Electronic Supplementary Information for

Photophysical properties of oligophenylenes end-capped with naphthyls with naphthyls in solution and solid state

Minoru Yamaji,[a,*], Kengo Suzuki,[b] and Hideki Okamoto[c]

[a] Division of Molecular Science, Graduate School of Science and Engineering, Gunma University, Ota, Gunma 373-0057, Japan
[b] Hamamatsu Photonics K.K., Joko-cho, Hamamatsu, Shizuoka 431-3196, Japan
[c] Department of Chemistry, Faculty of Environment, Life, Natural Sciences and Technology, Okayama University, Okayama, Okayama 700-8530, Japan

Contents

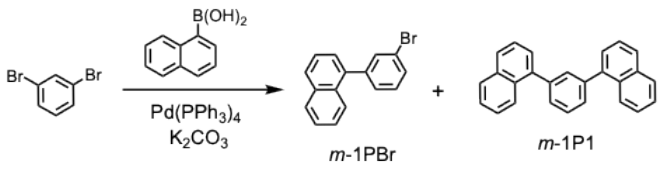
1. Materials and synthetic procedures.

1-1. Chemicals

Chloroform and ethanol (spectroscopic grade from Wako) were used as solvents for the spectral measurements as supplied. The studied DNpArs were prepared by the procedures described below.

1-2. Synthetic procedures for dinaphthylbenzenes

1-2-1. Synthesis of *m*-1P1 and *m*-1PBr



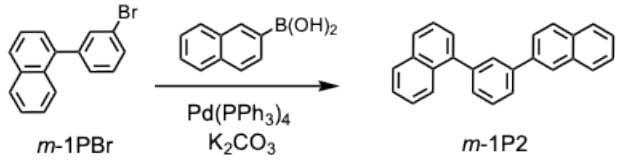
To a mixture of dimethoxyethane (20 ml) and H_2O (5 ml), 1,3-dibromobenzene (0.27 ml, 2.23 mmol), 1-naphthyl boronic acid (653 mg, 2.7 mmol) and K_2CO_3 (2.0 g, 15.1 mmol) were added, and the solution was bubbled with pure Ar for 20 min. After tetrakis(triphenylphosphinate)palladium (0) (258 mg, 10 % mol) was added, the solution was heated at 85 ℃ for 2 h. After cooling to room temperature, benzene (150 ml) was added. The solution was washed twice with brine (100 ml). Then, the organic layer was

separated, and dried with Na_2SO_4. After the organic solvent was evaporated, the crude products were separated by silica gel chromatography with a hexane/chloroform mixture (3:1, v/v) as the eluent to obtain ***m*-1PBr** (379 mg, 60%) and ***m*-1P1** (175 mg, 25 %). The products were further purified by recrystallization from hexane.

***m*-1PBr**: **^{1}H NMR** (600 MHz, $CDCl_3$) δ_H 7.92 (d, 1H, J = 8.0 Hz), 7.88 (d, 1H, J = 8.1 Hz), 7.85 (d, 1H, J = 8.3 Hz), 7.66 (m, 1H), 7.57 (brd, 1H, J = 8.0 Hz), 7.53 (d, 1H, J= 7.5 Hz), 7.50 (d, 1H, J = 7.7 Hz), 7.46 (t, 1H, J = 7.6 Hz), 7.43 (d, 1H, J = 7.5 Hz), 7.40 (d, 1H, J = 6.8 Hz), 7.36 (t, 1H, J = 7.8 Hz).
^{13}C NMR (151 MHz, $CDCl_3$) δ_C 142.97, 138.74, 133.86, 133.06, 131.45, 130.44, 129.92, 128.88, 128.49, 128.32, 127.12, 126.48, 126.09, 125.74, 125.45, 122.49.
HRMS (FAB)*: C*alcd for $C_{16}H_{11}{}^{79}Br$ 282.0044. Found *m/z* 282.0042 (M^+).

***m*-1P1**: **^{1}H NMR** (600 MHz, $CDCl_3$) δ_H 8.07 (d, 2H, J = 8.5 Hz), 7.92 (d, 2H, J = 8.1 Hz), 7.88 (d, 2H, J = 7.8 Hz), 7.67 (t, 1H, J = 1.6 Hz), 7.63 (dd, 1H, J = 8.6, 6.2 Hz), 7.60–7.58 (m, 2H), 7.57–7.45 (m, 8H).
^{13}C NMR (151 MHz, $CDCl_3$) δ_C 140.84, 140.09, 133.92, 131.82, 131.66, 129.09, 128.42, 128.28, 127.85, 127.20, 126.22, 126.09, 125.90, 125.51.
HRMS (FAB)*: C*alcd for $C_{26}H_{18}$ 330.1409. Found *m/z* 330.1419 (M^+).

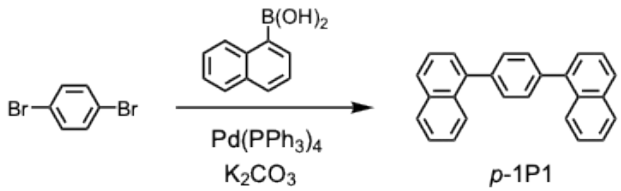
1-2-2. Synthesis of *m*-1P2



To a mixture of dimethoxyethane (12 ml) and H_2O (3 ml), ***m*-1PBr** (340 mg, 1.2 mmol), 2-naphthyl boronic acid (248 mg, 1.44 mmol) and K_2CO_3 (1.09 g, 6.0 mmol) were added, and the solution was bubbled with pure Ar for 20 min. After tetrakis(triphenylphosphinate)palladium (0) (139 mg, 10 % mol) was added, the solution was heated at 85 ℃ for 2 h. After cooling to room temperature, benzene (100 ml) was added. The solution was washed twice with brine (100 ml). Then, the organic layer was separated, and dried with Na_2SO_4. After the organic solvent was evaporated, the crude product was separated by silica gel chromatography with a hexane/chloroform mixture (3:1, v/v) as the eluent to obtain ***m*-1P2** (373 mg, 94 %). The products were further purified by recrystallization from hexane.

***m*-1P2**: **^{1}H NMR** (600 MHz, $CDCl_3$) δ_H 8.11 (s, 1H), 8.00 (d, 1H, J = 8.3 Hz), 7.95–7.85 (m, 6H), 7.83–7.79 (m, 2H), 7.62 (t, 1H, J = 7.6 Hz), 7.57 (t, 1H, J = 7.3 Hz), 7.55–7.43 (m, 6H).
^{13}C NMR (151 MHz, $CDCl_3$) δ_C 141.4964, 141.20, 140.26, 138.41, 133.96, 133.81, 132.80, 131.78, 129.27, 129.23, 128.96, 128.63, 128.46, 128.35, 127.94, 127.79, 127.14, 126.48, 126.42, 126.30, 126.17, 126.15, 126.07, 125.99, 125.73, 125.56.
HRMS (FAB)*:* Calcd for $C_{26}H_{18}$ 330.1409. Found *m/z* 330.1414 (M^+).

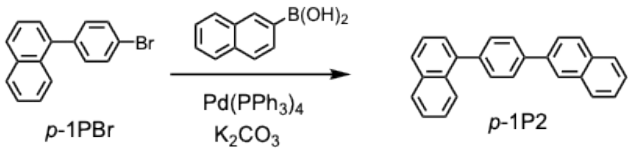
1-2-3. Synthesis of *p*-1P1



To a mixture of dimethoxyethane (8 ml) and H_2O (2 ml), 1,4-dibromobenzene (200 mg, 0.85 mmol), 2-naphthyl boronic acid (335 mg, 1.95 mmol) and K_2CO_3 (553 mg, 4.0 mmol) were added, and the solution was bubbled with pure Ar for 20 min. After tetrakis(triphenylphosphinate)palladium (0) (98 mg, 10 % mol) was added, the solution was heated at 85 ℃ for 3.5 h. After cooling to room temperature, benzene (100 ml) was added. The solution was washed twice with brine (100 ml). Then, the organic layer was separated, and dried with Na_2SO_4. After the organic solvent was evaporated, the crude product was separated by silica gel chromatography with a hexane/chloroform mixture (3:1, v/v) as the eluent to obtain ***p*-1P1** (231 mg, 83 %). The product was further purified by recrystallization from hexane.

