

Supporting Information
for
Catalytic transfer of carbon atoms enables spirofusion of C–C σ -bonds

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I. General Information

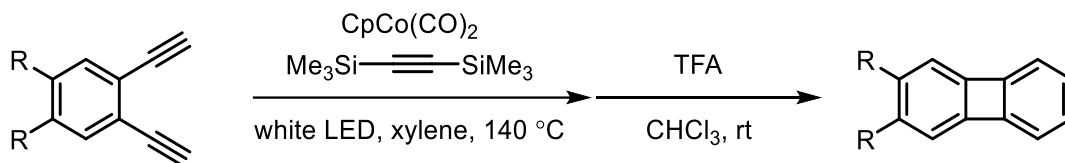
^1H and ^{13}C NMR spectra were recorded on a JEOL ECZL400S spectrometer in CDCl_3 . The chemical shifts in ^1H NMR spectra were recorded relative to CHCl_3 (δ 7.26). The chemical shifts in ^{13}C NMR spectra were recorded relative to CDCl_3 (δ 77.0). The chemical shifts in ^{19}F NMR spectra were recorded relative to benzotrifluoride (δ -63.72). The chemical shifts in ^{31}P NMR spectra were recorded relative to H_3PO_4 (δ 0.0). The data is reported as follows: chemical shift (δ) in ppm, coupling constant (Hz), and integration. Infrared spectra (IR) were obtained using a JASCO FT/IR-4200 spectrometer. Absorption is reported in reciprocal centimeters (cm^{-1}) with the following relative intensities: s (strong), m (medium), or w (weak). High resolution mass spectra (HRMS) were obtained using a JEOL JMS-T100LP spectrometer. Melting points were determined using a SRS Melting Point Apparatus MPA100. Differential scanning calorimetry (DSC) measurements were performed on a Rigaku ThermoPlus EVO2 DSCvesta. Column chromatography was performed with Biotage Isolera[®] equipped with Biotage[®] Sfar.

II. Materials

All commercially available reagents and solvents were supplied from TCI, BLD pharmatech, and Aldrich. Biphenylenes **1b** [CAS: 84509-67-1]¹, **1e** [CAS: 913332-00-0]², **1f** [CAS: 84509-68-2]¹, **1i** [CAS: 84509-69-3]¹, **1l** [CAS: 259-56-3]³, **1m** [CAS: 1436-33-5]⁴, **1o** [CAS: 55813-70-2]⁵, **1p** [CAS: 65513-20-4]⁶, and **1q** [CAS: 779345-87-8]⁷ were prepared according to the literature procedure. PINC- ^{13}C was prepared according to the literature method⁸.

III. Preparation of Starting Materials

Preparation of biphenylene **1c** and **1d**.

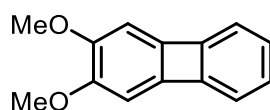


A two-necked flask equipped with a magnetic stir bar was charged with bis(trimethylsilyl)acetylene (BTMSA, 6.5 mL) and xylene (45 mL) and heated to $140\text{ }^\circ\text{C}$ under white LED irradiation. A solution of 1,2-diethynylarene (7.7 mmol) and CpCo(CO)_2 (211 mg, 1.18 mmol) in BTMSA (3 mL) and xylene (20 mL) was added dropwise over 7 h (3 mL/h) using a syringe pump. After completion of the addition, the reaction mixture was stirred at $140\text{ }^\circ\text{C}$ under irradiation overnight. The mixture was cooled to room

temperature, quenched with water (20 mL), and extracted with Et₂O (3 × 30 mL). The combined organic layers were dried over Na₂SO₄, filtered, and concentrated under reduced pressure.

To the residue were added trifluoroacetic acid (2.3 mL, 29.4 mmol) and CHCl₃ (2.5 mL), and the mixture was stirred at room temperature for 2 h. The reaction was quenched with water (20 mL) and extracted with Et₂O (3 × 30 mL). The combined organic layers were dried over Na₂SO₄, filtered, and concentrated. The crude product was purified by sublimation (10 mmHg) to afford the corresponding biphenylene.

2,3-Dimethoxybiphenylene (1c). [CAS: 92254-04-1]



The reaction was conducted according to the general procedure described above, except that 1,2-diethynylarene (4.6 mmol) was used.

White solid 71.8 mg (7%). R_f 0.48 (SiO₂, hexane/EtOAc = 4/1). M.p. 87–89 °C.

¹H NMR (CDCl₃, 400 MHz) δ: 6.61 (dd, *J* = 4.7, 2.9 Hz, 2H), 6.48 (s, 2H), 6.40 (dd, *J* = 4.7, 2.9 Hz, 2H), 3.82 (s, 6H).

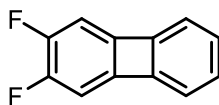
¹³C NMR (CDCl₃, 101 MHz) δ: 150.3, 148.5, 144.1, 127.6, 115.3, 106.0, 56.5.

IR (KBr): 3057 w, 3022 w, 2160 w, 2023 w, 1587 w, 1541 w, 1498 w, 1475 w, 1447 m, 1416 w, 1219 w, 1158 w, 1030 w, 806 w, 772 s.

MS, *m/z* (relative intensity, %): 213 (15), 212 (M⁺, 100), 198 (12), 197 (84), 169 (11), 168 (18), 151 (23), 141 (67), 139 (20), 127 (11), 126 (90), 115 (34), 91 (11), 76 (11), 75 (10), 63 (23).

HRMS (DART⁺, [M+H]⁺) Calcd for C₁₄H₁₃O₂: 213.0910. Found: 213.0911.

2,3-Fluorobiphenylene (1d). [CAS: 195201-95-7]



White solid 129.4 mg (9%). R_f 0.49 (SiO₂, hexane). M.p. 103–106 °C.

¹H NMR (CDCl₃, 400 MHz) δ: 6.77 (q, *J* = 2.5 Hz, 2H), 6.59 (dd, *J* = 4.7, 2.9 Hz, 2H), 6.51 (t, *J* = 7.6 Hz, 2H).

¹³C NMR (CDCl₃, 101 MHz) δ: 150.0 (dd, *J* = 249.5, 15.4 Hz), 148.2, 147.2 (t, *J* = 6.0 Hz), 129.0, 117.3, 109.8–109.4 (m).

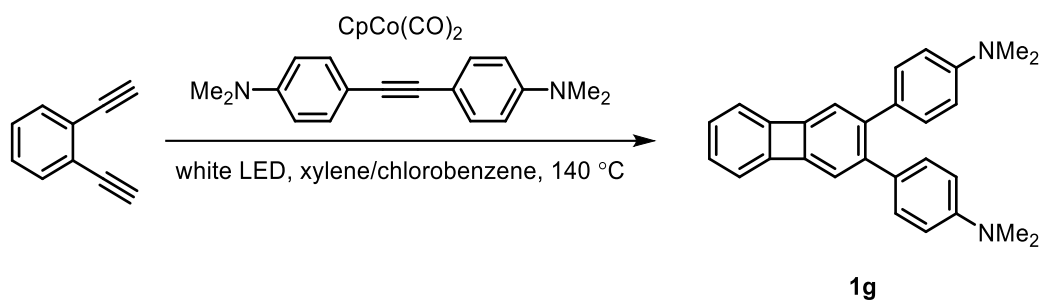
¹⁹F NMR (CDCl₃, 376 MHz) δ: –140.3–140.4 (m).

IR (KBr): 3076 w, 1667 w, 1599 w, 1471 w, 1454 w, 1434 m, 1409 w, 1382 w, 1345 w, 1308 w, 1269 m, 1203 w, 1169 w, 1142 w, 1103 w, 1059 w, 1048 w, 973 w, 930 w, 907 w, 867 m, 798 w, 783 m, 749 s.

MS, m/z (relative intensity, %): 189 (13), 188 (M^+ , 100), 187 (16), 168 (13), 94 (19).

HRMS (DART⁺, $[M+H]^+$) Calcd for $C_{12}H_7F_2$: 189.0510. Found: 189.0506.

Preparation of biphenylene 1g.



A two-necked flask equipped with a magnetic stir bar was charged with diarylacetylene (1.05 g, 3.97 mmol) and xylene (50 mL) and heated to 140 °C under white LED irradiation. A solution of 1,2-diethynylbenzene (1.68 g, 13.3 mmol), diarylacetylene (0.86 g, 3.25 mmol), $CpCo(CO)_2$ (0.72 g, 4.03 mmol) and chlorobenzene (40 mL) was added dropwise over 4 h (10 mL/h) using a syringe pump. After completion of the addition, the reaction mixture was stirred at 140 °C under irradiation overnight. The mixture was cooled to room temperature and purified by column chromatography on NH-silica gel (hexane/ $CHCl_3$ = 4/1). Further purification by GPC ($CHCl_3$) gave **1g** as a yellow solid (0.90 g, 32%).

4,4'-(Biphenylene-2,3-diyl)bis(*N,N*-dimethylaniline) (1g).

R_f 0.17 (SiO_2 , hexane/ $CHCl_3$ = 1/1). M.p. 198–199 °C.

1H NMR ($CDCl_3$, 400 MHz) δ : 7.00 (dt, J = 9.4, 2.5 Hz, 4H), 6.76 (dd, J = 4.8, 2.7 Hz, 2H), 6.71 (s, 2H), 6.66 (dd, J = 4.9, 2.9 Hz, 2H), 6.59 (d, J = 8.7 Hz, 4H), 2.92 (s, 12H).

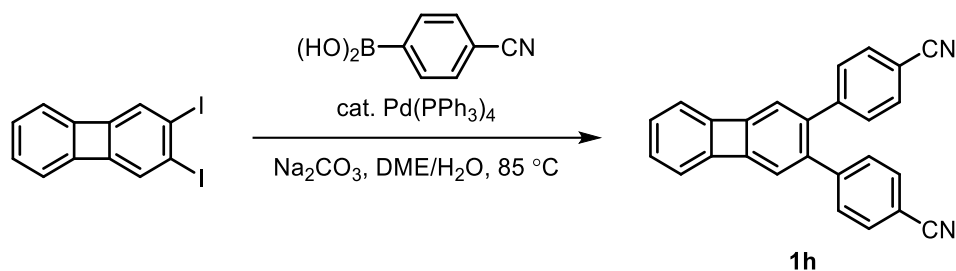
^{13}C NMR ($CDCl_3$, 101 MHz) δ : 151.1, 149.1, 148.8, 139.8, 130.3 (overlapped two peaks), 128.1, 120.2, 117.2, 112.0, 40.5.

IR (KBr): 3045 w, 2940 w, 2884 w, 2851 w, 2799 w, 1608 s, 1521 s, 1479 w, 1427 s, 1350 m, 1289 w, 1205 m, 1165 m, 1155 w, 1128 w, 1111 w, 1062 w, 969 w, 946 w.

MS, m/z (relative intensity, %): 391 (36), 390 (M^+ , 100), 195 (12).

HRMS (EI⁺, $[M]^+$) Calcd for $C_{28}H_{26}N_2$: 390.2096. Found: 390.2098.

Preparation of biphenylene 1h.



A two-necked flask was charged with 2,3-diiodobiphenylene (1.43 g, 3.54 mmol), 4-cyanophenylboronic acid (1.56 g, 10.6 mmol), Na_2CO_3 (1.95 g, 18.4 mmol), DME (90 mL) and H_2O (35 mL). The obtained mixture was degassed by passing through nitrogen for 30 min, followed by the addition of $\text{Pd(PPh}_3)_4$ (213.5 mg, 0.18 mmol). Then the reaction mixture was stirred at 85 °C for 15 h and then cooled to room temperature. The solvent was evaporated under reduced pressure, and the residue was extracted with EtOAc (3×50 mL), washed with brine, and dried over Na_2SO_4 . Purification by column chromatography on silica gel (hexane/EtOAc = 4/1) followed by GPC (CHCl_3) afforded **1h** as a yellow solid (192.7 mg, 15%).

4,4'-(Biphenylene-2,3-diyl)dibenzonitrile (1h).

R_f 0.39 (SiO_2 , hexane/EtOAc = 4/1). M.p. 249–250 °C.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ : 7.49 (d, J = 8.0 Hz, 4H), 7.14 (d, J = 8.0 Hz, 4H), 6.87–6.83 (m, 2H), 6.78–6.74 (m, 2H), 6.68 (s, 2H).

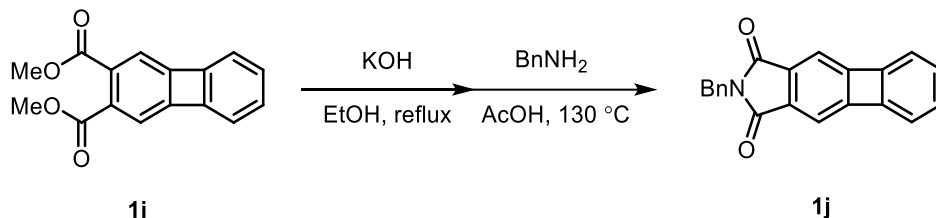
$^{13}\text{C NMR}$ (CDCl_3 , 101 MHz) δ : 151.7, 149.9, 145.8, 138.6, 131.9, 130.2, 129.2, 119.2, 118.5, 118.3, 110.7.

IR (KBr): 3060 w, 3045 w, 2222 s, 1604 s, 1505 m, 1430 m, 1380 w, 1340 w, 1277 w, 1208 m, 1179 m, 1153 s, 1110 m, 1063 w, 1022 w, 994 w, 973 w.

MS, m/z (relative intensity, %): 355 (29), 354 (M^+ , 100), 352 (19).

HRMS (EI^+ , $[\text{M}]^+$) Calcd for $\text{C}_{26}\text{H}_{14}\text{N}_2$: 354.1157. Found: 354.1158.

Preparation of biphenylene 1j.



