.932796
C	1.546301	0.859374	0.245629
C	1.120799	-0.292280	-0.454077
C	-0.069859	-0.323953	-1.209946
C	-0.540260	-1.516930	-1.770452
C	0.177065	-2.689468	-1.617474
C	1.379740	-2.672364	-0.934765
C	0.651205	2.050171	0.409864
C	-0.570766	1.726594	1.360100
C	-1.120633	0.349046	1.382348
C	-2.260013	-0.029606	0.610122
C	-0.580874	-0.572065	2.419884
O	0.122233	2.532497	-0.803338
C	1.060336	3.172878	-1.635735
C	-2.781128	-1.336853	0.666474
C	-2.912926	0.863795	-0.260869
N	-3.159989	-2.427975	0.713009
N	-3.397855	1.603142	-1.004128
H	3.675803	-2.394046	0.402800
H	4.481224	-0.326623	1.498884
H	3.086809	1.698332	1.464005
H	-0.597860	0.593067	-1.404277
H	-1.473549	-1.507189	-2.313208
H	-0.196481	-3.614886	-2.031473
H	1.948793	-3.586415	-0.822254
H	1.228053	2.855977	0.879720
H	-0.242576	1.995915	2.368136
H	-1.320620	2.459570	1.055345
H	0.512282	-0.643934	2.377679
H	-0.814274	-0.216299	3.433694
H	-0.983886	-1.579313	2.332248
H	0.510363	3.566898	-2.486942
H	1.549090	4.001131	-1.110810
H	1.831018	2.482763	-1.995995

ortho-G--pro-R (GS)

C	-2.0486512	-1.2890614	1.0648746
C	-1.2121541	-1.7922219	2.0926692
C	0.0267414	-1.2413827	2.3215258
C	0.4789780	-0.1671461	1.5262982
C	-0.3006972	0.3566648	0.5137925
C	-1.5935532	-0.1938708	0.2555176
C	-2.4465874	0.2685616	-0.7814072
C	-3.6766751	-0.3098786	-1.0052277
C	-4.1214325	-1.3840100	-0.2038785
C	-3.3215127	-1.8590979	0.8095287
C	0.2606590	1.4633345	-0.3585745
C	0.9564684	0.8939952	-1.6297330
C	2.1660795	0.0749895	-1.3019648
C	2.0870789	-1.2864744	-1.2302785
C	3.4662352	0.7709449	-1.0184198
O	1.2291158	2.2679994	0.3161600
C	0.6382330	3.1222283	1.2991604
C	3.2290505	-2.0626423	-0.8626866
C	0.8850841	-2.0057254	-1.5116540
N	4.1741383	-2.6649553	-0.5529301
N	-0.0846303	-2.5976472	-1.7581432
H	-1.5670503	-2.6268776	2.6918281
H	0.6670316	-1.6332342	3.1063125
H	1.4592927	0.2638533	1.7080247
H	-2.1300126	1.0882094	-1.4186491
H	-4.3087197	0.0602676	-1.8074100
H	-5.0913229	-1.8342022	-0.3938432
H	-3.6499347	-2.6903574	1.4284837
H	-0.5535626	2.1160118	-0.7059664
H	0.2151409	0.2940403	-2.1663002
H	1.2517292	1.7439511	-2.2544141
H	3.3539334	1.8514011	-1.0970544
H	3.8187197	0.5301139	-0.0091631
H	4.2421149	0.4293769	-1.7142958
H	1.4539845	3.7015719	1.7348353
H	-0.0891757	3.8014660	0.8312035
H	0.1358634	2.5398036	2.0817794

ortho-G--pro-R (EX)

C	-2.022406	-0.185088	1.011761
C	-1.332811	-0.646188	2.152250
C	-0.045964	-0.217815	2.433177
C	0.590754	0.644451	1.571633
C	-0.036688	1.092920	0.384633
C	-1.371524	0.706676	0.114614
C	-2.066134	1.102911	-1.033454
C	-3.356394	0.651660	-1.287552
C	-3.982674	-0.207903	-0.410397
C	-3.312173	-0.630758	0.731002
C	0.836649	1.795771	-0.603635
C	1.556002	0.725268	-1.488560
C	2.119925	-0.441408	-0.758608
C	1.358389	-1.636502	-0.684040
C	3.546706	-0.401272	-0.322422
O	1.826745	2.572328	0.030822
C	1.352827	3.785397	0.567781
C	1.757590	-2.714078	0.137029
C	0.140941	-1.797232	-1.365404
N	2.092609	-3.565913	0.839596
N	-0.877478	-1.861346	-1.914149
H	-1.828136	-1.345830	2.812603
H	0.467134	-0.588876	3.308396
H	1.595131	0.981982	1.768271
H	-1.603136	1.771483	-1.742225
H	-3.860222	0.969174	-2.189342
H	-4.980227	-0.568602	-0.616179
H	-3.786020	-1.327774	1.409636
H	0.250876	2.446576	-1.260450
H	0.833248	0.407321	-2.244427
H	2.337773	1.287032	-2.004305
H	3.805865	0.561433	0.122651
H	3.768915	-1.182614	0.404176
H	4.238899	-0.551301	-1.164282
H	2.211496	4.311357	0.978578
H	0.892372	4.406504	-0.208271
H	0.620651	3.624434	1.366890