***p*-1P1**: **^{1}H NMR** (600 MHz, $CDCl_3$) δ_H 8.09 (d, 2H, J = 8.2 Hz), 7.95 (d, 2H, J = 7.8 Hz), 7.91 (d, 2H, J = 7.9 Hz), 7.64 (s, 4H), 7.59 (t, 2H, J = 7.2 Hz), 7.56–7.48 (m, 6H).
^{13}C NMR (151 MHz, $CDCl_3$) δ_C 140.10, 139.82, 134.01, 131.77, 130.12, 128.49, 127.89, 127.22, 126.27, 126.22, 125.99, 125.61.
HRMS (FAB): Calcd for $C_{26}H_{18}$ 330.1409. Found *m/z* 330.1406 (M^+).

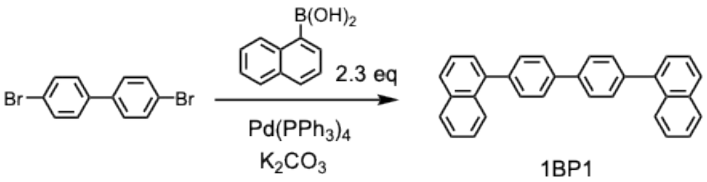
1-2-4. Synthesis of *p*-1P2



To a mixture of dimethoxyethane (6 ml) and H_2O (2 ml), 1-(4-bromophenyl)naphthalene (***p*-1PBr**, 137 mg, 0.48 mmol), 2-naphthyl boronic acid (100 mg, 0.58 mmol) and K_2CO_3 (200 mg, 6.6 mmol) were added, and the solution was bubbled with pure Ar for 20 min. After tetrakis(triphenylphosphinate)palladium (0) (56 mg, 10 % mol) was added, the solution was heated at 85 ℃ for 2 h. After cooling to room temperature, benzene (100 ml) was added. The solution was washed twice with brine (100 ml). Then, the organic layer was separated, and dried with Na_2SO_4. After the organic solvent was evaporated, the crude product was separated by silica gel chromatography with a hexane/chloroform mixture (3:1, v/v) as the eluent to obtain ***p*-1P2** (144 mg, 90 %). The product was further purified by recrystallization from hexane.

***p*-1P2**: **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.19 (brs, 1H), 8.05 (d, 1H, J = 8.4 Hz), 8.00 (d. 1H, J = 8.4 Hz), 8.99–7.97 (m, 2H), 7.95–7.88 (m, 5H), 7.67 (m, 2H), 7.69–7.48 (m, 6H).
^{13}C NMR (CDCl, 151 MHz) δ 140.13, 140.00, 139.96, 138.29, 133.98, 133.87, 132.82, 131.74, 130.76, 128.68, 128.48, 128.39, 127.90, 127.83, 127.41, 127.12, 126.51, 126.26, 126.17, 126.15, 125.99, 125.96, 125.67, 125.59.
HRMS (FAB): *C*alcd. for $C_{26}H_{18}$ 330.1409. Found *m/z* 330.1405 (M^+).

1-2-5. Synthesis of 1BP1

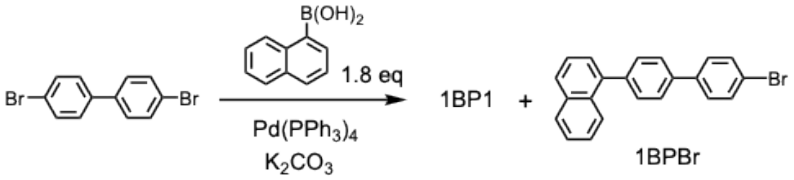


To a mixture of dimethoxyethane (10 ml) and H_2O (2 ml), 4,4'-dibromobiphenyl (312 mg, 1.0 mmol), 1-naphthyl boronic acid (396 mg, 2.3 mmol) and K_2CO_3 (661 mg, 5.0 mmol) were added, and the solution was bubbled with pure Ar for 20 min. After tetrakis(triphenylphosphinate)palladium (0) (115 mg, 10 % mol) was added, the solution was heated at 85 ℃ for 5 h. After cooling to room temperature, benzene (100 ml) was added. The solution was washed twice with brine (100 ml). Then, the organic layer was

separated, and dried with Na_2SO_4. After the organic solvent was evaporated, the crude product was separated by silica gel chromatography with a hexane/chloroform mixture (3:1, v/v) as the eluent to obtain **1BP1** (289 mg, 71 %). The product was further purified by recrystallization from hexane.

1BP1: **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.03 (d, 2H, *J* = 8.3 Hz), 7.94 (d, 2H, *J* = 8.1 Hz), 7.90 (d, 2H,*J* = 8.1 Hz), 7.86 (m, 4H), 7.64 (m, 4H), 7.57 (dd, 2H, *J* = 7.8, 7.1 Hz), 7.55–7.46 (m, 6H).
^{13}C NMR ($CDCl_3$, 151 MHz) δ 139.98, 139.96, 139.85, 133.98, 131.73, 130.74, 128.48, 127.89, 127.12, 126.26, 126.16, 125.98, 125.58.
HRMS (FAB)*: C*alcd. for $C_{32}H_{22}$ 406.1722. Found *m/z* 406.1721 (M^+).

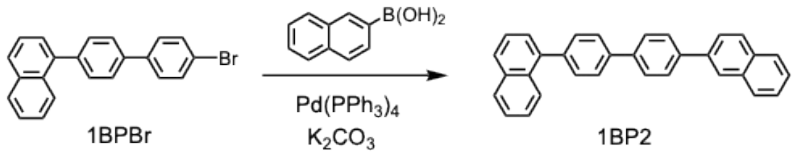
1-2-6. Synthesis of 1BPBr



To a mixture of dimethoxyethane (25 ml) and H_2O (5 ml), 4,4'-dibromobiphenyl (780 mg, 2.5 mmol), 1-naphthyl boronic acid (774 mg, 4.5 mmol) and K_2CO_3 (1.65 g, 12.5 mmol) were added, and the solution was bubbled with pure Ar for 20 min. After tetrakis(triphenylphosphinate)palladium (0) (288 mg, 10 % mol) was added, the solution was heated at 85 ℃ for 2 h. After cooling to room temperature, benzene (200 ml) was added. The solution was washed twice with brine (100 ml). Then, the organic layer was separated, and dried with Na_2SO_4. After the organic solvent was evaporated, the crude product was separated by silica gel chromatography with a hexane/chloroform mixture (3:1, v/v) as the eluent to obtain **1BPBr** (386 mg, 43 %). The product was further purified by recrystallization from hexane.

1BPBr: **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 7.96 (d, 1H, *J* =7.9 Hz), 7.92 (d, 1H, *J* = 7.9 Hz), 7.89 (d, 1H, = 7.9 Hz), 7.69 (m, 2H), 7.56–7.43 (m, 10H).
^{13}C NMR ($CDCl_3$, 151 MHz) δ 140.31, 139.87, 139.75, 138.99, 133.95, 132.10, 131.65, 130.77, 128.85, 128.48, 127.96, 127.08, 126.94, 126.28, 126.05, 126.00, 125.56, 121.78.
HRMS (FAB)*: C*alcd. for $C_{22}H_{15}{}^{79}Br$ 358.0357. Found *m/z* 358.0360 (M^+).

1-2-7. Synthesis of 1BP2

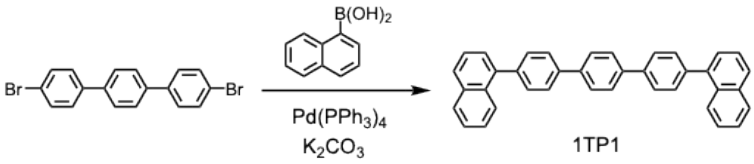


To a mixture of dimethoxyethane (10 ml) and H_2O (2 ml), **1BPBr** (383 mg, 0.98 mmol), 2-naphthyl boronic acid (203 mg, 1.18 mmol) and K_2CO_3 (650 mg, 4.9 mmol) were added, and the solution was bubbled with pure Ar for 20 min. After tetrakis(triphenylphosphinate)palladium (0) (113 mg, 10 % mol) was added, the solution was heated at 85 ℃ for 2 h. After cooling to room temperature, benzene (100 ml) was added. The solution was washed twice with brine (100 ml). Then, the organic layer was separated, and dried with Na_2SO_4. After the organic solvent was evaporated, the crude product was separated by silica gel chromatography with a hexane/chloroform mixture (3:1, v/v) as the eluent to obtain **1BP2** (276 mg, 85 %). The product was further purified by recrystallization from hexane.