To a stirred solution of **1i** (1.00 g, 3.72 mmol) in EtOH (50 mL) was added KOH (1.96 g, 34.9 mmol). The reaction mixture was refluxed for 2 h and then cooled to room temperature. The mixture was quenched with 3 M aqueous HCl (15 mL). After evaporation of the solvent, the residue was extracted with EtOAc (3×30 mL), washed with brine, dried over Na_2SO_4 , and concentrated under reduced

pressure to afford the crude anhydride. The crude product was used in the next step without further purification.

A two-necked flask was charged with the anhydride, benzylamine (0.44 mL, 4.02 mmol), and AcOH (3 mL) and heated at 130 °C for 3 h under nitrogen atmosphere. After cooling to room temperature, water was added to the mixture, and the resulting precipitate was collected by filtration. Further purification by recrystallization from CHCl₃/hexane gave **1j** as a yellow solid (367.0 mg, 32%).

2-Benzyl-1*H*-benzo[3,4]cyclobuta[1,2-*f*]isoindole-1,3(2*H*)-dione (1j**).**

R_f 0.49 (SiO₂, hexane/EtOAc = 4/1). M.p. 240–241 °C.

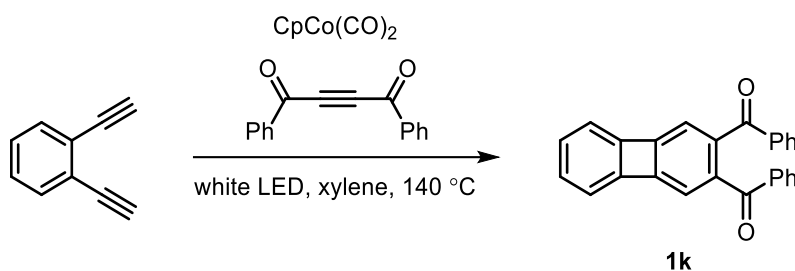
¹H NMR (CDCl₃, 400 MHz) δ: 7.41–7.39 (m, 2H), 7.34–7.24 (m, 3H), 6.98 (s, 2H), 6.92–6.88 (m, 2H), 6.82–6.79 (m, 2H), 4.77 (s, 2H).

¹³C NMR (CDCl₃, 101 MHz) δ: 168.0, 158.2, 148.5, 136.5, 133.5, 130.3, 128.7, 128.5, 127.8, 119.3, 111.1, 41.5.

IR (KBr): 3091 m, 3054 w, 2302 w, 2224 s, 1767 s, 1725 m, 1704 m, 1659 m, 1637 w, 1449 m, 1441 s, 1426 s, 1333 w, 1134 w, 1065 w, 1046 w, 976 m, 938 w.

HRMS (EI⁺, [M⁺]) Calcd for C₂₀H₁₃: 253.1012. Found: 253.1008.

Preparation of biphenylene **1k.**



A two-necked flask equipped with a magnetic stir bar was charged with xylene (60 mL) and heated to 140 °C under white LED irradiation. A solution of 1,2-diethynylbenzene (1.07 g, 8.49 mmol), dibenzoylacetylene (2.33 g, 9.95 mmol), CpCo(CO)₂ (0.69 g, 3.81 mmol) and xylene (20 mL) was added dropwise over 4 h (7 mL/h) using a syringe pump. After completion of the addition, the reaction mixture was stirred at 140 °C under irradiation overnight. The mixture was cooled to room temperature and purified by column chromatography on silica gel (hexane/EtOAc = 85/15). Further purification by recrystallization from CHCl₃/hexane gave **1k** as a yellow solid (0.75 g, 24%).

Biphenylene-2,3-diylbis(phenylmethanone) (1k**).**

R_f 0.20 (SiO₂, hexane/EtOAc = 9/1). M.p. 154–156 °C.

¹H NMR (CDCl₃, 400 MHz) δ: 7.72–7.70 (m, 4H), 7.52–7.48 (m, 2H), 7.37 (t, *J* = 7.7 Hz, 4H), 6.90–6.86 (m, 2H), 6.83 (s, 2H), 6.79–6.76 (m, 2H).

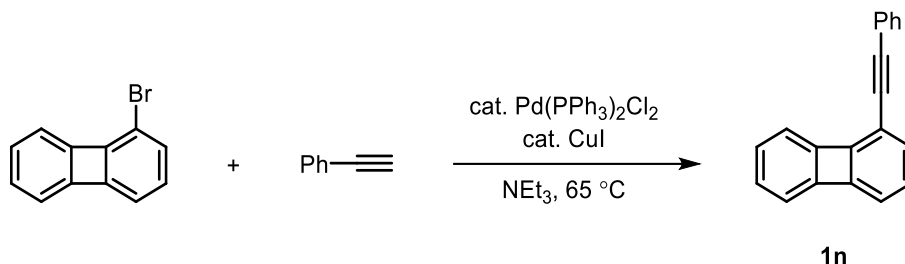
¹³C NMR (CDCl₃, 101 MHz) δ: 196.2, 153.5, 149.4, 141.1, 137.1, 133.0, 129.8, 129.6, 128.3, 118.9, 117.6.

IR (KBr): 3059 w, 2350 w, 2252 w, 1657 s, 1597 m, 1578 m, 1572 w, 1448 s, 1403 m, 1378 w, 1314 m, 1284 s, 1238 s, 1177 m, 1159 w, 1132 w, 1001 w, 976 w, 946 m.

MS, m/z (relative intensity, %): 361 (30), 360 (M^+ , 100), 359 (11), 331 (13), 284 (21), 283 (95), 255 (30), 226 (35), 105 (21), 77 (18).

HRMS (EI⁺, [M^+]) Calcd for $C_{26}H_{16}O_2$: 360.1150. Found: 360.1151.

Preparation of biphenylene 1n.



A two-necked flask was charged with 1-bromobiphenylene (432.9 mg, 1.87 mmol) and NEt_3 (20 mL). The obtained mixture was degassed by passing through nitrogen for 30 min, followed by the addition of phenylacetylene (267.3 mg, 2.62 mmol), CuI (58.7 mg, 0.31 mmol) and $Pd(PPh_3)_2Cl_2$ (156.7 mg, 0.22 mmol). Then the reaction mixture was stirred at 65 °C for 43 h and then cooled to room temperature. The resulting mixture was passed through a pad of Celite with EtOAc. Purification by column chromatography on silica gel (hexane/EtOAc = 9/1) followed by GPC ($CHCl_3$) afforded **1n** as a yellow solid (210.7 mg, 45%).

1-(Phenylethynyl)biphenylene (1n).

R_f 0.41 (SiO_2 , hexane). M.p. 71–72 °C.

1H NMR ($CDCl_3$, 400 MHz) δ : 7.53–7.50 (m, 2H), 7.38–7.34 (m, 3H), 6.82–6.77 (m, 4H), 6.76–6.71 (m, 1H), 6.67–6.65 (m, 1H), 6.58 (d, J = 6.9 Hz, 1H).

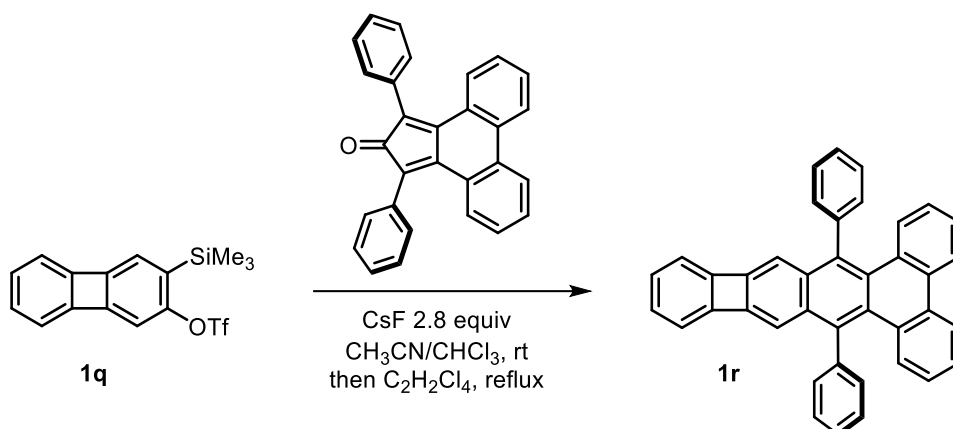
^{13}C NMR ($CDCl_3$, 101 MHz) δ : 153.2, 151.1, 150.6, 150.5, 131.6, 130.5, 128.8, 128.6, 128.44, 128.36, 128.34, 123.1, 118.0, 117.7, 116.7, 112.8, 92.0, 85.8.

IR (KBr): 3063 m, 3032 m, 2360 m, 2341 w, 1881 w, 1837 w, 1828 w, 1792 w, 1661 w, 1599 m, 1572 w, 1489 s, 1443 s, 1409 s, 1369 m, 1313 m, 1277 w, 1256 s, 1200 w, 1177 w, 1153 s, 1141 m, 1114 w, 1087 w, 1069 w, 1026 w, 1019 w, 992 w, 969 s, 916 m.

MS, m/z (relative intensity, %): 253 (22), 252 (M^+ , 100), 250 (35), 126 (15), 125 (12).

HRMS (DART⁺, [$M+H$]⁺) Calcd for $C_{20}H_{13}$: 253.1012. Found: 253.1008.

Preparation of π -extended biphenylene.



In the nitrogen-filled glovebox, a two-necked flask equipped with magnetic stir bar was charged with **1q** (463.0 mg, 1.24 mmol), phencyclone (478.7 mg, 1.25 mmol), CH₃CN (35 mL), and CHCl₃ (15 mL). To that solution, CsF (528.3 mg, 3.48 mmol) was added and stirred at room temperature for 20 h. The solvent was evaporated and residue was suspended in CHCl₃/Et₂O (3/1) and passed through a SiO₂. The resulting material was redissolved in C₂H₂Cl₄ and refluxed overnight. The crude product was purified by flash column chromatography on silica gel to afford **1r** as a yellow solid (560.2 mg, 90%).

9,16-Diphenylbenzo[*f*]benzo[3,4]cyclobuta[1,2-*l*]tetraphene (1r**).**

R_f 0.59 (SiO₂, hexane/toluene = 1/1). M.p. 295–300 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.31 (d, J = 7.6 Hz, 2H), 7.54–7.46 (m, 12H), 7.35 (t, J = 7.2 Hz, 2H), 7.06 (s, 2H), 7.01–6.90 (m, 6H).

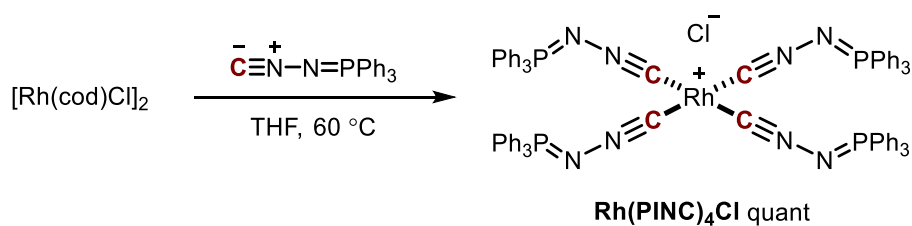
¹³C NMR (CDCl₃, 101 MHz) δ : 150.5, 146.4, 141.9, 136.2, 133.0, 132.5, 131.7, 130.9, 129.9 (overlapped two peaks), 129.4, 128.9, 127.5, 126.4, 125.6, 123.2, 119.6, 113.5.

IR (KBr): 3057 w, 2368 w, 2343 w, 2331 w, 2179 w, 2162 w, 2022 w, 1490 w, 1440 w, 1418 w, 1398 w, 1220 w, 1155 w, 877 w, 810 w, 772 s.

MS, m/z (relative intensity, %): 505 (42), 504 (M⁺, 100), 503 (11), 427 (11), 426 (18), 424 (11).

HRMS (EI⁺, [M]⁺) Calcd for C₄₀H₂₄: 504.1878. Found: 504.1873.

Preparation of Rh(PINC)₄Cl.



In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with [Rh(cod)Cl]₂ (24.7 mg, 0.050 mmol), PINC (121 mg, 0.40 mmol), and THF (3.0 mL). The

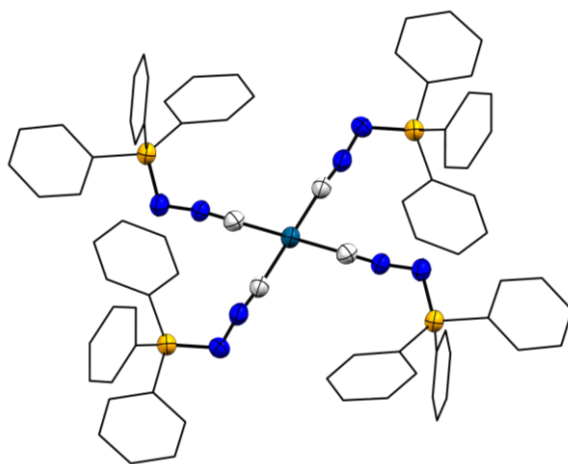
resulting mixture was stirred at 60 °C overnight. Complete consumption of the starting material was confirmed by ^1H NMR spectroscopy. After removal of the solvent under reduced pressure, the residue was purified by recrystallization from CHCl_3 /hexane to afford $\text{Rh}(\text{PINC})_4\text{Cl}$ as yellow crystals. Single crystals suitable for X-ray diffraction were obtained from this recrystallization.

^1H NMR (CDCl_3 , 400 MHz) δ : 7.67–7.46 (m, 60H).

^{13}C NMR (CDCl_3 , 101 MHz) δ : 133.4 (d, $J = 2.9$ Hz), 132.7 (d, $J = 9.6$ Hz), 129.3 (d, $J = 12.0$ Hz), 124.9 (d, $J = 98.7$ Hz).

^{31}P NMR (CDCl_3 , 162 MHz) δ : 28.3.