ortho-G--pro-S (GS)

C	2.4367312	-1.3510230	-0.3203214
C	1.8369847	-2.4203973	-1.0334258
C	0.5691523	-2.2913828	-1.5507766
C	-0.1545944	-1.0931239	-1.3661270
C	0.3851623	-0.0276496	-0.6729429
C	1.7069044	-0.1269786	-0.1379570
C	2.3384068	0.9274973	0.5755192
C	3.6112098	0.7841475	1.0840257
C	4.3219784	-0.4239371	0.9081116
C	3.7445110	-1.4652131	0.2178962
C	-0.4518342	1.2210388	-0.4490603
C	-1.0605044	1.3108935	0.9823989
C	-2.0289792	0.2061084	1.2838321
C	-3.3619098	0.3651345	1.0368482
C	-1.4882918	-1.0555159	1.8757098
O	-1.5480969	1.3061793	-1.3493523
C	-1.1754105	1.7828617	-2.6438803
C	-4.3011529	-0.6844718	1.2868017
C	-3.9104380	1.5903740	0.5418933
N	-5.0614616	-1.5411364	1.4866264
N	-4.3779464	2.5891787	0.1749893
H	2.3996666	-3.3411777	-1.1646855
H	0.1137410	-3.1109502	-2.0989786
H	-1.1617412	-1.0002118	-1.7605910
H	1.8182432	1.8694293	0.7184926
H	4.0734843	1.6067929	1.6220718
H	5.3238408	-0.5249459	1.3149585
H	4.2848745	-2.3973897	0.0723961
H	0.1820969	2.1130848	-0.5714738
H	-0.2369147	1.2763704	1.7028860
H	-1.5562249	2.2834407	1.0531343
H	-0.6648004	-1.4363461	1.2623664
H	-1.0669970	-0.8339665	2.8655230
H	-2.2517181	-1.8282907	1.9814143
H	-2.0948638	1.8281834	-3.2290780
H	-0.7348229	2.7874413	-2.5717159
H	-0.4582850	1.1059513	-3.1275291

ortho-G--pro-S (EX)

C	-1.214596	-1.841463	0.500503
C	-2.324464	-2.305846	-0.201370
C	-3.144745	-1.417222	-0.881352
C	-2.828625	-0.071735	-0.908818
C	-1.737441	0.435180	-0.200001
C	-0.967874	-0.443862	0.588929
C	0.134865	-0.001376	1.352737
C	1.082720	-0.927330	1.836915
C	0.889569	-2.285301	1.659287
C	-0.252715	-2.741098	1.029651
C	-1.262682	1.827298	-0.497311
C	0.055284	1.766810	-1.341165
C	1.300181	1.382803	-0.622083
C	1.964456	0.146148	-0.862757
C	2.045663	2.450466	0.115256
O	-1.035029	2.634822	0.632030
C	-2.202311	2.926511	1.360635
C	3.273194	-0.079989	-0.376002
C	1.352841	-0.940622	-1.508222
N	4.333002	-0.246024	0.056425
N	0.807583	-1.849651	-1.977877
H	-2.516334	-3.370315	-0.247360
H	-4.002973	-1.783627	-1.428638
H	-3.424570	0.605269	-1.508727
H	0.220878	1.041860	1.606279
H	1.958241	-0.562797	2.355637
H	1.631590	-2.988682	2.010535
H	-0.409461	-3.803247	0.890549
H	-2.020066	2.311129	-1.129475
H	-0.142219	1.101228	-2.184183
H	0.177987	2.776238	-1.747364
H	1.374949	3.252048	0.417835
H	2.543692	2.060074	1.006932
H	2.837848	2.885697	-0.507749
H	-1.918519	3.607691	2.160582
H	-2.953348	3.413058	0.726266
H	-2.644566	2.023499	1.797172