1BP2: **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.14 (s, 1H), 8.02 (d, 1H, *J* = 8.3 Hz), 7.99–7.79 (m, 12H), 7.62 (m, 4H), 7.59–7.45 (m, 6H).

^{13}C NMR (CDCl, 151 MHz) δ 140.21, 140.02, 139.94, 139.68, 138.11, 133.97, 133.84, 132.81, 131.72, 130.73, 128.66, 128.47, 128.37, 127.98, 127.89, 127.82, 127.71, 127.11, 127.05, 126.51, 126.26, 126.15, 125.98, 125.85, 125.58.
HRMS (FAB)*: Calcd.* for $C_{32}H_{22}$ 406.1722. Found *m/z* 406.1721 (M^+).

1-2-8. Synthesis of 1TP1



To a mixture of dimethoxyethane (10 ml) and H_2O (2 ml), 4,4'-dibromo-*p*-terphenyl (620 mg, 1.6 mmol), 1-naphthyl boronic acid (494 mg, 2.87 mmol) and K_2CO_3 (1.05 g, 7.9 mmol) were added, and the solution was bubbled with pure Ar for 20 min. After tetrakis(triphenylphosphinate)palladium (0) (185 mg, 10 % mol) was added, the solution was heated at 85 ℃ for 2 h. After cooling to room temperature, benzene (200 ml) was added. The solution was washed twice with brine (100 ml). Then, the organic layer was separated, and dried with Na_2SO_4. After the organic solvent was evaporated, the crude product was separated by silica gel chromatography with a hexane/chloroform mixture (3:1, v/v) as the eluent to obtain **1TP1** (284 mg, 37 %). The product was further purified by recrystallization from hexane.

1TP1: **^{1}H NMR** ($CDCl_3$, 600 MHz) δ 8.01 (d, 2H, *J* = 8.0 Hz), 7.94 (d, 2H, *J* = 7.9 Hz), 7.90 (d, 2H, *J* = 7.9 Hz), 7.83 (s, 4H), 7.81 (d, 4H, *J* = 7.8 Hz), 7.62 (d, 4H, *J* = 7.8 Hz), 7.57 (t, 2H, *J* = 7.6 Hz), 7.55-7.46, m, 6H).
^{13}C NMR ($CDCl_3$, 151 MHz) δ 140.01, 139.95(2C), 139.69, 133.97, 131.72, 130.74, 128.48, 127.89, 127.71, 127.12, 127.04, 126.26, 126.16, 125.99, 125.59.
HRMS (FAB)*: Calcd.* for $C_{38}H_{26}$ 482.2035. Found *m/z* 482.2035 (M^+).

2. ^{1}H and ^{13}C NMR spectra of the synthesized compounds.

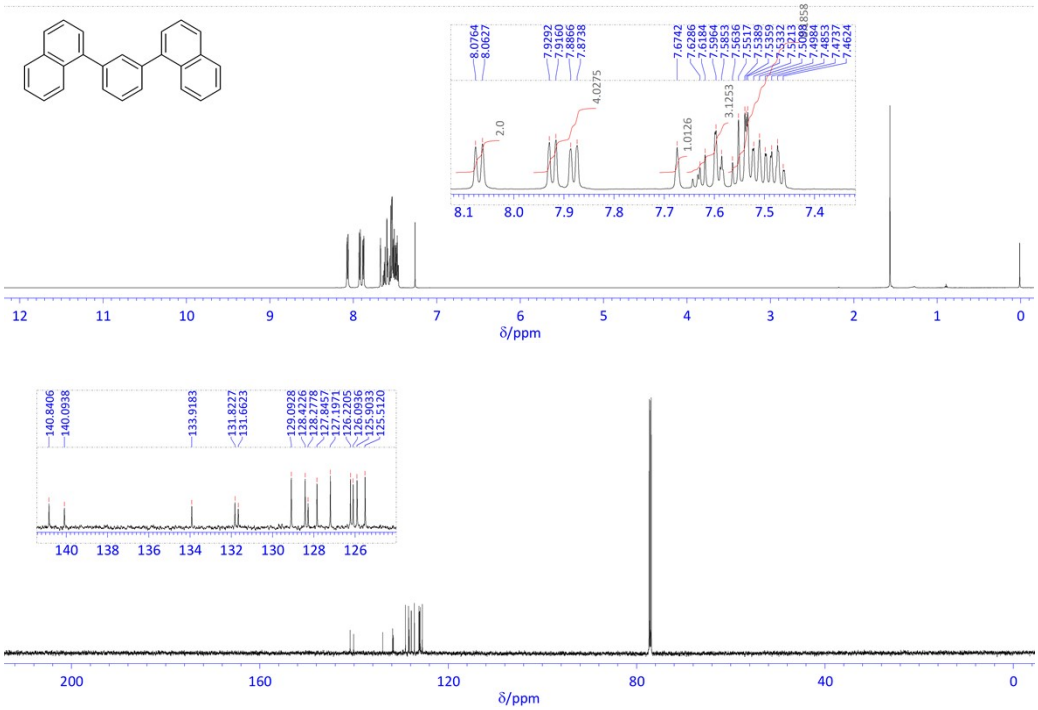


Fig. S1. ^{1}H (600 MHz, $CDCl_3$, upper) and ^{13}C (151 MHz, $CDCl_3$, lower) NMR spectra of ***m*-1P1**.

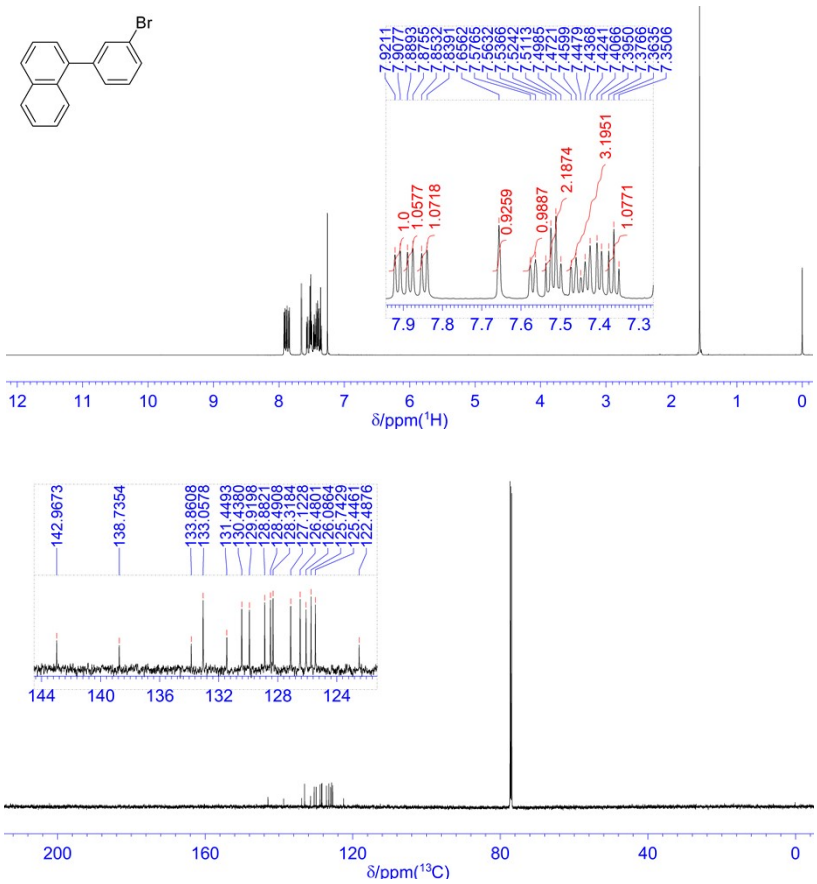


Fig. S2. ^{1}H (600 MHz, $CDCl_3$, upper) and ^{13}C (151 MHz, $CDCl_3$, lower) NMR spectra of *m*-**1PBr**.