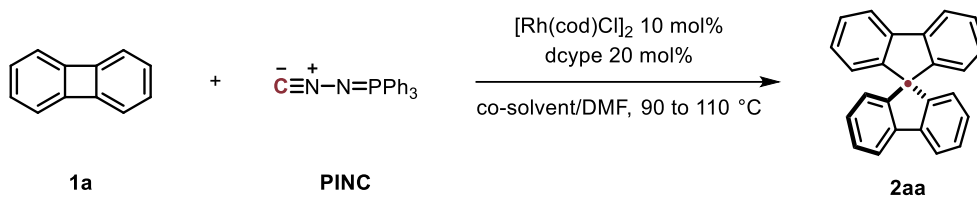
HRMS (ESI $^+$, $[\text{M}]^+$) Calcd for $\text{C}_{76}\text{H}_{60}\text{N}_8\text{P}_4\text{Rh}$: 1311.2941. Found: 1311.2970.



Crystal data for $\text{Rh}(\text{PINC})_4\text{Cl}$, orthorhombic, space group $P2_1/b2_1/c2_1/n$, $a = 15.6132(3)$ Å, $b = 14.2441(2)$ Å, $c = 39.3584(7)$ Å, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 8753.2(3)$ Å 3 , $T = 123$ K, $Z = 8$, R_1 (wR_2) = 0.0778 (0.2453) for 408 parameters and 8727 unique reflections. GOF = 1.066. CCDC 2526082. Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms and the counter anion are omitted for clarity.

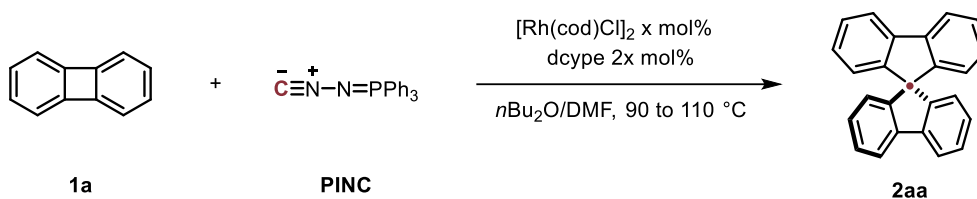
IV. Optimization Studies

Table S1. Solvent effect.



Entry	co-solvent	Yield of 2aa (%)
1	<i>n</i> Bu ₂ O	72
2	DMF	56
3	toluene	9

Table S2. Catalyst loading.

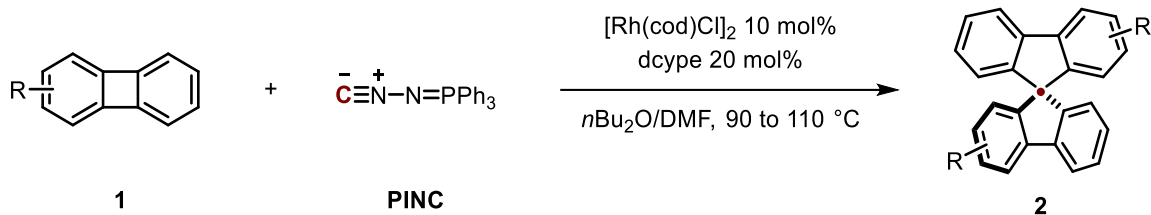


Entry	Catalyst loading (mol%)	Dropwise rate of PINC (mmol/h)	Yield of 2aa (%)
1	10	0.10	72
2	5	0.05	16
3 ^a	5	0.05	57
4 ^a	3	0.03	56
5 ^a	1	0.03	9

^a Reaction conducted at 110 °C throughout, instead of the standard temperature program (90 to 110 °C).

V. General Procedures

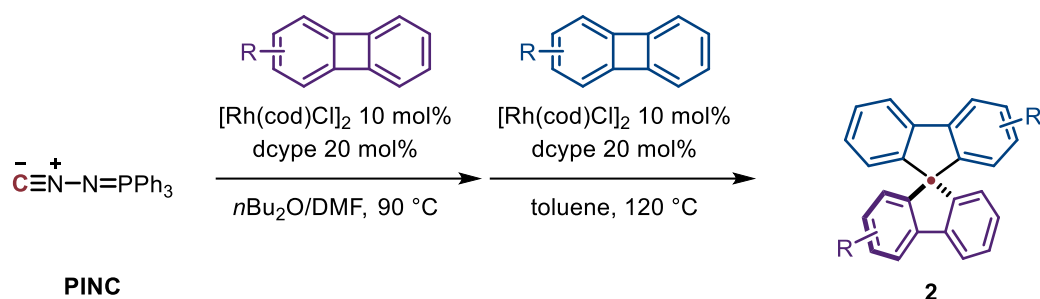
Homo-spirofusion



In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with [Rh(cod)Cl]₂ (4.9 mg, 0.01 mmol), dcype (8.5 mg, 0.02 mmol), biphenylene **1** (0.25 mmol),

*n*Bu₂O (0.6 mL) and DMF (0.1 mL) and heated to 90 °C using an oil bath. A solution of PINC (30.2 mg, 0.10 mmol) in DMF (0.5 mL) was added dropwise over 1 h (0.5 mL/h) using a syringe pump. After completion of the addition, the reaction mixture was stirred at 90 °C for 1.5 h and then heated to 110 °C and stirred for 24 h. The reaction mixture was cooled to room temperature and purified by flash column chromatography on silica gel to afford spirobifluorene **2**.

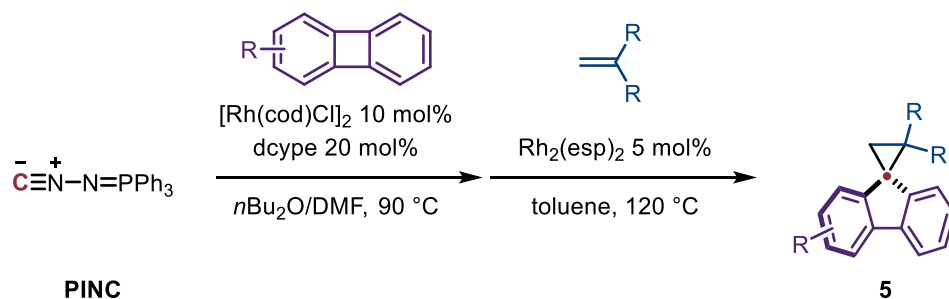
Cross-spirofusion via σ -bonds activation



In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with [Rh(cod)Cl]₂ (9.8 mg, 0.02 mmol), dcype (16.9 mg, 0.04 mmol), biphenylene **1** (purple, 0.24 mmol), *n*Bu₂O (1.2 mL) and DMF (0.2 mL) and heated to 90 °C in an oil bath. A solution of PINC (60.4 mg, 0.20 mmol) in DMF (1.0 mL) was added dropwise over 1 h (1.0 mL/h) using a syringe pump. After completion of the addition, the reaction mixture was stirred at 90 °C for 1.5 h. The reaction mixture was cooled to room temperature, concentrated under reduced pressure, and the residue was recrystallized from CHCl₃/hexane to afford the phosphazine **4**.

The resulting phosphazine (0.2 mmol) was dissolved in toluene (1.0 mL), and [Rh(cod)Cl]₂ (4.9 mg, 0.01 mmol), dcype (8.5 mg, 0.02 mmol), biphenylene **1** (blue, 0.10 mmol) were added. The mixture was then heated at 120 °C in an aluminum heating block for 24 h. The reaction mixture was cooled to room temperature and purified by flash column chromatography on silica gel to afford spirobifluorene **2**.

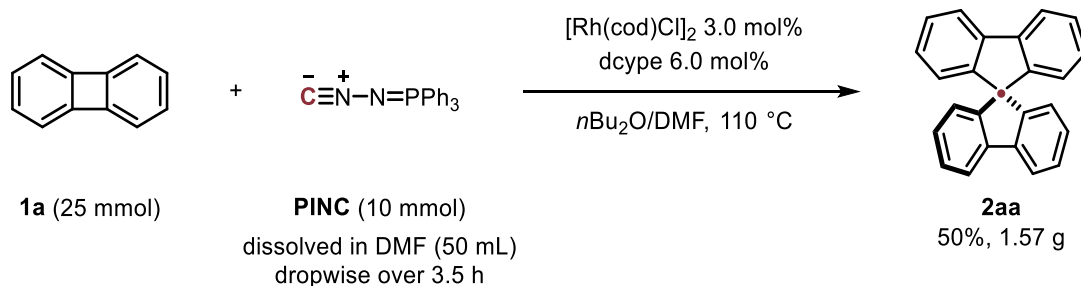
Cross-spirofusion via σ - and π -bond activation.



In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with [Rh(cod)Cl]₂ (9.8 mg, 0.02 mmol), dcype (16.9 mg, 0.04 mmol), biphenylene **1** (purple, 0.24 mmol), *n*Bu₂O (1.2 mL) and DMF (0.2 mL) and heated to 90 °C in an oil bath. A solution of PINC (60.4 mg, 0.20 mmol) in DMF (1.0 mL) was added dropwise over 1 h (1.0 mL/h) using a syringe pump. After completion of the addition, the reaction mixture was stirred at 90 °C for 1.5 h. The reaction mixture was cooled to room temperature, concentrated under reduced pressure, and the residue was recrystallized from CHCl₃/hexane to afford the phosphazine **4**.

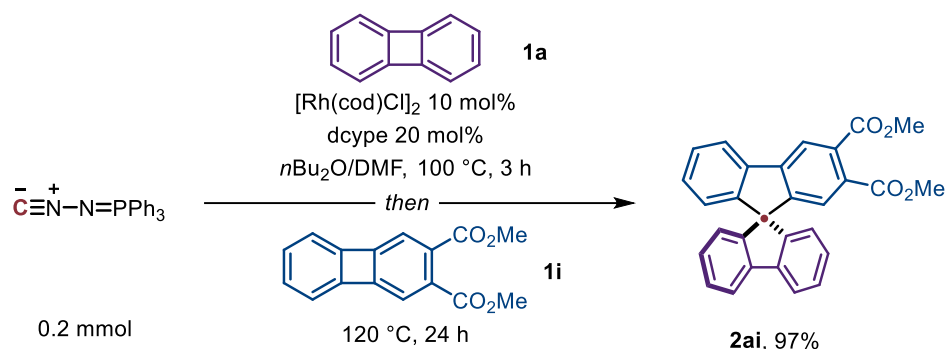
The resulting phosphazine (0.15 mmol) was dissolved in toluene (1.5 mL), and Rh₂(esp)₂ (5.7 mg, 0.0075 mmol), alkene (blue, 0.30 mmol) were added. The mixture was then heated at 120 °C in an aluminum heating block for 24 h. The reaction mixture was cooled to room temperature and purified by flash column chromatography on silica gel to afford spiro[2.4]heptane **5**.

VI. Large-Scale Experiment



A 200 mL two-necked flask equipped with a magnetic stir bar was charged with [Rh(cod)Cl]₂ (147.3 mg, 0.30 mmol), dcype (253.6 mg, 0.60 mmol), *n*Bu₂O (3 mL) and DMF (3 mL) and the mixture was stirred at room temperature for several minutes under nitrogen atmosphere. To the resulting mixture, a solution of biphenylene (3.86 g, 25.4 mmol) in *n*Bu₂O (57 mL) and DMF (7 mL) was added in one portion and heated to 110 °C. A solution of PINC (3.02 g, 10.0 mmol) in DMF (50 mL) was added dropwise over 3.5 h (14 mL/h) using a syringe pump. After completion of the addition, the reaction mixture was stirred at 110 °C for 44 h. The reaction mixture was cooled to room temperature and purified by column chromatography on silica gel to afford spirobifluorene **2aa** (1.57 g, 50%).

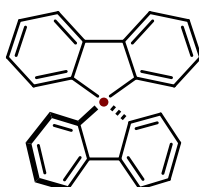
VII. One-Pod Cross-Spirofusion Experiment



In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with $[\text{Rh}(\text{cod})\text{Cl}]_2$ (5.0 mg, 0.010 mmol), dcype (7.9 mg, 0.019 mmol), biphenylene **1a** (31.6 mg, 0.21 mmol), $n\text{Bu}_2\text{O}$ (1.2 mL) and DMF (0.2 mL) and heated to 100 °C in an oil bath. A solution of PINC (61.5 mg, 0.20 mmol) in DMF (1.0 mL) was added dropwise over 2 h (0.5 mL/h) using a syringe pump. After completion of the addition, the reaction mixture was stirred at 100 °C for 1 h and cooled to room temperature. Biphenylene **1i** (25.4 mg, 0.095 mmol) was added to the mixture in a glovebox, and the resulting mixture was stirred at 120 °C for 24 h in an oil bath. The reaction mixture was cooled to room temperature and purified by flash column chromatography on silica gel to afford spirobifluorene **2ai** (39.7 mg, 97%).

VIII. Spectroscopic Data of Products

9,9'-Spiro[bi]fluorene (**2aa**). [CAS: 159-66-0]



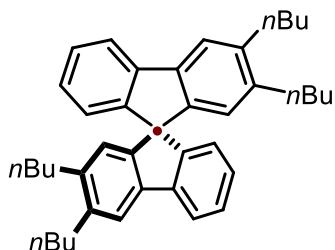
White solid 17.2 mg (53%).

^1H NMR (CDCl_3 , 400 MHz) δ : 7.86 (d, $J = 7.6$ Hz, 4H), 7.38 (td, $J = 97.5, 1.1$ Hz, 4H), 7.12 (td, $J = 7.4, 1.1$ Hz, 4H), 6.75 (d, $J = 7.6$ Hz, 4H).

^{13}C NMR (CDCl_3 , 101 MHz) δ : 148.7, 141.7, 127.8, 127.7, 124.0, 120.0, 65.9.

HRMS (DART⁺, $[\text{M}+\text{H}]^+$) Calcd for $\text{C}_{25}\text{H}_{17}$: 317.1325. Found: 317.1338.

2,2',3,3'-Tetrabutyl-9,9'-spiro[bi]fluorene (**2bb**).