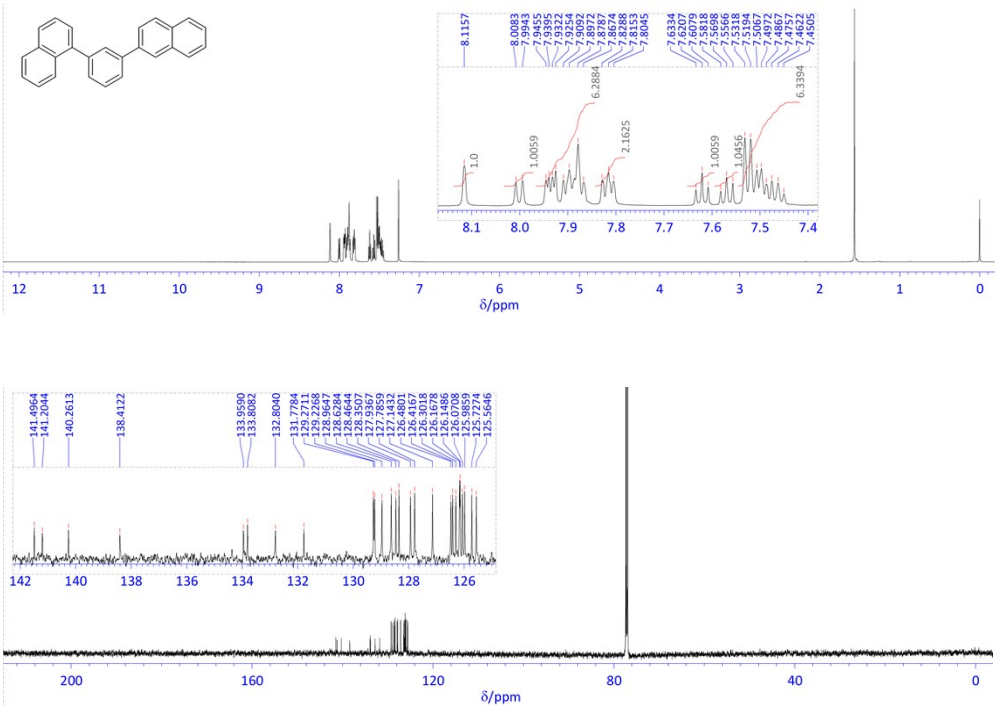


Fig. S3. ^{1}H (600 MHz, $CDCl_3$, upper) and ^{13}C (151 MHz, $CDCl_3$, lower) NMR spectra of ***m*-1P2**.

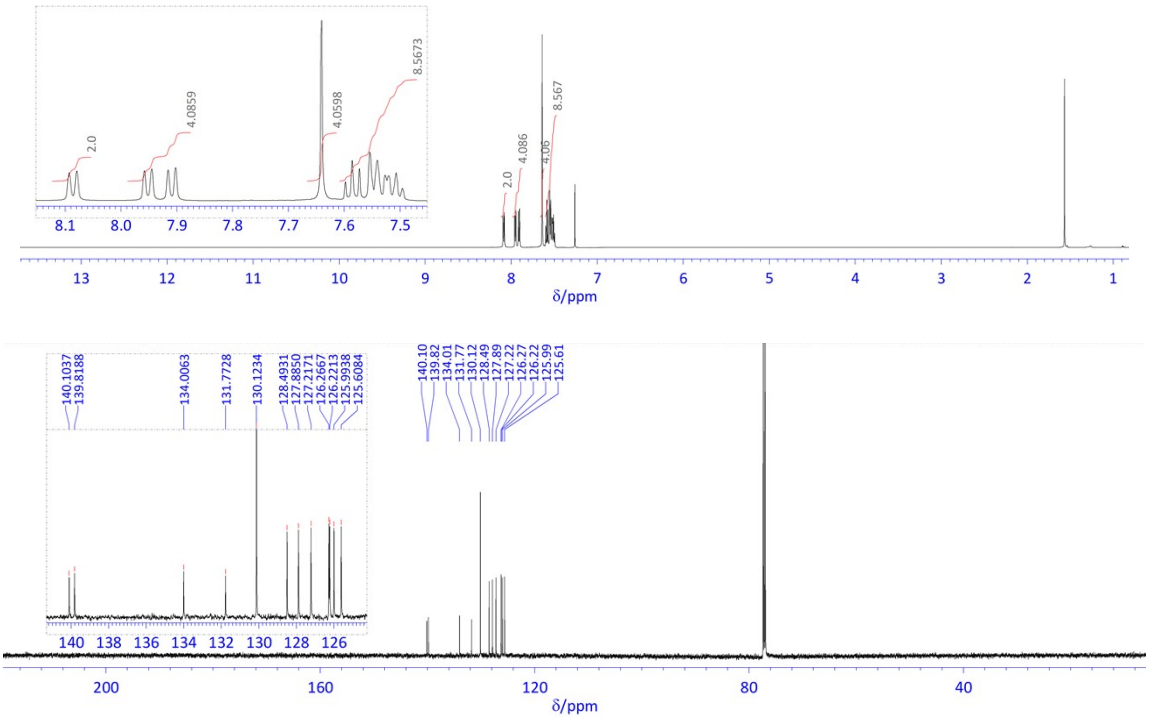


Fig. S4. ^{1}H (600 MHz, $CDCl_3$, upper) and ^{13}C (151 MHz, $CDCl_3$, lower) NMR spectra of ***p*-1P1**.

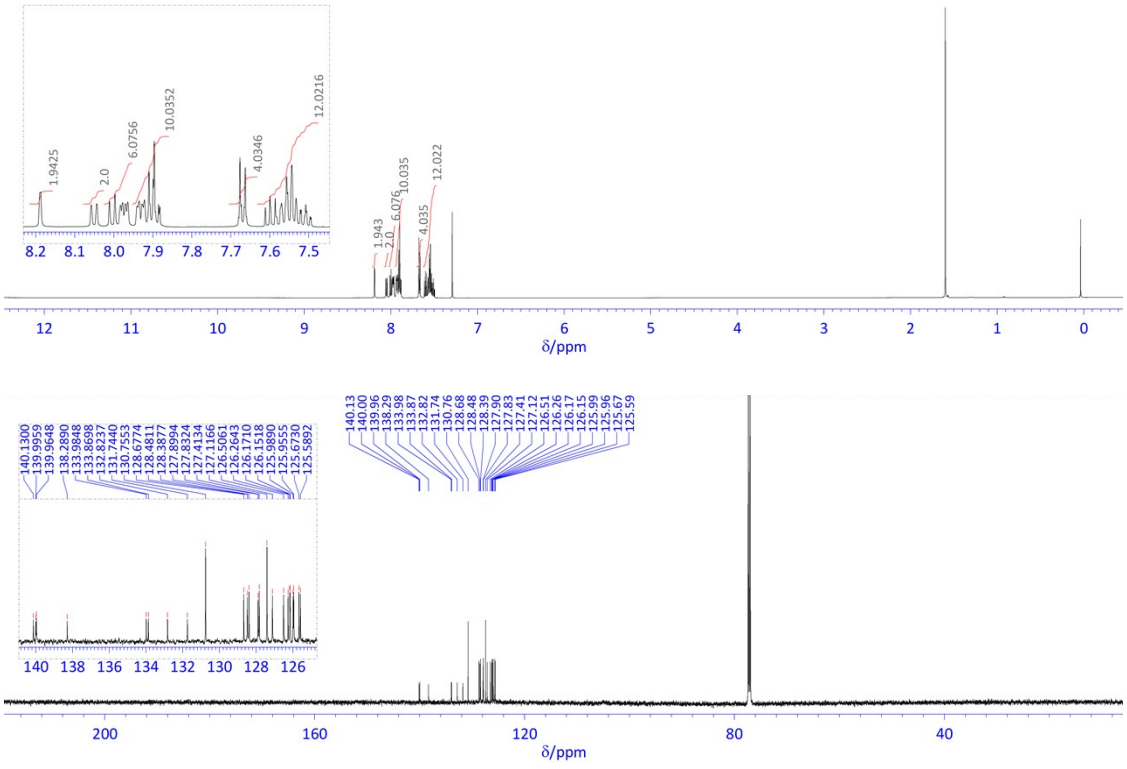


Fig. S5. ^{1}H (600 MHz, $CDCl_3$, upper) and ^{13}C (151 MHz, $CDCl_3$, lower) NMR spectra of ***p*-1P2**.

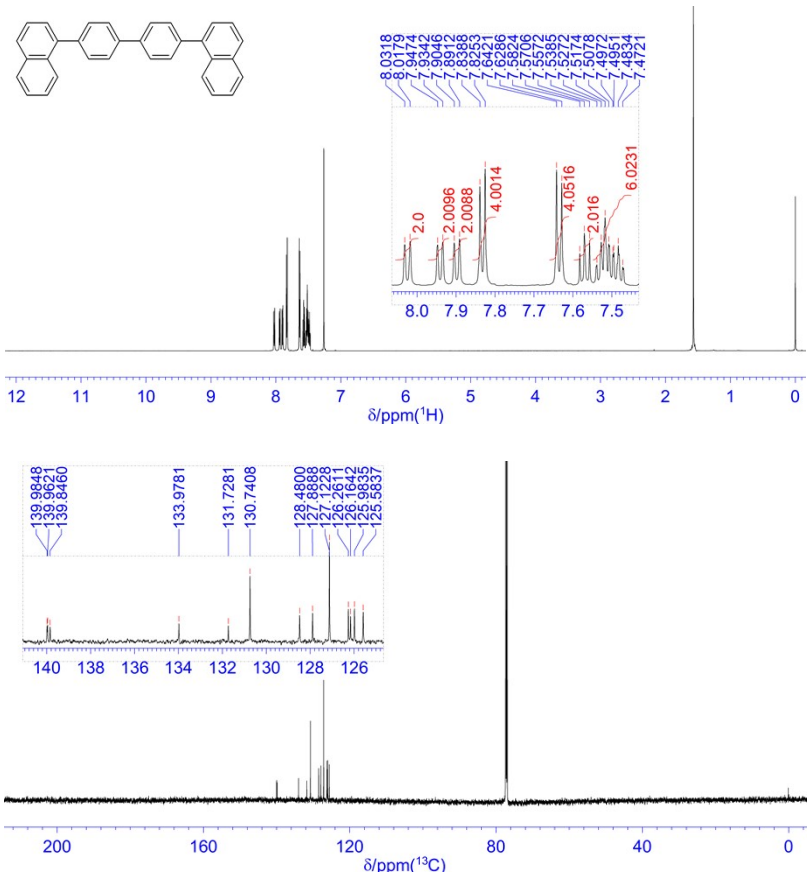


Fig. S6. ^{1}H (600 MHz, $CDCl_3$, upper) and ^{13}C (151 MHz, $CDCl_3$, lower) NMR spectra of **1BP1**.

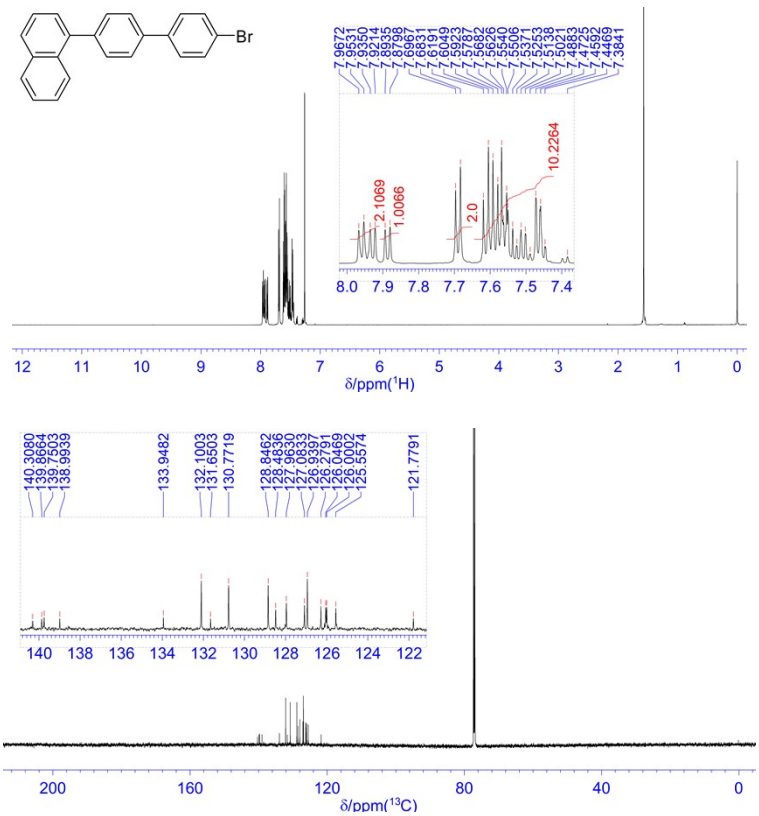


Fig. S7. ^{1}H (600 MHz, $CDCl_3$, upper) and ^{13}C (151 MHz, $CDCl_3$, lower) NMR spectra of **1BPBr**.

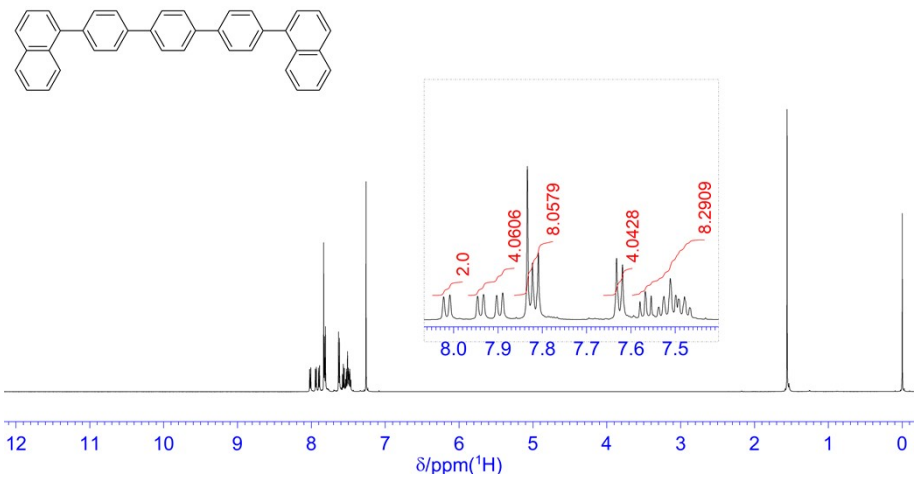


Fig. S8. ^{1}H (600 MHz, $CDCl_3$, upper) and ^{13}C (151 MHz, $CDCl_3$, lower) NMR spectra of **1TP1**.

3. Decay profiles of fluorescence of the DArNps in chloroform and the solid state.

Fig. S9 shows decay profiles of fluorescence for DNpArs in chloroform.