Yellow solid 29.0 mg (54%). R_f 0.24 (SiO₂, hexane). M.p. 73–77 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 7.77 (d, J = 7.6 Hz, 2H), 7.60 (s, 2H), 7.31 (td, J = 7.5, 1.1 Hz, 2H), 7.03 (td, J = 7.5, 1.1 Hz, 2H), 6.67 (d, J = 7.3 Hz, 2H), 6.50 (s, 2H), 2.70–2.66 (m, 4H), 2.51–2.37 (m, 4H), 1.71–1.63 (m, 4H), 1.52–1.43 (m, 4H), 1.39–1.31 (m, 4H), 1.26–1.17 (m, 4H), 1.00 (t, J = 7.3 Hz, 6H), 0.81 (t, J = 7.2 Hz, 6H).

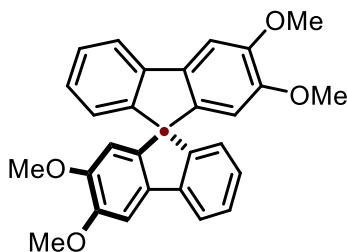
¹³C NMR (CDCl₃, 101 MHz) δ : 149.6, 146.6, 141.9, 140.6, 139.9, 139.5, 127.3, 127.0, 124.6, 123.9, 120.2, 119.4, 65.5, 33.6, 33.5, 32.8, 32.7, 23.0, 22.7, 14.1, 13.9.

IR (KBr): 2955 s, 2929 s, 2870 m, 2360 w, 2336 w, 1610 w, 1510 s, 1467 m, 1449 m, 1378 w, 1362 w, 1233 s, 1178 m, 1152 s, 1103 w, 1079 m, 1011 s, 923 w.

MS, m/z (relative intensity, %): 541 (44), 540 (M⁺, 100), 483 (21), 455 (27), 186 (15), 185 (46).

HRMS (EI⁺, [M]⁺) Calcd for C₄₁H₄₈: 540.3756. Found: 540.3770.

2,2',3,3'-Tetramethoxy-9,9'-spirobi[fluorene] (2cc). [CAS: 1422643-54-6]

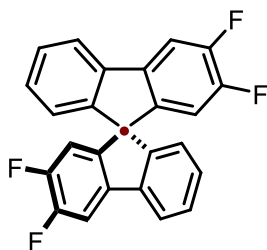


White solid 26.0 mg (61%).

¹H NMR (CDCl₃, 400 MHz) δ : 7.71 (d, J = 7.6 Hz, 2H), 7.34–7.31 (m, 4H), 7.03 (td, J = 7.5, 1.0 Hz, 2H), 6.66 (d, J = 7.6 Hz, 2H), 6.23 (s, 2H), 4.03 (s, 6H), 3.64 (s, 6H).

¹³C NMR (CDCl₃, 101 MHz) δ : 149.5, 149.3, 149.1, 141.9, 140.8, 134.3, 127.5, 126.5, 123.6, 118.8, 106.8, 102.9, 65.8, 56.2, 56.0.

2,2',3,3'-Tetrafluoro-9,9'-spirobi[fluorene] (2dd).



Pale yellow solid 21.1 mg (55%). R_f 0.37 (SiO_2 , hexane). M.p. 203–204 °C.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ : 7.74 (d, J = 7.6 Hz, 2H), 7.60 (dd, J = 10.0, 7.2 Hz, 2H), 7.40 (td, J = 7.6, 1.1 Hz, 2H), 7.14 (td, J = 7.5, 1.1 Hz, 2H), 6.71 (d, J = 7.6 Hz, 2H), 6.52 (dd, J = 9.6, 7.3 Hz, 2H).

$^{13}\text{C NMR}$ (CDCl_3 , 101 MHz) δ : 151.9 (dd, J = 60.2, 12.0 Hz), 149.4 (dd, J = 59.5, 12.3 Hz), 148.0 (d, 1.9 Hz), 143.5 (dd, J = 5.8, 2.9 Hz), 140.0 (dd, J = 2.4, 1.4 Hz), 137.9 (dd, J = 7.0, 3.1 Hz), 128.4, 128.3, 124.0, 120.1, 113.0 (d, J = 18.8 Hz), 108.9 (d, J = 18.8 Hz), 65.3–65.2 (m).

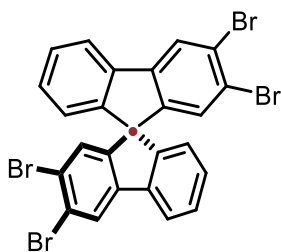
$^{19}\text{F NMR}$ (CDCl_3 , 376 MHz) δ : –140.0–140.1 (m), –140.4–140.5 (m).

IR (KBr): 2362 w, 1608 w, 1492 s, 1454 s, 1422 w, 1362 m, 1303 w, 1290 w, 1261 w, 1198 w, 1170 w, 1025 w, 869 w, 784 s.

MS, m/z (relative intensity, %): 389 (25), 388 (M^+ , 100), 387 (50), 369 (12), 367 (16).

HRMS (DART $^+$, $[\text{M}+\text{H}]^+$) Calcd for $\text{C}_{25}\text{H}_{13}\text{F}_4$: 389.0948. Found: 389.0941.

2,2',3,3'-Tetrabromo-9,9'-spirobi[fluorene] (2ee).



White solid 37.7 mg (59%). R_f 0.33 (SiO_2 , hexane). M.p. 307–308 °C.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ : 8.09 (d, J = 4.0 Hz, 2H), 7.79 (d, J = 7.6 Hz, 2H), 7.41 (td, J = 7.6, 1.1 Hz, 2H), 7.19 (td, J = 7.5, 1.1 Hz, 2H), 6.95 (s, 2H), 6.72 (d, J = 7.8 Hz, 2H).

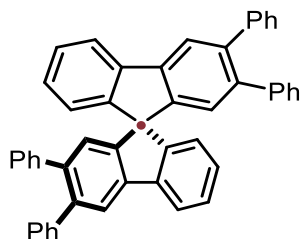
$^{13}\text{C NMR}$ (CDCl_3 , 101 MHz) δ : 148.1, 147.5, 142.6, 139.5, 129.2, 129.0, 128.6, 125.2, 124.6, 124.2, 123.6, 120.6, 64.9.

IR (KBr): 3058 w, 3012 w, 2924 w, 1945 w, 1921 w, 1712 w, 1591 w, 1556 w, 1459 m, 1435 s, 1358 m, 1271 m, 1215 w, 1155 w, 1109 w, 1092 m.

MS, m/z (relative intensity, %): 636 (17), 635 (17), 634 (67), 632 (M^+ , 100), 630 (67), 628 (17), 555 (14), 554 (13), 553 (41), 552 (12), 551 (39), 549 (15), 471 (17), 393 (26), 391 (27), 312 (17), 311 (47), 309 (16), 276 (26), 275 (28), 196 (23), 195 (22), 156 (19), 155 (71), 154 (28).

HRMS (EI $^+$, $[\text{M}^+]$) Calcd for $\text{C}_{25}\text{H}_{12}\text{Br}_4$: 627.7672. Found: 627.7685.

2,2',3,3'-Tetraphenyl-9,9'-spirobi[fluorene] (2ff).



Pale orange solid 46.3 mg (75%). R_f 0.26 (SiO_2 , hexane). M.p. 187–188 °C.

^1H NMR (CDCl_3 , 400 MHz) δ : 7.89–7.87 (m, 4H), 7.41 (td, J = 7.4, 0.9 Hz, 2H), 7.27–7.24 (m, 10H), 7.19 (td, J = 7.6, 0.9 Hz, 2H), 7.11–7.09 (m, 6H), 7.03–7.01 (m, 4H), 6.90–6.88 (m, 4H).

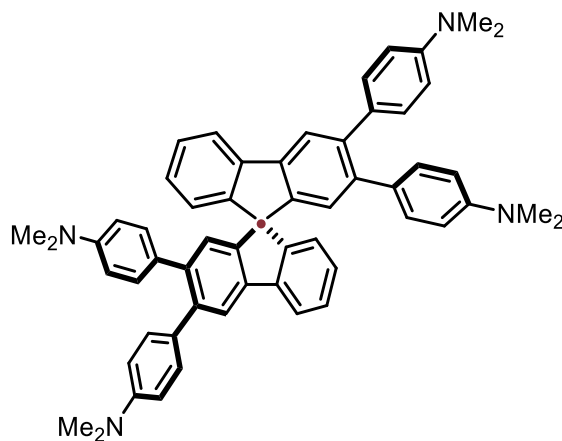
^{13}C NMR (CDCl_3 , 101 MHz) δ : 149.3, 147.9, 141.8, 141.5, 141.4, 141.1, 140.4, 140.3, 130.0, 129.9, 128.0, 127.89, 127.86, 127.7, 126.5, 126.3, 126.1, 124.3, 122.1, 120.1, 65.8.

IR (KBr): 3060 w, 3023 w, 2197 w, 2179 w, 2163 w, 2154 w, 2030 w, 2017 w, 2003 w, 1972 w, 1600 w, 1466 w, 1447 w, 1219 m, 890 w, 771 s.

MS, m/z (relative intensity, %): 622 (13), 621 (51), 620 (M^+ , 100), 543 (16), 310 (12).

HRMS (EI^+ , $[\text{M}]^+$) Calcd for $\text{C}_{49}\text{H}_{32}$: 620.2504. Found: 620.2498.

4,4',4'',4'''-(9,9'-Spirobi[fluorene]-2,2',3,3'-tetrayl)tetrakis(*N,N*-dimethylaniline) (2gg).



Brown solid 24.4 mg (30%). R_f 0.10 (SiO_2 , CHCl_3). M.p. 280–282 °C.

^1H NMR (CDCl_3 , 400 MHz) δ : 7.82–7.79 (m, 4H), 7.35 (td, J = 7.5, 1.0 Hz, 2H), 7.19–7.16 (m, 4H), 7.11 (td, J = 7.5, 1.1 Hz, 2H), 6.94–6.91 (m, 4H), 6.85 (d, J = 7.6 Hz, 2H), 6.80 (s, 2H), 6.68 (d, J = 8.5 Hz, 4H), 6.51 (d, J = 8.2 Hz, 4H), 2.95 (s, 12H), 2.84 (s, 12H).

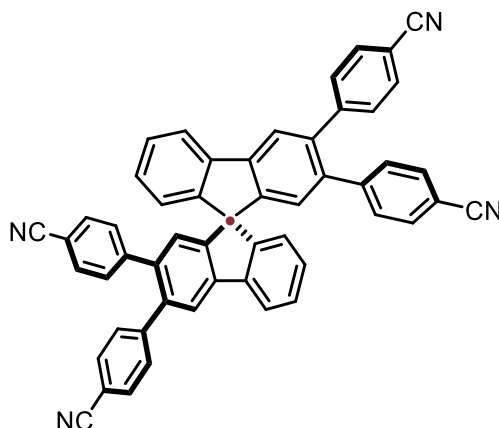
^{13}C NMR (CDCl_3 , 101 MHz) δ : 149.5, 148.9, 148.8, 147.4, 141.9, 140.2, 140.0, 139.8, 130.7 (overlapped two peaks), 130.5 (overlapped two peaks), 127.5, 127.4, 126.1, 124.2, 121.8, 119.7, 112.2, 112.0, 65.7, 40.62, 40.56.

IR (KBr): 3037 w, 3021 w, 2884 w, 2851 w, 2796 w, 2360 w, 2332 w, 1735 w, 1679 w, 1609 s, 1522 s, 1483 m, 1465 w, 1444 m, 1428 w, 1352 m, 1219 w, 1196 m, 1166 m, 1130 w, 1061 w.

MS, m/z (relative intensity, %): 794 (19), 792 (M^+ , 100), 416 (10), 404 (11), 396 (24), 376 (17).

HRMS (EI⁺, [M^+]) Calcd for $C_{57}H_{52}N_4$: 792.4192. Found: 792.4187.

4,4',4'',4'''-(9,9'-Spirobi[fluorene]-2,2',3,3'-tetrayl)tetrabenzonitrile (2hh).



Pale yellow solid 58.8 mg (79%). R_f 0.09 (SiO_2 , toluene/ $CHCl_3$ = 1/1). M.p. 230–231 °C.

1H NMR ($CDCl_3$, 400 MHz) δ : 7.91 (d, J = 7.6 Hz, 2H), 7.88 (s, 2H), 7.58 (dd, J = 6.6, 1.8 Hz, 4H), 7.48–7.40 (m, 6H), 7.31 (dd, J = 6.8, 1.7 Hz, 4H), 7.23 (td, J = 7.6, 0.9 Hz, 2H), 7.06 (dd, J = 6.6, 1.8 Hz, 4H), 6.86–6.84 (m, 4H).

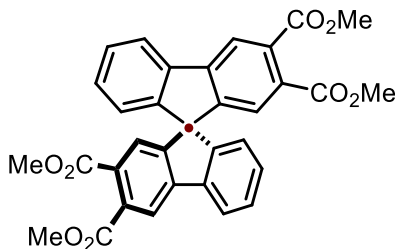
^{13}C NMR ($CDCl_3$, 101 MHz) δ : 148.8, 148.7, 145.6, 145.3, 142.7, 140.3, 138.9, 138.4, 132.1, 131.8, 130.6, 130.5, 129.0, 128.4, 125.9, 124.3, 122.3, 120.6, 118.5, 118.4, 111.1, 110.8, 65.8.

IR (KBr): 3063 w, 3041 w, 2360 m, 2332 w, 2227 s, 1605 s, 1506 w, 1466 m, 1449 m, 1389 w, 1179 w, 1110 w, 1018 w, 965 w, 911 m.

MS, m/z (relative intensity, %): 722 (16), 721 (55), 720 (M^+ , 100), 618 (17), 361 (12), 360 (19).

HRMS (EI⁺, [M^+]) Calcd for $C_{53}H_{28}N_4$: 720.2314. Found: 720.2310.