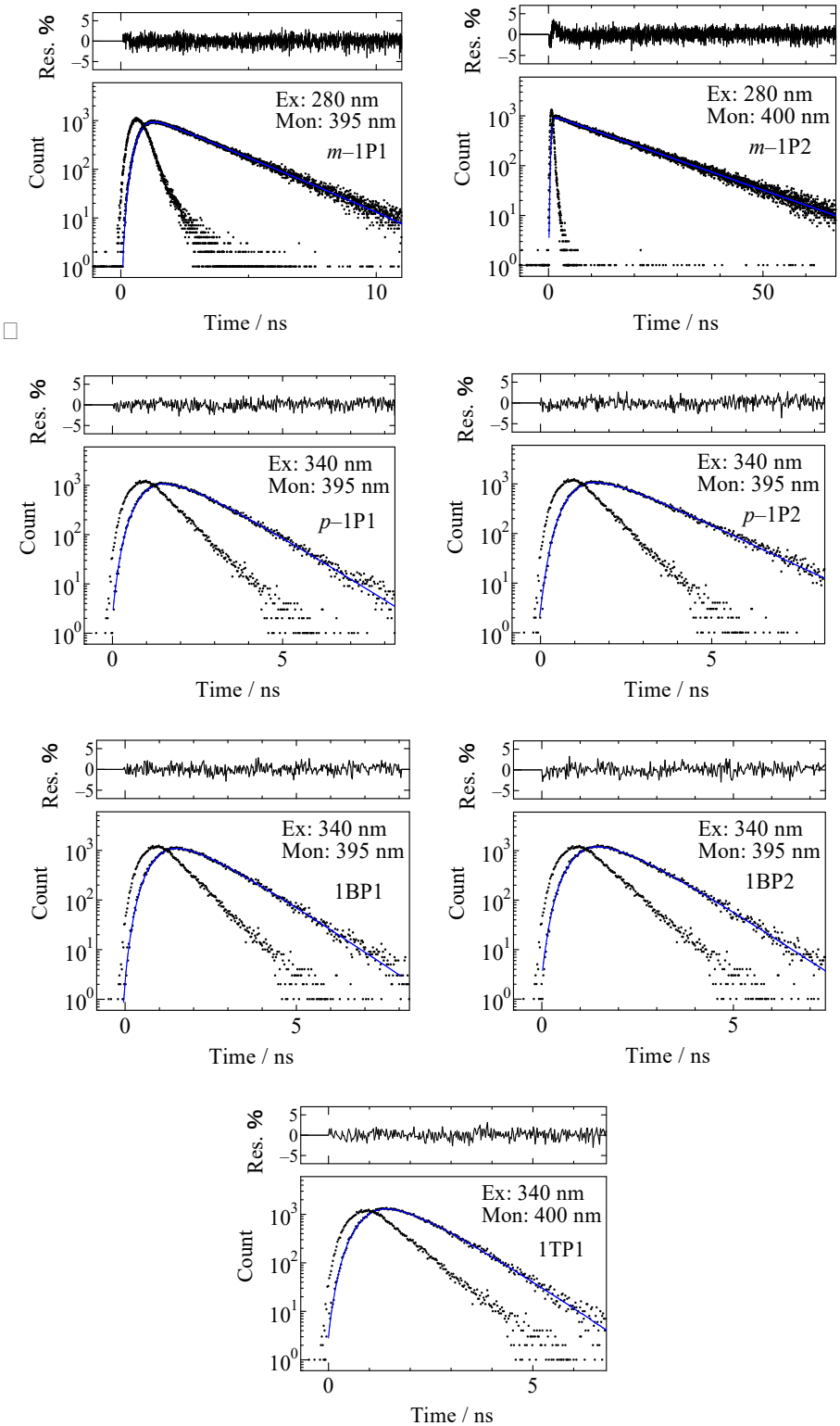


Fig. S9. Decay profiles of fluorescence for DNpArs in chloroform at 295 K. Ex and Mon in the figures indicate the excitation and monitoring wavelengths, respectively.

Fig. S10 shows decay profiles of DNpArs in the solid state.

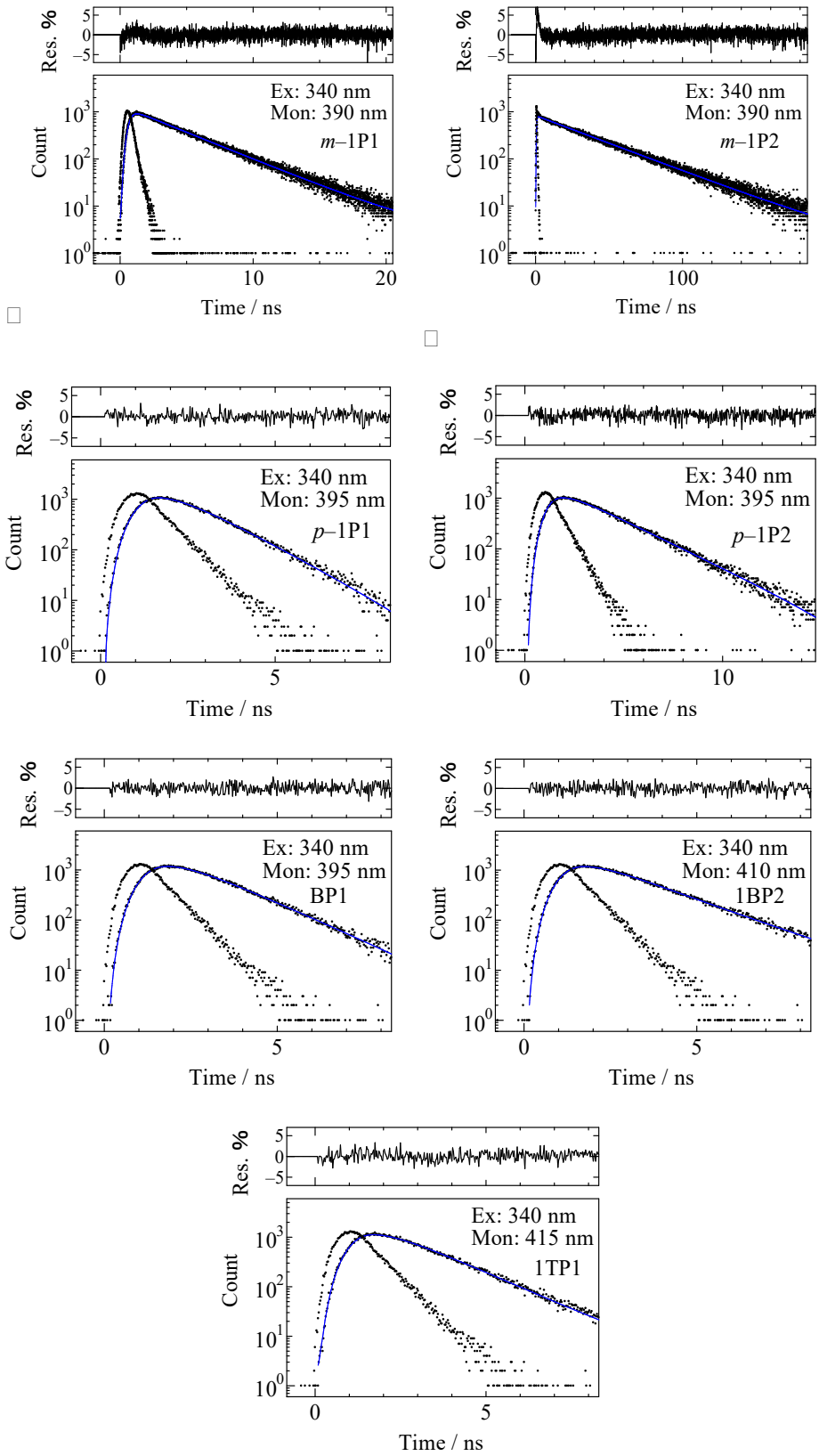


Fig. S10. Decay profiles of fluorescence for DNpArs in the solid state at 295 K. Ex and Mon in the figures indicate the excitation and monitoring wavelengths, respectively.

4. Results of DFT calculations of the DNpArs; optimized atom coordinates in vacuum.

The calculation was carried out at the DFT level, using the Gaussian 09 software package [1]. The geometries of DPNs were fully optimized by using the 6-31+G(d) base set at the B3LYP method. Atom coordinates for the optimized geometries of DArNps in vacuum are as follows.

Table S1. Atom coordinates for the optimized geometry of ***m*-1P1**.

Atom	X	Y	Z
C	3.647231	0.001898	0.013607
C	4.793915	0.485698	0.732555
C	4.672310	1.640729	1.551659
C	3.464899	2.291301	1.667300
C	2.336012	1.826361	0.952540
C	-3.473942	-2.181717	1.806963
C	-4.678358	-1.534118	1.650700
C	-4.795076	-0.432639	0.760140
C	-3.646623	-0.000880	0.011529
C	-2.406718	-0.711846	0.168734
C	2.404116	0.715929	0.125713
C	-2.343197	-1.768002	1.064191
C	-1.167944	-0.391560	-2.010038
C	0.001363	-0.093219	-2.712143
C	1.169477	0.250833	-2.029212
C	-0.000876	-0.001984	0.066239
C	-1.183844	-0.347963	-0.606174
C	1.183114	0.299844	-0.625420
C	3.792283	-1.188758	-0.754942
C	5.002275	-1.845990	-0.834582
C	6.136993	-1.349822	-0.147502
C	6.028784	-0.212255	0.621614
C	-6.026639	0.262883	0.605956
C	-6.129912	1.350219	-0.233323
C	-4.993479	1.796113	-0.951339
C	-3.786650	1.139218	-0.831207
H	5.548154	1.997777	2.089021
H	3.373176	3.172519	2.297048
H	1.396539	2.367295	1.032773

H	-3.386015	-3.021813	2.491103
H	-5.555530	-1.852360	2.209848
H	-1.406052	-2.306756	1.178867
H	-2.068085	-0.675456	-2.548791
H	0.002252	-0.128769	-3.798894
H	2.070273	0.499015	-2.584264
H	-0.001802	0.033461	1.152828
H	2.929801	-1.588834	-1.277458
H	5.084693	-2.755133	-1.424929
H	7.086815	-1.873305	-0.220896
H	6.890923	0.168688	1.165084
H	-6.890141	-0.078751	1.172878
H	-7.077169	1.872830	-0.339011
H	-5.072025	2.666564	-1.597869
H	-2.922875	1.501378	-1.378686

Table S2. Atom coordinates for the optimized geometry of ***m*-1P2**.

Atom	X	Y	Z
C	-6.016731	0.158511	-1.371286
C	-5.917240	-1.122613	-1.867582
C	-4.762968	-1.896474	-1.594342
C	-3.743070	-1.384039	-0.820095
C	5.525752	-1.341058	-0.713858
C	6.759495	-0.872394	-1.112235
C	7.024822	0.520867	-1.129000
C	6.049362	1.417963	-0.747783
C	-1.659070	-1.440443	1.695529
C	-0.287784	0.178999	0.544681
C	-1.561298	-0.272717	0.920429
C	-0.506684	-2.127631	2.080188
C	0.753757	-1.667836	1.695791
C	0.882710	-0.505537	0.916491
C	2.501484	1.384347	0.460068
C	-2.776848	0.503106	0.532981

C	2.218845	-0.014340	0.487708
C	3.217958	-0.894273	0.102041
C	4.498931	-0.441553	-0.311379
C	4.767167	0.966011	-0.332913
C	3.732296	1.856061	0.065101
C	-2.903641	1.812553	0.968675
C	-4.044079	2.591217	0.660535
C	-5.065985	2.053531	-0.088477
C	-4.979979	0.721183	-0.575808
C	-3.819083	-0.070570	-0.274045
H	-6.893237	0.765905	-1.587089
H	-6.716674	-1.538085	-2.475742
H	-4.678234	-2.900375	-2.002772
H	-2.859745	-1.984890	-0.630674
H	5.321178	-2.409558	-0.701095
H	7.535192	-1.570813	-1.415780
H	8.001295	0.878688	-1.445222
H	6.249797	2.487276	-0.760597
H	-2.636399	-1.795345	2.011579
H	-0.212928	1.063121	-0.082949
H	-0.590470	-3.018995	2.697177
H	1.644384	-2.196872	2.023869
H	1.735821	2.085139	0.781372
H	3.019903	-1.963670	0.085703
H	3.929877	2.925988	0.062327
H	-2.116866	2.241884	1.583888
H	-4.110930	3.611478	1.029565
H	-5.950659	2.641898	-0.322035

Table S3. Atom coordinates for the optimized geometry of ***p*-1P1**.

Atom	X	Y	Z
C	3.838194	0.151283	0.154211
C	5.206577	-0.288143	0.137138
C	5.545354	-1.503016	-0.518178

C	4.575467	-2.254248	-1.142172
C	3.225349	-1.832802	-1.117719
C	-4.575505	2.254231	-1.142173
C	-5.545380	1.502979	-0.518186
C	-5.206583	0.288115	0.137138
C	-3.838189	-0.151280	0.154225
C	-2.837428	0.665804	-0.477557
C	2.837417	-0.665781	-0.477572
C	-3.225376	1.832814	-1.117709
C	-1.391586	0.299213	-0.464085
C	-0.682033	0.144625	0.739768
C	0.682052	-0.144507	0.739763
C	0.682149	-0.148459	-1.665964
C	-0.682180	0.148420	-1.665960
C	1.391580	-0.299180	-0.464094
C	3.544167	1.400862	0.771897
C	4.534313	2.156831	1.363974
C	5.876866	1.706054	1.370483
C	6.201362	0.512218	0.764846
C	-6.201353	-0.512266	0.764841
C	-5.876833	-1.706089	1.370493
C	-4.534268	-2.156829	1.364006
C	-3.544135	-1.400842	0.771929
H	6.584410	-1.825037	-0.522682
H	4.837373	-3.181294	-1.645742
H	2.466898	-2.452205	-1.589741
H	-4.837427	3.181270	-1.645748
H	-6.584443	1.824975	-0.522705
H	-2.466935	2.452226	-1.589736
H	-1.202517	0.265586	1.686399
H	1.202553	-0.265414	1.686392
H	1.208219	-0.255889	-2.611389
H	-1.208270	0.255791	-2.611381
H	2.523158	1.767542	0.764099
H	4.283384	3.109150	1.824341

H	6.648447	2.307870	1.843820
H	7.232171	0.164408	0.750827
H	-7.232172	-0.164484	0.750808
H	-6.648404	-2.307920	1.843827
H	-4.283319	-3.109134	1.824391
H	-2.523117	-1.767493	0.764148

Table S4. Atom coordinates for the optimized geometry of ***p*-1P2**.

Atom	X	Y	Z
C	-6.373122	1.322067	0.118854
C	-5.848365	2.560502	0.415784
C	-4.447844	2.716305	0.556901
C	-3.602067	1.641030	0.381191
C	5.363535	1.925552	-0.271177
C	6.740959	1.960191	-0.228655
C	7.480882	0.769560	-0.012206
C	6.827125	-0.432504	0.159055
C	-1.773359	-0.703313	-0.076837
C	0.351750	-1.454639	0.854771
C	-1.041893	-1.498627	0.820447
C	-1.051211	0.134512	-0.944231
C	0.341388	0.175525	-0.912831
C	1.075005	-0.614029	-0.008854
C	3.319174	-1.748365	0.253803
C	-3.260175	-0.797755	-0.136429
C	2.558695	-0.560756	0.032463
C	3.241133	0.633751	-0.138638
C	4.658978	0.700691	-0.101475
C	5.407998	-0.500813	0.121450
C	4.694091	-1.718111	0.295355
C	-3.842942	-2.031564	-0.382438
C	-5.245610	-2.185686	-0.479902
C	-6.072541	-1.095192	-0.332976
C	-5.530264	0.190003	-0.060913
C	-4.106260	0.350024	0.052159

H	-7.448741	1.188519	0.023956
H	-6.505460	3.415552	0.552583
H	-4.036968	3.689879	0.812212
H	-2.532831	1.774602	0.507280
H	4.795312	2.838477	-0.436909
H	7.266238	2.902594	-0.361429
H	8.566696	0.809142	0.019023
H	7.391937	-1.347288	0.326292
H	0.882137	-2.060689	1.584818
H	-1.574460	-2.143745	1.514981
H	-1.586459	0.738976	-1.672090
H	0.869314	0.806781	-1.622949
H	2.799288	-2.696072	0.364488
H	2.685818	1.558199	-0.280772
H	5.254238	-2.637405	0.453526
H	-3.201901	-2.896876	-0.530892
H	-5.662739	-3.168341	-0.684822
H	-7.151789	-1.202465	-0.417309

Table S5. Atom coordinates for the optimized geometry of **1BP1**.