Tetramethyl 9,9'-spirobi[fluorene]-2,2',3,3'-tetracarboxylate (2ii).



Orange solid 38.8 mg (71%). R_f 0.48 (SiO_2 , hexane/EtOAc = 1/1). M.p. 209–210 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.13 (s, 2H), 7.91 (d, J = 7.6 Hz, 2H), 7.45 (td, J = 7.6, 0.9 Hz, 2H), 7.21 (td, J = 7.6, 0.9 Hz, 2H), 7.07 (s, 2H), 6.72 (d, J = 7.6 Hz, 2H), 3.97 (s, 6H), 3.77 (s, 6H).

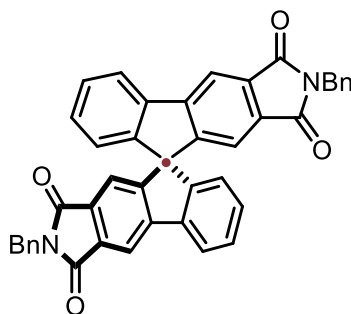
¹³C NMR (CDCl₃, 101 MHz) δ : 168.6, 167.1, 149.8, 147.9, 145.0, 139.7, 133.4, 130.5, 129.6, 128.7, 124.9, 124.2, 121.2, 120.4, 65.7, 52.8, 52.5.

IR (KBr): 3023 w, 2951 w, 2365 w, 2333 w, 2168 w, 2120 w, 2094 w, 1988 w, 1870 w, 1725 s, 1615 w, 1569 w, 1471 w, 1450 w, 1435 m, 1403 w, 1354 w, 1304 m, 1271 s, 1227 m, 1156 w, 1144 w, 1119 m, 1070 w, 966 w.

MS, m/z (relative intensity, %): 549 (35), 548 (M⁺, 100), 518 (14), 517 (39), 490 (29), 489 (82), 313 (21), 244 (23), 243 (48).

HRMS (EI⁺, [M]⁺) Calcd for C₃₃H₂₄O₈: 548.1471. Found: 548.1485.

2,2'-Dibenzyl-1*H*,1'*H*-9,9'-spirobi[indeno[1,2-*f*]isoindole]-1,1',3,3'(2*H*,2'*H*)-tetraone (2jj).



The reaction was conducted according to the general procedure described above, except that *n*Bu₂O (1.0 mL) and DMF (2.5 mL) was used as the initial solvent, and the reaction mixture was heated at 140 °C in an oil bath for 72 h after the completion of heating at 90 °C.

Orange solid 24.0 mg (38%). R_f 0.27 (SiO₂, hexane/EtOAc = 4/1). M.p. 335–337 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.29 (s, 2H), 7.98 (d, J = 7.1 Hz, 2H), 7.50 (t, J = 7.6 Hz, 2H), 7.37 (d, J = 7.6 Hz, 4H), 7.29–7.21 (m, 8H), 7.08 (s, 2H), 6.77 (dd, J = 7.7, 0.6 Hz, 2H), 4.81 (s, 4H).

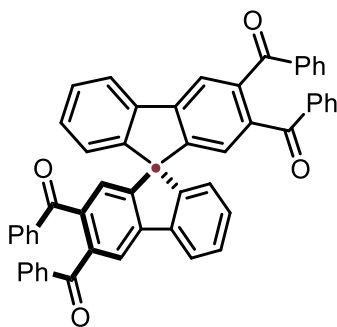
¹³C NMR (CDCl₃, 101 MHz) δ : 167.6, 167.5, 153.4, 147.9, 147.2, 139.8, 136.2, 133.0, 131.5, 130.2, 129.1, 128.6, 128.4, 127.8, 124.3, 121.6, 119.2, 115.3, 65.9, 41.6.

IR (KBr): 3464 w, 3061 w, 3032 w, 1768 m, 1702 s, 1613 w, 1496 w, 1455 w, 1430 m, 1387 s, 1346 m, 1184 w, 1155 w, 1120 m, 1102 w, 1067 w, 1027 w, 996 w, 947 w.

MS, m/z (relative intensity, %): 636 (12), 635 (48), 634 (M⁺, 100), 543 (14), 278 (13), 91 (13).

HRMS (EI⁺, [M]⁺) Calcd for C₄₃H₂₆N₂O₄: 634.1893. Found: 634.1869.

9,9'-Spirobi[fluorene]-2,2',3,3'-tetrayltetrakis(phenylmethanone) (2kk).



Orange solid 31.7 mg (43%). R_f 0.09 (SiO₂, hexane/EtOAc = 3/1). M.p. 208–210 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.04 (s, 2H), 7.86 (d, J = 7.6 Hz, 2H), 7.74 (d, J = 7.6 Hz, 4H), 7.54–7.51 (m, 6H), 7.46–7.38 (m, 8H), 7.28–7.24 (m, 6H), 7.08 (s, 2H), 6.87 (d, J = 7.6 Hz, 2H).

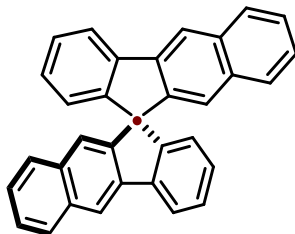
¹³C NMR (CDCl₃, 101 MHz) δ : 196.5, 195.9, 149.6, 148.2, 144.3, 141.0, 139.9, 139.3, 137.25, 137.23, 133.2, 133.0, 129.8, 129.7, 129.6, 128.7, 128.4, 128.2, 125.5, 124.3, 121.4, 121.3, 66.0.

IR (KBr): 3058 w, 2928 w, 2851 w, 2167 w, 1660 s, 1597 m, 1579 w, 1557 w, 1447 m, 1395 w, 1349 m, 1315 m, 1297 m, 1270 s, 1177 w, 1158 w, 1074 w, 1026 w, 1002 w, 941 w, 920 w.

MS, m/z (relative intensity, %): 734 (15), 733 (46), 732 (M⁺, 78), 705 (31), 704 (56), 676 (10), 656 (23), 655 (47), 628 (22), 627 (27), 599 (16), 387 (12), 313 (20), 289 (14), 105 (100), 78 (16), 77 (34).

HRMS (EI⁺, [M⁺]) Calcd for C₅₃H₃₂O₄: 732.2301. Found: 732.2283.

11,11'-Spirobi[benzo[*b*]fluorene] (2II). [CAS: 24969-55-9]



White solid 20.2 mg (50%). R_f 0.63 (SiO₂, hexane/toluene = 3/1). M.p. 163–165 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.31 (s, 2H), 8.04 (d, J = 7.6 Hz, 2H), 7.96 (d, J = 8.2 Hz, 2H), 7.52 (d, J = 8.0 Hz, 2H), 7.46–7.41 (m, 4H), 7.35–7.31 (m, 2H), 7.21 (s, 2H), 7.16 (td, J = 7.5, 1.0 Hz, 2H), 6.79 (d, J = 7.6 Hz, 2H).

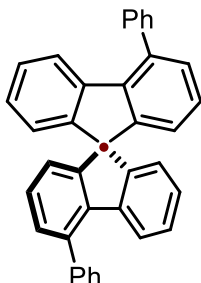
¹³C NMR (CDCl₃, 101 MHz) δ : 150.4, 148.2, 140.9, 140.1, 133.7, 133.6, 128.7, 128.2 (overlapped two peaks), 128.0, 125.8, 125.6, 124.6, 123.1, 120.6, 118.1, 65.0.

IR (KBr): 3051 w, 2920 w, 2849 w, 2363 w, 2338 w, 2177 w, 2158 w, 2006 w, 1994 w, 1968 w, 1723 w, 1606 w, 1502 w, 1465 w, 1434 w, 1227 w, 1211 w, 952 w, 881 w, 840 w, 786 s.

MS, m/z (relative intensity, %): 417 (31), 416 (M⁺, 100), 415 (36), 414 (12), 413 (20), 207 (15), 206 (12).

HRMS (EI⁺, [M]⁺) Calcd for C₃₃H₂₀: 416.1565. Found: 416.1554.

4,4'-Diphenyl-9,9'-spirobi[fluorene] (2mm).



Orange solid 16.3 mg (35%). R_f 0.74 (SiO₂, hexane/CHCl₃ = 1/1). M.p. 202–203 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 7.65 (d, J = 6.9 Hz, 4H), 7.60–7.50 (m, 6H), 7.23 (dd, J = 7.4, 1.3 Hz, 2H), 7.16 (t, J = 7.4 Hz, 2H), 7.07–7.02 (m, 6H), 6.82–6.77 (m, 4H).

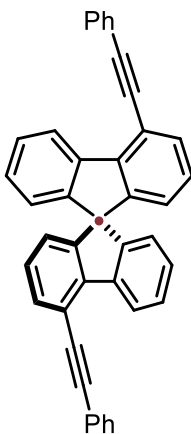
¹³C NMR (CDCl₃, 101 MHz) δ : 149.6, 149.3, 141.6, 141.0, 138.6, 137.8, 129.7, 129.2, 128.5, 127.6, 127.5, 127.3, 127.2, 123.9, 123.0, 122.9, 65.4.

IR (KBr): 3057 w, 3024 w, 2161 w, 2023 w, 1959 w, 1602 w, 1586 w, 1498 w, 1477 w, 1447 s, 1416 m, 1339 w, 1283 w, 1216 m, 1158 w, 1071 w, 1030 w, 1003 w, 971 w, 930 w.

MS, m/z (relative intensity, %): 469 (39), 468 (M⁺, 100), 467 (21), 391 (11), 234 (11).

HRMS (EI⁺, [M]⁺) Calcd for C₃₇H₂₄: 468.1878. Found: 468.1876.

4,4'-Bis(phenylethynyl)-9,9'-spirobi[fluorene] (2nn).



Pale yellow solid 16.2 mg (32%). R_f 0.71 (SiO₂, hexane/toluene = 1/1). M.p. 237–239 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.68 (d, J = 7.8 Hz, 2H), 7.74–7.71 (m, 4H), 7.54 (dd, J = 7.7, 1.0 Hz, 2H), 7.49–7.40 (m, 8H), 7.17 (td, J = 7.6, 1.1 Hz, 2H), 7.10 (t, J = 7.7 Hz, 2H), 6.77 (d, J = 7.6 Hz, 2H), 6.73 (dd, J = 7.6, 1.1 Hz, 2H).

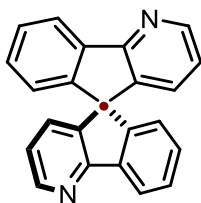
¹³C NMR (CDCl₃, 101 MHz) δ : 149.0, 148.6, 141.6, 141.4, 132.2, 131.6, 128.6 (overlapped two peaks), 128.3, 127.9, 127.4, 124.1, 123.8, 123.3, 122.9, 116.6, 93.8, 88.3, 65.0.

IR (KBr): 3060 w, 2926 w, 1971 w, 1597 m, 1507 w, 1492 s, 1481 w, 1449 s, 1418 s, 1286 w, 1252 w, 1156 w, 1097 w, 1071 m, 1026 w, 1002 w, 969 w, 929 w, 913 w.

MS, m/z (relative intensity, %): 517 (42), 516 (M⁺, 100), 515 (28), 514 (11), 513 (15), 258 (12).

HRMS (EI⁺, [M⁺]) Calcd for C₄₁H₂₄: 516.1878. Found: 516.1868.

5,5'-Spiro[indeno[1,2-*b*]pyridine] (2oo). [CAS: 502494-22-6]



Yellow solid 20.6 mg (66%). R_f 0.26 (SiO₂, hexane/EtOAc = 2/1). M.p. 183–186 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.62 (dd, J = 4.6, 2.1 Hz, 2H), 8.17 (d, J = 7.6 Hz, 2H), 7.48 (td, J = 7.6, 0.9 Hz, 2H), 7.26 (td, J = 7.6, 1.2 Hz, 2H), 7.09–7.03 (m, 4H), 6.78 (d, J = 7.8 Hz, 2H).

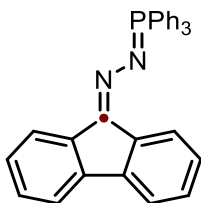
¹³C NMR (CDCl₃, 101 MHz) δ : 160.7, 149.4, 147.9, 141.7, 140.7, 131.5, 130.1, 128.7, 123.9, 122.2, 121.2, 61.6.

IR (KBr): 3052 w, 2961 w, 1606 w, 1591 w, 1582 w, 1567 w, 1466 w, 1450 w, 1405 s, 1219 w, 1168 w, 1107 w, 1013 w, 947 w.

MS, m/z (relative intensity, %): 319 (31), 318 (M⁺, 100), 317 (49), 316 (20), 315 (11), 290 (10), 159 (18), 145 (12), 131 (11).

HRMS (DART⁺, [M+H]⁺) Calcd for C₂₃H₁₅N₂: 319.1230. Found: 319.1215.

1-(9*H*-Fluoren-9-ylidene)-2-(triphenyl- λ^5 -phosphaneylidene)hydrazine (4a). [CAS: 751-35-9]



Yellow solid 66.9 mg (74%).

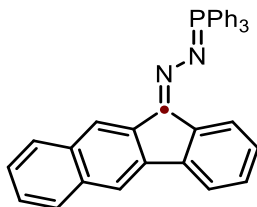
¹H NMR (CDCl₃, 400 MHz) δ : 9.13–9.11 (m, 1H), 7.85–7.80 (m, 6H), 7.77–7.75 (m, 1H), 7.70–7.67 (m, 2H), 7.60 (td, J = 7.4, 1.5 Hz, 3H), 7.53–7.49 (m, 6H), 7.40–7.33 (m, 2H), 7.27–7.17 (m, 2H).

¹³C NMR (CDCl₃, 101 MHz) δ : 139.3, 138.7 (d, J = 106.4 Hz), 133.5 (d, J = 8.2 Hz), 132.2 (d, J = 2.9 Hz), 131.18, 131.16, 129.0, 128.6 (d, J = 11.6 Hz), 128.1, 127.4, 127.04, 127.00, 126.5, 126.3, 119.7, 119.2, 119.1.