Atom	X	Y	Z
C	5.926402	0.363104	-0.147672
C	7.339233	0.297822	0.108654
C	7.851043	-0.712999	0.966671
C	7.005496	-1.632019	1.545335
C	5.612769	-1.563949	1.307529
C	-7.005351	-1.631878	-1.545645
C	-7.850955	-0.712920	-0.966967
C	-7.339232	0.297810	-0.108792
C	-5.926424	0.363070	0.147677
C	-5.058313	-0.587654	-0.493761
C	5.058355	-0.587696	0.493741
C	-5.612648	-1.563825	-1.307703
C	-3.578152	-0.555916	-0.316006
C	-2.818164	0.576902	-0.655077

C	-1.429745	0.576039	-0.532793
C	-1.500312	-1.689290	0.271993
C	-2.889542	-1.688803	0.148255
C	-0.739617	-0.556745	-0.065215
C	5.456866	1.353464	-1.057700
C	6.323090	2.246518	-1.653123
C	7.710646	2.198218	-1.373813
C	8.203412	1.239748	-0.516058
C	-8.203479	1.239659	0.515942
C	-7.710805	2.198029	1.373861
C	-6.323277	2.246301	1.653315
C	-5.456988	1.353324	1.057872
C	0.739641	-0.556762	0.065373
C	1.429795	0.576013	0.532929
C	2.818218	0.576860	0.655175
C	3.578184	-0.555963	0.316080
C	2.889549	-1.688840	-0.148174
C	1.500315	-1.689315	-0.271866
H	8.922041	-0.750395	1.153476
H	7.399131	-2.406140	2.199101
H	4.955250	-2.277644	1.797463
H	-7.398922	-2.405932	-2.199529
H	-8.921936	-0.750299	-1.153877
H	-4.955079	-2.277458	-1.797661
H	-3.319008	1.458678	-1.046386
H	-0.870149	1.457205	-0.836219
H	-1.002289	-2.572421	0.664027
H	-3.453468	-2.572477	0.436664
H	4.399067	1.395160	-1.294646
H	5.938829	2.989522	-2.347493
H	8.383556	2.909904	-1.845291
H	9.269703	1.183879	-0.307155
H	-9.269749	1.183809	0.306926
H	-8.383766	2.909656	1.845355
H	-5.939090	2.989222	2.347815

H	-4.399214	1.394995	1.294936
H	0.870221	1.457197	0.836342
H	3.319090	1.458643	1.046436
H	3.453460	-2.572511	-0.436621
H	1.002275	-2.572435	-0.663905

Table S6. Atom coordinates for the optimized geometry of **1BP2**

Atom	X	Y	Z
C	8.490988	1.350615	-0.290089
C	7.980439	2.507475	-0.836264
C	6.584175	2.635585	-1.035720
C	5.727975	1.618034	-0.669885
C	-7.677063	1.698672	1.050906
C	-9.052760	1.729163	0.967582
C	-9.745103	0.760078	0.197175
C	-9.046664	-0.221802	-0.473502
C	3.874761	-0.584715	0.203857
C	1.763435	-1.494123	-0.609904
C	3.155770	-1.535016	-0.539652
C	3.142240	0.406655	0.879293
C	1.750663	0.445492	0.812030
C	1.029553	-0.502950	0.064292
C	-5.496521	-1.303431	-0.995372
C	5.359680	-0.669884	0.310609
C	-4.782857	-0.332109	-0.230408
C	-5.509448	0.643878	0.434099
C	-6.926735	0.700739	0.367658
C	-7.628174	-0.280432	-0.406666
C	-6.869505	-1.276435	-1.080578
C	5.929030	-1.832541	0.807050
C	7.328476	-1.967962	0.962745
C	8.165417	-0.929778	0.621848
C	7.637283	0.278007	0.090623
C	6.216988	0.416047	-0.082145
C	-0.452481	-0.459110	-0.008983

C	-1.143638	0.762897	-0.089729
C	-2.534307	0.803509	-0.163118
C	-3.300557	-0.375545	-0.155937
C	-2.609363	-1.597640	-0.076670
C	-1.218485	-1.638189	-0.003530
H	9.563518	1.236188	-0.147420
H	8.645780	3.317269	-1.124608
H	6.185094	3.540530	-1.486970
H	4.662622	1.726117	-0.843680
H	-7.145246	2.441721	1.641459
H	-9.613158	2.498236	1.493065
H	-10.829974	0.794241	0.138724
H	-9.575257	-0.967046	-1.064251
H	1.241502	-2.225119	-1.221997
H	3.697854	-2.301660	-1.087811
H	3.667989	1.138437	1.487312
H	1.213871	1.204348	1.375476
H	-4.939507	-2.059760	-1.541549
H	-4.992794	1.378322	1.047912
H	-7.392433	-2.019136	-1.679547
H	5.279436	-2.649928	1.109714
H	7.734761	-2.891951	1.366190
H	9.241953	-1.020896	0.748821
H	-0.583861	1.693631	-0.133765
H	-3.032239	1.764392	-0.263696
H	-3.168041	-2.529147	-0.036000
H	-0.721147	-2.599903	0.092919

Table S7. Atom coordinates for the optimized geometry of **1TP1**

Atom	X	Y	Z
C	8.068370	0.532933	-0.093395
C	9.494373	0.422762	0.049842
C	10.062524	-0.800999	0.496513
C	9.258573	-1.880577	0.784050
C	7.853807	-1.773376	0.657992

C	-9.258639	-1.880579	-0.783926
C	-10.062560	-0.800972	-0.496400
C	-9.494363	0.422789	-0.049787
C	-8.068355	0.532924	0.093417
C	-7.246083	-0.598006	-0.243507
C	7.246062	-0.597974	0.243549
C	-7.853867	-1.773401	-0.657918
C	-5.757945	-0.547857	-0.164965
C	-5.010654	0.384299	-0.905408
C	-3.617440	0.386012	-0.864759
C	-3.657952	-1.474178	0.659406
C	-5.051965	-1.477155	0.616723
C	-2.909529	-0.542717	-0.080665
C	7.539022	1.755494	-0.597960
C	8.362565	2.816606	-0.911384
C	9.764669	2.714115	-0.740148
C	10.313727	1.539628	-0.274983
C	-10.313675	1.539695	0.275009
C	-9.764568	2.714188	0.740107
C	-8.362454	2.816642	0.911296
C	-7.538952	1.755492	0.597894
C	-1.425479	-0.541404	-0.039122
C	-0.696462	0.660623	-0.019826
C	0.696430	0.660629	0.019926
C	1.425459	-0.541393	0.039064
C	0.696387	-1.743429	0.018369
C	-0.696392	-1.743435	-0.018583
C	2.909512	-0.542699	0.080626
C	3.617392	0.385907	0.864890
C	5.010607	0.384202	0.905562
C	5.757919	-0.547815	0.164967
C	5.051967	-1.477005	-0.616872
C	3.657956	-1.474029	-0.659587
H	11.143004	-0.870584	0.601694
H	9.695205	-2.816667	1.122683

H	7.230835	-2.625181	0.918813
H	-9.695299	-2.816673	-1.122515
H	-11.143044	-0.870530	-0.601553
H	-7.230920	-2.625228	-0.918729
H	-5.527044	1.097370	-1.542931
H	-3.070041	1.097803	-1.477360
H	-3.145028	-2.187140	1.299854
H	-5.604925	-2.196815	1.215384
H	6.468569	1.845574	-0.749593
H	7.932974	3.736857	-1.299228
H	10.403994	3.558061	-0.986334
H	11.390996	1.445419	-0.155078
H	-11.390948	1.445512	0.155127
H	-10.403858	3.558167	0.986267
H	-7.932818	3.736899	1.299077
H	-6.468486	1.845547	0.749476
H	-1.226858	1.609466	-0.018908
H	1.226817	1.609477	0.019131
H	1.226116	-2.692122	0.048720
H	-1.226110	-2.692130	-0.049060
H	3.069969	1.097584	1.477601
H	5.526981	1.097159	1.543225
H	5.604952	-2.196563	-1.215634
H	3.145045	-2.186883	-1.300167

5. Reference

1. A. C. S. D. B. Crystallography, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision D.01*, (2010) Gaussian, Inc., Wallingford CT.