^{31}P NMR (CDCl_3 , 162 MHz) δ : 20.1.

HRMS (DART+, $[\text{M}+\text{H}]^+$) Calcd for $\text{C}_{31}\text{H}_{24}\text{N}_2\text{P}$: 455.1671. Found: 455.1650.

1-(11*H*-benzo[*b*]fluoren-11-ylidene)-2-(triphenyl- λ^5 -phosphaneylidene)hydrazine (4l).



Yellowish brown solid 24.0 mg (24%). M.p. 181–185 °C (decomp).

^1H NMR (CDCl_3 , 400 MHz) δ : 9.69 (s, 1H), 8.14 (s, 1H), 7.94 (d, $J = 7.6$ Hz, 1H), 7.91–7.83 (m, 8H), 7.75 (d, $J = 7.3$ Hz, 1H), 7.66–7.59 (m, 3H), 7.56–7.49 (m, 6H), 7.48–7.41 (m, 2H), 7.31 (td, $J = 7.3$, 1.3 Hz, 1H), 7.28–7.24 (m, 1H).

^{13}C NMR (CDCl_3 , 101 MHz) δ : 139.5 (d, $J = 289.0$ Hz), 137.7, 137.1, 134.1, 133.5 (d, $J = 8.2$ Hz), 133.3, 132.2 (d, $J = 1.0$ Hz), 130.14, 130.13, 129.6, 129.21, 129.16, 128.7 (d, $J = 11.1$ Hz), 128.2, 127.4, 126.7, 126.5, 125.7, 124.9, 120.0, 117.2.

^{31}P NMR (CDCl_3 , 162 MHz) δ : 20.1.

IR (KBr): 3057 w, 2359 w, 2342 w, 1542 w, 1437 w, 1220 w, 1148 w, 1114 w, 1037 w, 1021 w, 997 w, 957 w, 898 w, 869 w, 772 s.

MS, m/z (relative intensity, %): 504 (M^+ , 0.4), 278 (13), 277 (34), 263 (20), 262 (100), 261 (17), 244 (11), 230 (21), 215 (17), 214 (33), 213 (17), 185 (10), 184 (12), 183 (57), 108 (18), 107 (11).

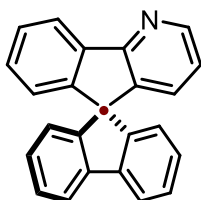
HRMS (EI^+ , $[\text{M}^+]$) Calcd for $\text{C}_{35}\text{H}_{25}\text{N}_2\text{P}$: 504.1755. Found: 504.1742.

Selected peaks in NMR assigned to the cis-trans isomer

^1H NMR (CDCl_3 , 400 MHz) δ : 9.26–9.24 (m, 1H), 8.11 (d, $J = 3.9$ Hz, 1H), 7.39–7.36 (m, 1H).

^{31}P NMR (CDCl_3 , 162 MHz) δ : 19.7.

Spiro[fluorene-9,5'-indeno[1,2-*b*]pyridine] (2ao). [CAS: 868393-17-3]



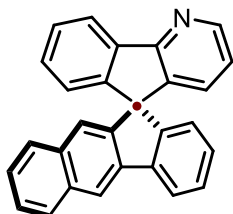
Pale yellow solid 21.0 mg (67%).

^1H NMR (CDCl_3 , 400 MHz) δ : 8.59 (dd, $J = 4.8$, 1.6 Hz, 1H), 8.17–8.15 (m, 1H), 7.87–7.85 (m, 2H), 7.46 (td, $J = 7.5$, 1.0 Hz, 1H), 7.39 (td, $J = 7.5$, 1.0 Hz, 2H), 7.23 (td, $J = 7.6$, 1.1 Hz, 1H), 7.12 (td, $J = 7.5$, 1.1 Hz, 2H), 7.06–6.99 (m, 2H), 6.79–6.72 (m, 3H).

¹³C NMR (CDCl₃, 101 MHz) δ : 160.8, 149.2, 149.1, 147.5, 143.0, 141.8, 140.7, 131.5, 129.9, 128.3, 128.05, 127.96, 124.0, 123.9, 122.1, 121.0, 120.2, 63.8.

HRMS (DART+, [M+H]⁺) Calcd for C₂₄H₁₆N: 318.1277. Found: 318.1284.

Spiro[benzo[*b*]fluorene-11,5'-indeno[1,2-*b*]pyridine] (2lo). [CAS: 2437210-86-9]



The reaction was conducted according to the general procedure described above, except that phosphazine **4l** (0.10 mmol) and biphenylene **1o** (0.15 mmol) were used, DMF/*n*Bu₂O was used as the solvent, and the reaction mixture was heated at 110 °C in an oil bath.

Orange solid 24.4 mg (68%). R_f 0.11 (SiO₂, hexane/EtOAc = 3/1). M.p. 135–137 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.62 (d, *J* = 3.9 Hz, 1H), 8.28 (s, 1H), 8.22 (d, *J* = 7.6 Hz, 1H), 8.02 (d, *J* = 7.6 Hz, 1H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.50–7.42 (m, 3H), 7.38–7.34 (m, 1H), 7.23 (d, *J* = 7.3 Hz, 1H), 7.19–7.16 (m, 2H), 7.10–7.08 (m, 1H), 7.02 (dd, *J* = 7.6, 4.8 Hz, 1H), 6.81 (d, *J* = 7.6 Hz, 1H), 6.76 (d, *J* = 7.6 Hz, 1H).

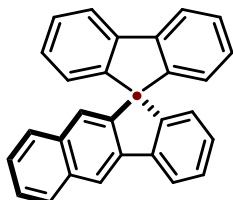
¹³C NMR (CDCl₃, 101 MHz) δ : 160.2, 150.3, 148.6, 147.8, 145.4, 144.3, 141.2, 140.0 (overlapped two peaks), 133.6, 133.5, 132.2, 130.2, 128.7, 128.40, 128.36, 128.15, 128.12, 126.1, 125.8, 124.3, 124.2, 122.8, 122.3, 121.2, 120.8, 118.4, 63.3.

IR (KBr): 3054 w, 3011 w, 2156 w, 2029 w, 2016 w, 2006 w, 1972 w, 1591 w, 1582 w, 1569 w, 1504 w, 1465 w, 1444 w, 1435 w, 1407 m, 1219 m, 1168 w, 1145 w, 877 w, 771 s.

MS, *m/z* (relative intensity, %): 368 (27), 367 (M⁺, 100), 366 (39), 365 (18), 364 (16), 184 (10), 183 (15).

HRMS (DART+, [M+H]⁺) Calcd for C₂₈H₁₈N: 368.1434. Found: 368.1429.

Spiro[benzo[*b*]fluorene-11,9'-fluorene] (2la). [CAS: 1198597-71-5]



The reaction was conducted according to the general procedure described above, except that phosphazine **4l** (0.10 mmol) and biphenylene **1a** (0.15 mmol) were used, DMF/*n*Bu₂O was used as the solvent, and the reaction mixture was heated at 110 °C in an oil bath.

White solid 30.1 mg (88%). R_f 0.64 (SiO₂, hexane). M.p. 144–145 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.29 (s, 1H), 8.02 (d, J = 7.8 Hz, 1H), 7.96 (d, J = 8.2 Hz, 1H), 7.91 (d, J = 7.6 Hz, 2H), 7.56 (d, J = 8.0 Hz, 1H), 7.47–7.33 (m, 5H), 7.21 (s, 1H), 7.19–7.10 (m, 3H), 6.80–6.76 (m, 3H).

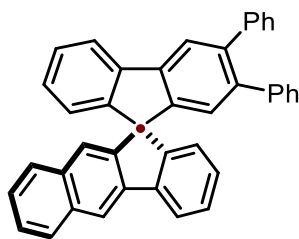
¹³C NMR (CDCl₃, 101 MHz) δ : 149.9, 149.3, 146.9, 141.5, 141.1, 140.3, 133.61, 133.57, 128.6, 128.1 (overlapped two peaks), 127.93, 127.84, 127.7, 125.8, 125.5, 124.3 (overlapped two peaks), 122.7, 120.6, 120.0, 118.1, 65.4.

IR (KBr): 3059 w, 3015 w, 1956 w, 1604 w, 1581 w, 1503 w, 1474 w, 1465 w, 1446 w, 1434 w, 1335 w, 1311 w, 1283 w, 1251 w, 1215 w, 1189 w, 1154 w, 1145 w, 1102 w, 1020 w, 952 w, 876 w, 790 w, 749 s.

MS, m/z (relative intensity, %): 367 (31), 366 (M⁺, 100), 365 (51), 364 (14), 363 (29), 183 (11), 182 (17), 181 (13).

HRMS (DART⁺, [M+H]⁺) Calcd for C₂₉H₁₉: 367.1481. Found: 367.1480.

2',3'-Diphenylspiro[benzo[*b*]fluorene-11,9'-fluorene] (2lf).



The reaction was conducted according to the general procedure described above, except that phosphazine **4l** (0.10 mmol) and biphenylene **1f** (0.15 mmol) were used, DMF/*n*Bu₂O was used as the solvent, and the reaction mixture was heated at 110 °C in an oil bath.

Pink solid 44.8 mg (87%). R_f 0.18 (SiO₂, hexane). M.p. 148–150 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.28 (s, 1H), 8.00 (d, J = 7.6 Hz, 1H), 7.96–7.90 (m, 3H), 7.61 (d, J = 8.0 Hz, 1H), 7.47–7.33 (m, 5H), 7.27–7.23 (m, 5H), 7.19 (td, J = 7.4, 0.8 Hz, 1H), 7.14 (td, J = 7.5, 0.8 Hz, 1H), 7.04 (dd, J = 6.9, 2.7 Hz, 3H), 6.96–6.94 (m, 2H), 6.88 (d, J = 7.6 Hz, 1H), 6.83–6.79 (m, 2H).

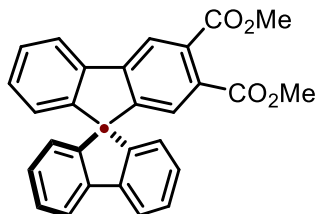
¹³C NMR (CDCl₃, 101 MHz) δ : 150.4, 149.3, 149.2, 146.9, 141.8, 141.4, 141.11, 141.07, 140.9, 140.4, 140.29, 140.28, 133.62, 133.61, 130.0, 129.8, 128.6, 128.1, 128.01, 127.99, 127.91 (overlapped two peaks), 127.8, 127.6, 126.5, 126.29, 126.25, 125.8, 125.5, 124.5, 124.3, 122.9, 122.0, 120.7, 120.1, 118.1, 65.4.

IR (KBr): 3056 w, 3021 w, 2354 w, 1732 w, 1600 w, 1504 w, 1466 w, 1447 w, 1435 w, 1218 w, 1020 w, 892 w, 880 w, 771 s.

MS, m/z (relative intensity, %): 519 (46), 518 (M⁺, 100), 517 (17), 441 (14), 259 (11).

HRMS (EI⁺, [M]⁺) Calcd for C₄₁H₂₆: 518.2035. Found: 518.2041.

Dimethyl 9,9'-spirobi[fluorene]-2,3-dicarboxylate (2ai).



White solid 42.5 mg (98%). R_f 0.35 (SiO₂, hexane/EtOAc = 2/1). M.p. 198–201 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.15 (s, 1H), 7.91–7.86 (m, 3H), 7.43–7.38 (m, 3H), 7.19 (td, J = 7.5, 1.0 Hz, 1H), 7.15–7.11 (m, 3H), 6.77 (d, J = 7.6 Hz, 1H), 6.70 (d, J = 7.6 Hz, 2H), 3.97 (s, 3H), 3.76 (s, 3H).

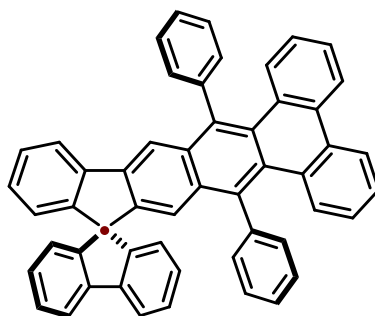
¹³C NMR (CDCl₃, 101 MHz) δ : 168.6, 167.5, 151.6, 149.7, 147.1, 144.9, 141.9, 139.7, 132.7, 130.6, 129.4, 128.2 (overlapped two peaks), 128.0, 124.9, 124.2, 124.0, 120.9, 120.3, 120.2, 65.9, 52.7, 52.4.

IR (KBr): 3063 w, 3020 w, 2951 w, 1720 s, 1615 w, 1568 w, 1472 w, 1447 m, 1434 m, 1403 w, 1353 w, 1304 m, 1270 s, 1233 m, 1173 w, 1147 w, 1119 m, 1091 w, 1064 w, 966 w.

MS, m/z (relative intensity, %): 433 (30), 432 (M⁺, 100), 401 (28), 374 (24), 373 (73), 314 (37), 313 (53), 200 (19), 157 (24), 150 (19).

HRMS (DART⁺, [M+H]⁺) Calcd for C₂₉H₂₁O₄: 433.1434. Found: 433.1435.

9,17-Diphenylspiro[benzo[f]indeno[1,2-*l*]tetraphene-15,9'-fluorene] (2ar).



The reaction was conducted according to the general procedure described above, except that phosphazine **4a** (0.24 mmol), [Rh(cod)Cl]₂ (0.005 mmol), dcype (0.01 mmol), and biphenylene **1k** (0.06 mmol) were used, and the reaction mixture was heated in toluene (2.5 mL) at 110 °C in an oil bath for 48 h.

Orange solid 12.9 mg (34%). R_f 0.35 (SiO₂, hexane/toluene = 3/2). M.p. 278–282 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 8.31 (s, 1H), 8.24 (t, J = 7.3 Hz, 2H), 7.84–7.79 (m, 3H), 7.67 (dd, J = 7.9, 1.5 Hz, 2H), 7.63–7.56 (m, 3H), 7.49 (d, J = 8.2 Hz, 1H), 7.38–7.17 (m, 12H), 7.15–7.11 (m, 3H), 7.01–6.97 (m, 1H), 6.90–6.86 (m, 1H), 6.82 (d, J = 7.6 Hz, 2H), 6.74 (d, J = 7.6 Hz, 1H).

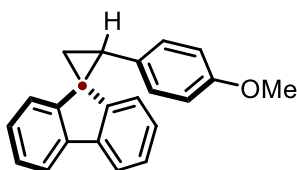
^{13}C NMR (CDCl_3 , 101 MHz) δ : 149.8, 149.7, 146.9, 141.8, 141.5, 141.2, 140.9, 140.1, 135.32, 135.27, 132.9, 132.6, 132.2, 131.91, 131.90, 131.8, 131.3 (overlapped two peaks), 130.4, 130.3, 129.2, 129.1, 128.8, 128.62, 128.57, 127.82, 127.76, 127.71 (overlapped two peaks), 127.6, 127.5, 126.7, 126.6, 125.8, 125.6, 124.3, 124.1, 123.2, 121.5, 120.9, 120.0, 116.8, 65.6.

IR (KBr): 3058 w, 2366 w, 2344 w, 2332 w, 2058 w, 1991 w, 1444 w, 1220 w, 1074 w, 808 w, 772 s.

MS, m/z (relative intensity, %): 670 (16), 669 (57), 668 (M^+ , 100), 334 (10).

HRMS (EI^+ , $[\text{M}]^+$) Calcd for $\text{C}_{53}\text{H}_{32}$: 668.2504. Found: 668.2515.

2-(4-Methoxyphenyl)spiro[cyclopropane-1,9'-fluorene] (5aa). [CAS: 3047731-26-7]



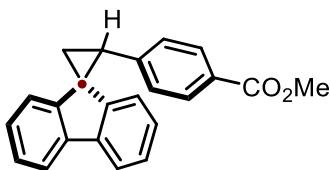
White solid 23.1 mg (58%). R_f 0.09 (SiO_2 , hexane).

^1H NMR (CDCl_3 , 400 MHz) δ : 7.84 (dd, $J = 7.6, 0.9$ Hz, 1H), 7.80 (d, $J = 7.6$ Hz, 1H), 7.40–7.33 (m, 2H), 7.26–7.23 (m, 1H), 7.18 (d, $J = 6.9$ Hz, 1H), 7.08 (d, $J = 8.7$ Hz, 2H), 6.94 (t, $J = 7.6$ Hz, 1H), 6.80 (d, $J = 8.7$ Hz, 2H), 6.18 (d, $J = 7.8$ Hz, 1H), 3.79 (s, 3H), 3.31 (t, $J = 8.4$ Hz, 1H), 2.21–2.14 (m, 2H).

^{13}C NMR (CDCl_3 , 101 MHz) δ : 158.4, 148.4, 144.4, 140.4, 139.6, 131.2, 129.2, 126.8, 126.0, 125.9, 125.7, 121.7, 119.8, 119.6, 118.5, 113.5, 55.2, 35.6, 34.3, 22.7.

HRMS (DART^+ , $[\text{M}+\text{H}]^+$) Calcd for $\text{C}_{22}\text{H}_{19}\text{O}$: 299.1430. Found: 299.1419.

Methyl 4-(spiro[cyclopropane-1,9'-fluorene]-2-yl)benzoate (5ab).



White solid 16.0 mg (24%). R_f 0.40 (SiO_2 , hexane/ $\text{EtOAc} = 10/1$). M.p. 217–219 °C.

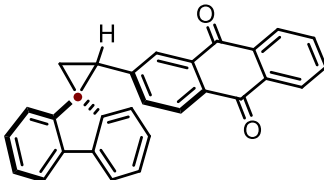
^1H NMR (CDCl_3 , 400 MHz) δ : 7.95 (dd, $J = 6.6, 1.6$ Hz, 2H), 7.85 (dd, $J = 6.8, 1.3$ Hz, 1H), 7.80 (d, $J = 7.8$ Hz, 1H), 7.43–7.34 (m, 2H), 7.26–7.19 (m, 4H), 6.91 (td, $J = 7.6, 0.9$ Hz, 1H), 6.14 (d, $J = 7.8$ Hz, 1H), 3.91 (s, 3H), 3.37 (t, $J = 8.5$ Hz, 1H), 2.28–2.23 (m, 2H).

^{13}C NMR (CDCl_3 , 101 MHz) δ : 167.0, 147.8, 143.7, 142.5, 140.4, 139.7, 130.1, 129.5, 128.7, 126.9, 126.3, 126.1, 126.0, 121.4, 119.9, 119.8, 118.6, 52.1, 35.8, 34.7, 22.0.

IR (KBr): 3064 w, 3019 w, 2951 w, 2354 w, 2121 w, 1997 w, 1717 s, 1609 w, 1448 m, 1435 m, 1407 w, 1308 w, 1279 s, 1223 w, 1178 w, 1111 m, 1020 w, 973 w, 938 w, 862 w.

MS, m/z (relative intensity, %): 327 (20), 326 (M^+ , 79), 311 (27), 268 (22), 267 (100), 266 (40), 265 (71), 263 (13), 253 (10), 252 (43), 189 (11), 165 (20), 148 (19), 133 (21), 132 (20), 126 (15), 120 (11).
HRMS (DART⁺, $[M+H]^+$) Calcd for $C_{23}H_{19}O_2$: 327.1380. Found: 327.1365.

2-(Spiro[cyclopropane-1,9'-fluoren]-2-yl)anthracene-9,10-dione (5ac).



White solid 31.6 mg (56%). R_f 0.43 (SiO_2 , hexane/EtOAc = 4/1). M.p. 203–207 °C.

1H NMR ($CDCl_3$, 400 MHz) δ : 8.32–8.30 (m, 2H), 8.23 (s, 1H), 8.18 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 7.1 Hz, 1H), 7.80 (d, J = 6.0 Hz, 3H), 7.50 (d, J = 8.0 Hz, 1H), 7.44–7.36 (m, 2H), 7.26–7.22 (m, 2H), 6.88 (t, J = 7.6 Hz, 1H), 6.19 (d, J = 7.6 Hz, 1H), 3.43 (t, J = 8.2 Hz, 1H), 2.41–2.34 (m, 2H).

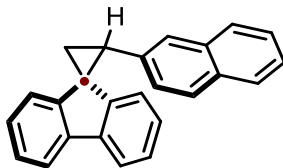
^{13}C NMR ($CDCl_3$, 101 MHz) δ : 183.2, 182.8, 147.4, 144.3, 143.1, 140.6, 139.7, 136.0, 134.1, 134.0, 133.50, 133.46, 133.3, 132.1, 128.1, 127.4, 127.21, 127.17, 127.0, 126.5, 126.3, 126.2, 121.1, 120.03, 119.96, 118.6, 36.3, 34.9, 21.8.

IR (KBr): 3067 w, 3019 w, 1673 s, 1594 m, 1480 w, 1448 w, 1417 w, 1326 m, 1291 s, 1216 w, 1159 w, 1094 w, 988 w, 973 w, 932 w, 909 w, 861 w.

MS, m/z (relative intensity, %): 399 (31), 398 (M^+ , 100), 397 (17), 381 (10), 339 (10), 165 (11).

HRMS (EI⁺, $[M]^+$) Calcd for $C_{29}H_{18}O_2$: 398.1307. Found: 398.1301.

2-(Naphthalen-2-yl)spiro[cyclopropane-1,9'-fluorene] (5ad). [CAS: 3047731-29-0]



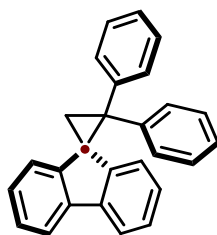
White solid 17.2 mg (39%). R_f 0.10 (SiO_2 , hexane).

1H NMR ($CDCl_3$, 400 MHz) δ : 7.89–7.86 (m, 1H), 7.82–7.81 (m, 4H), 7.68 (dd, J = 8.4, 2.4 Hz, 1H), 7.51–7.37 (m, 4H), 7.26–7.19 (m, 2H), 7.14 (d, J = 8.5 Hz, 1H), 6.84–6.79 (m, 1H), 6.18–6.16 (m, 1H), 3.52 (t, J = 8.4 Hz, 1H), 2.39–2.35 (m, 1H), 2.33–2.29 (m, 1H).

^{13}C NMR ($CDCl_3$, 101 MHz) δ : 148.2, 144.1, 140.3, 139.7, 134.8, 133.2, 132.5, 128.7, 128.2, 127.8, 127.73, 127.67, 126.8, 126.1, 126.04, 125.97, 125.8, 125.7, 121.5, 119.8, 119.7, 118.6, 35.7, 35.2, 22.5.

HRMS (DART⁺, $[M+H]^+$) Calcd for $C_{25}H_{19}$: 319.1481. Found: 319.1478.

2,2-Diphenylspiro[cyclopropane-1,9'-fluorene] (5ae).



Pink solid 20.0 mg (29%). R_f 0.20 (SiO₂, hexane). M.p. 216–218 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 7.81 (d, J = 7.6 Hz, 2H), 7.28–7.18 (m, 12H), 6.90 (t, J = 7.6 Hz, 2H), 5.91 (d, J = 7.8 Hz, 2H), 2.62 (s, 2H).

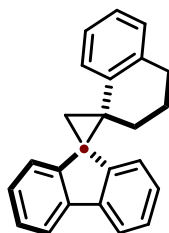
¹³C NMR (CDCl₃, 101 MHz) δ : 145.0, 142.6, 140.4, 128.4 (overlapped two peaks), 126.8, 125.9, 125.6, 123.1, 119.4, 48.4, 40.2, 29.4.

IR (KBr): 3060 w, 3028 w, 2353 w, 2159 w, 2029 w, 1974 w, 1739 w, 1732 w, 1715 w, 1494 w, 1446 w, 1219 w, 797 w, 772 s.

MS, m/z (relative intensity, %): 345 (30), 344 (M⁺, 100), 343 (11), 329 (13), 267 (35), 266 (41), 265 (65), 263 (12), 253 (41), 252 (32), 179 (18), 178 (22), 166 (12), 165 (41), 163 (10), 133 (10).

HRMS (DART⁺, [M+H]⁺) Calcd for C₂₇H₂₁: 345.1638. Found: 345.1628.

3'',4''-Dihydro-2''*H*-dispiro[fluorene-9,1'-cyclopropane-2',1''-naphthalene] (5af).



White solid 33.8 mg (77%). R_f 0.16 (SiO₂, hexane). M.p. 131–134 °C.

¹H NMR (CDCl₃, 400 MHz) δ : 7.83 (d, J = 7.3 Hz, 1H), 7.70 (d, J = 7.6 Hz, 1H), 7.54 (d, J = 7.3 Hz, 1H), 7.44 (d, J = 7.6 Hz, 1H), 7.38 (td, J = 7.4, 1.0 Hz, 1H), 7.33–7.28 (m, 2H), 7.16–7.11 (m, 2H), 6.90 (d, J = 7.3 Hz, 1H), 6.80 (td, J = 7.6, 1.0 Hz, 1H), 6.45 (d, J = 7.8 Hz, 1H), 2.72 (d, J = 6.0 Hz, 1H), 2.56–2.50 (m, 1H), 2.22 (d, J = 6.0 Hz, 1H), 2.18–2.13 (m, 1H), 2.02–1.94 (m, 1H), 1.50–1.25 (m, 3H).

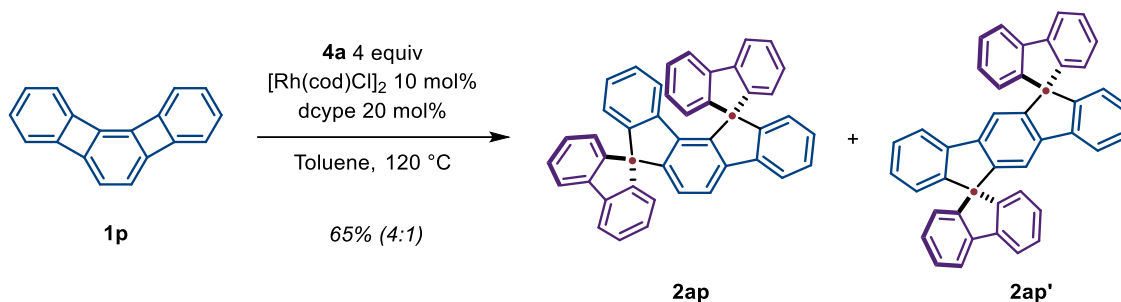
¹³C NMR (CDCl₃, 101 MHz) δ : 146.1, 144.4, 141.1, 140.6, 140.0, 139.7, 127.4, 126.7, 126.0, 125.8, 125.4 (overlapped two peaks), 125.2, 124.9, 121.7, 120.9, 120.0, 119.1, 40.5, 39.8, 27.7, 27.1, 23.5, 19.5.

IR (KBr): 3061 w, 3019 w, 2986 w, 2937 w, 2865 w, 1479 w, 1446 m, 1220 w, 1156 w, 1113 w, 1048 w, 998 w, 772 s.

MS, m/z (relative intensity, %): 308 (M⁺, 31), 178 (13), 166 (48), 165 (100), 143 (39), 142 (17), 141 (15), 130 (25), 128 (50), 115 (18), 44 (28).

HRMS (DART⁺, [M+H]⁺) Calcd for C₂₄H₂₁: 309.1638. Found: 309.1642.

IX. Double Spirofusion via Sequential Carbon-Atom Transfer



In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with $[\text{Rh}(\text{cod})\text{Cl}]_2$ (5.2 mg, 0.01 mmol), dcype (8.4 mg, 0.02 mmol), **1p** (23.1 mg, 0.10 mmol), **4a** (184.6 mg, 0.41 mmol) and toluene (1 mL) and heated to 120 °C using an aluminum block and stirred for 24 h. The reaction mixture was cooled to room temperature and purified by flash column chromatography on silica gel to afford the mixture of **2ap** and **2ap'**. Separation by GPC gave pure **2ap** and **2ap'**.

Dispiro[fluorene-9,7'-indeno[1,2-*a*]fluorene-12',9''-fluorene] (**2ap**). [CAS: 1265593-08-5]

Pale yellow solid 29.6 mg (52%). R_f 0.22 (SiO_2 , hexane/toluene = 4/1).

^1H NMR (CD_2Cl_2 , 400 MHz) δ : 8.08 (dt, $J = 7.6, 0.9$ Hz, 2H), 7.87 (dt, $J = 7.6, 0.9$ Hz, 2H), 7.79 (dt, $J = 7.5, 0.9$ Hz, 1H), 7.70 (d, $J = 7.8$ Hz, 1H), 7.48 (td, $J = 7.5, 1.1$ Hz, 2H), 7.38 (td, $J = 7.5, 1.1$ Hz, 2H), 7.30 (td, $J = 7.5, 1.1$ Hz, 1H), 7.19 (td, $J = 7.5, 1.1$ Hz, 2H), 7.11 (td, $J = 7.5, 1.1$ Hz, 2H), 7.05 (td, $J = 7.5, 1.1$ Hz, 1H), 6.92 (dt, $J = 7.6, 0.9$ Hz, 2H), 6.85–6.79 (m, 2H), 6.73 (td, $J = 7.6, 1.3$ Hz, 1H), 6.64 (dt, $J = 7.5, 0.8$ Hz, 2H), 6.54 (dt, $J = 7.6, 0.8$ Hz, 1H), 6.49 (ddd, $J = 7.5, 1.2, 0.7$ Hz, 1H), 6.45–6.42 (m, 1H).

^{13}C NMR (CD_2Cl_2 , 101 MHz) δ : 150.4, 149.7, 149.4, 147.8, 144.2, 142.5, 142.1, 141.0, 140.7, 140.6, 139.3, 128.6, 128.5, 128.20, 128.16, 128.12, 127.8, 127.6, 127.5, 124.22, 124.18, 124.05, 123.97, 123.6, 123.3, 121.0, 120.5, 120.2, 119.6, 66.9, 66.4.

HRMS (DART⁺, $[\text{M}+\text{H}]^+$) Calcd for $\text{C}_{44}\text{H}_{27}$: 555.2107. Found: 555.2129.

Dispiro[fluorene-9,6'-indeno[1,2-*b*]fluorene-12',9''-fluorene] (**2ap'**). [CAS: 475436-98-7]

Pale yellow solid 7.2 mg (13%). R_f 0.22 (SiO_2 , hexane/toluene = 4/1).

^1H NMR (CDCl_3 , 400 MHz) δ : 7.91 (d, $J = 7.6$ Hz, 4H), 7.52 (d, $J = 7.6$ Hz, 2H), 7.42 (td, $J = 7.5, 1.0$ Hz, 4H), 7.22–7.14 (m, 8H), 7.01 (td, $J = 7.4, 1.1$ Hz, 2H), 6.80 (d, $J = 7.6$ Hz, 4H), 6.66 (d, $J = 7.6$ Hz, 2H).

^{13}C NMR (CD_2Cl_2 , 101 MHz) δ : 149.5, 149.30, 149.26, 142.35, 142.30, 141.9, 128.24, 128.23, 128.1, 128.0, 124.4, 124.0, 120.6, 120.4, 120.2, 115.9, 66.2.

HRMS (DART+, $[\text{M}+\text{H}]^+$) Calcd for $\text{C}_{44}\text{H}_{27}$: 555.2107. Found: 555.2082.

Proposed formation of the rearranged byproduct **2ap'**

A plausible pathway for the formation of the rearranged byproduct is shown in Figure S1. On the basis of the reported preferential activation of the bay C–C bond in angular phenylenes, the first oxidative addition is tentatively proposed to occur at the corresponding inner C–C bond of **1p**⁹. Subsequent reaction with the diazo species generates a rhodium–carbene intermediate, which undergoes carbene insertion and reductive elimination to furnish the mono-spiro intermediate.

From this intermediate, oxidative addition of the remaining biphenylene motif can in principle occur at either the outer or inner C–C bond. Oxidative addition at the outer C–C bond leads directly to the major inner–outer double-spiro-fused product **2ap**. In contrast, oxidative addition at the inner C–C bond generates a highly congested rhodacyclic intermediate **A**. In this case, approach of the diazo species and formation of the corresponding rhodium–carbene complex may be sterically disfavored. The rhodacycle may instead undergo formal protodemetalation of one Rh–C bond, followed by intramolecular C–H activation to regenerate a less congested rhodacyclic intermediate **B** with the metalation site relocated to a different aryl carbon. Subsequent reaction with the diazo species, carbene insertion, and reductive elimination would then furnish the rearranged double-spiro-fused byproduct **2ap'**.

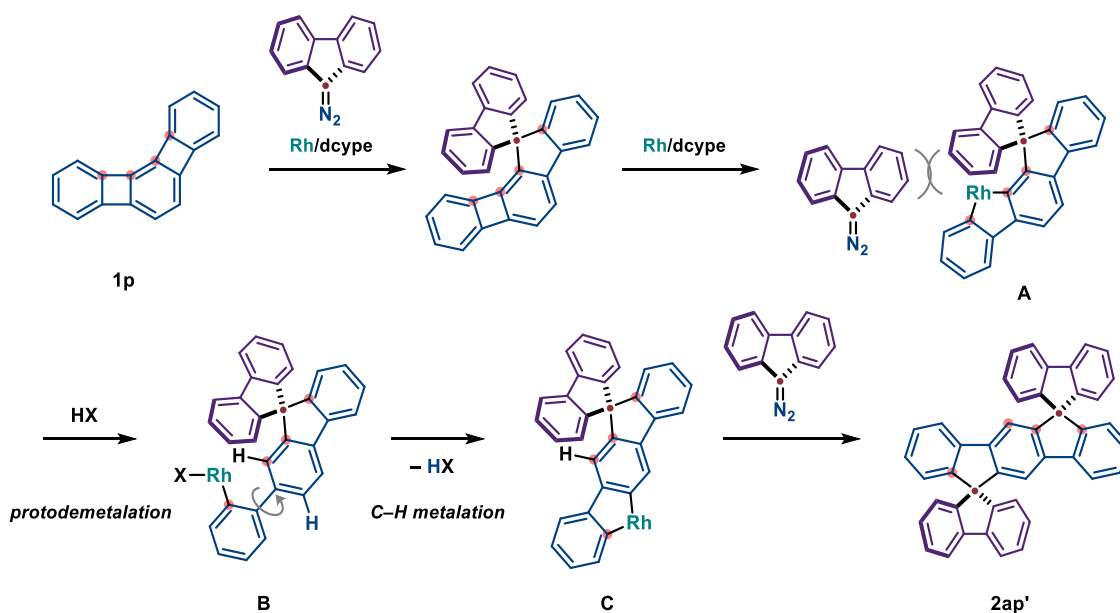
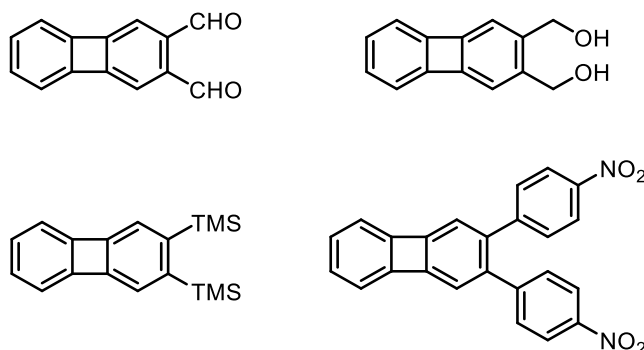


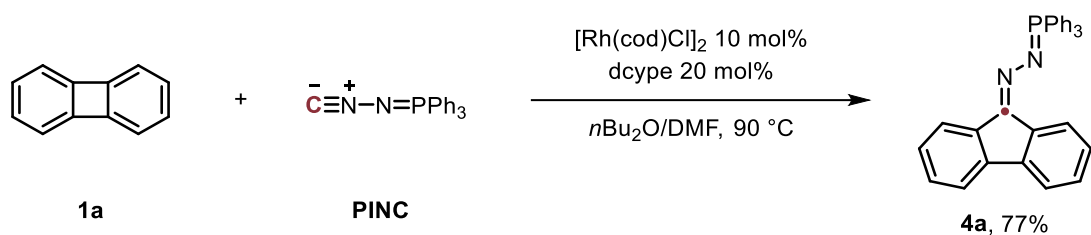
Figure S1. Proposed pathway for the formation of the rearranged byproduct.

X. Unsuccessful Substrates



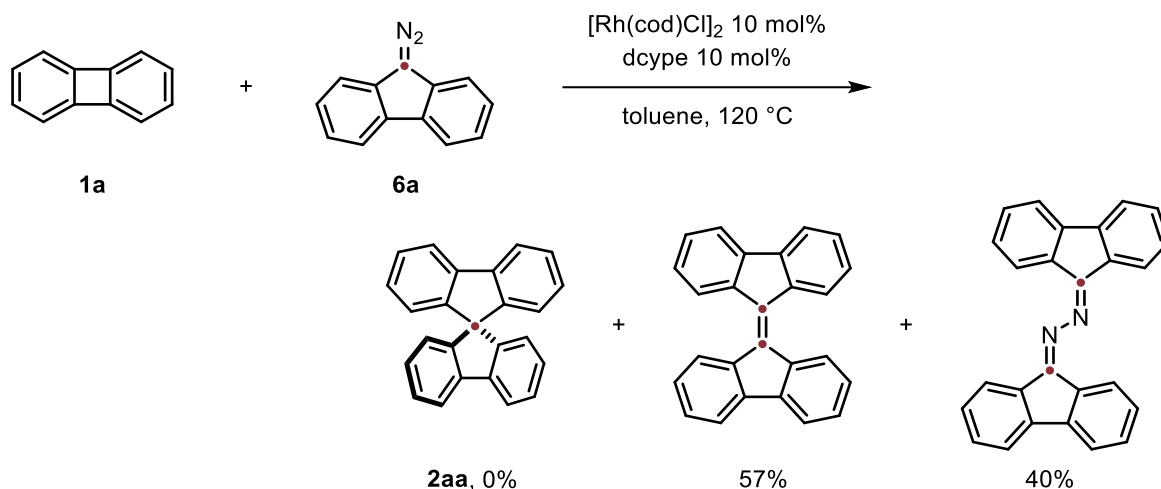
XI. Control Experiments

Reaction of biphenylene with PINC under mild condition



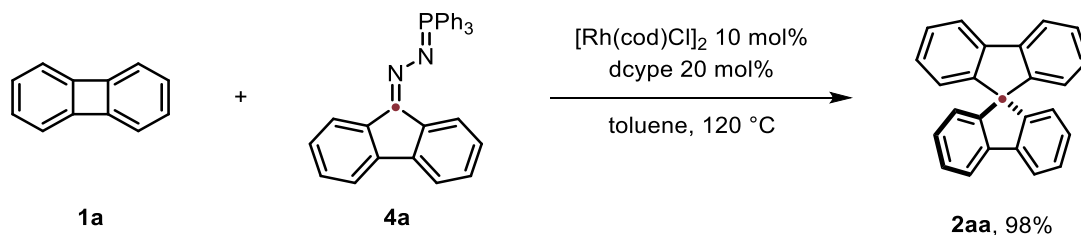
In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with $[\text{Rh}(\text{cod})\text{Cl}]_2$ (4.7 mg, 0.01 mmol), dcype (10.9 mg, 0.03 mmol), biphenylene **1a** (21.9 mg, 0.14 mmol), $n\text{Bu}_2\text{O}$ (0.6 mL) and DMF (0.1 mL) and heated to 90 °C in an oil bath. A solution of PINC (28.9 mg, 0.10 mmol) in DMF (1.0 mL) was added dropwise over 1 h (1.0 mL/h) using a syringe pump. After completion of the addition, the reaction mixture was stirred at 90 °C for 1.5 h. The crude was analyzed by ^1H NMR using 1,3,5-trimethoxybenzene as an internal standard.

Reaction of biphenylene with diazo compound



In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with $[\text{Rh}(\text{cod})\text{Cl}]_2$ (5.8 mg, 0.012 mmol), dcype (5.2 mg, 0.012 mmol), **1a** (28.2 mg, 0.19 mmol), **6a** (24.0 mg, 0.12 mmol) and toluene (1 mL) and heated to 120 °C using an aluminum block and stirred for 20 h. The crude was analyzed by ^1H NMR using 1,3,5-trimethoxybenzene as an internal standard.

Reaction of biphenylene with phosphazine



In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with $[\text{Rh}(\text{cod})\text{Cl}]_2$ (5.9 mg, 0.01 mmol), dcype (8.4 mg, 0.02 mmol), **1a** (14.5 mg, 0.10 mmol), **4a** (90.9 mg, 0.20 mmol) and toluene (0.1 mL) and heated to 120 °C using an aluminum block and stirred for 24 h. The reaction mixture was cooled to room temperature and purified by flash column chromatography on silica gel to afford spirobifluorene **2aa** as a white solid (29.4 mg, 98%).

XII. Studies on the Formation and Effect of PPh_3

Formation of PPh_3 under the standard condition

To determine the fate of the phosphorus-containing fragment derived from PINC, the standard reaction was carried out and the crude reaction mixture was analyzed by quantitative ^{31}P NMR spectroscopy using triphenyl phosphate. PPh_3 was detected as the major phosphorus-containing product in 50% yield, together with $\text{O}=\text{PPh}_3$ (5%) and unreacted PINC (3%).

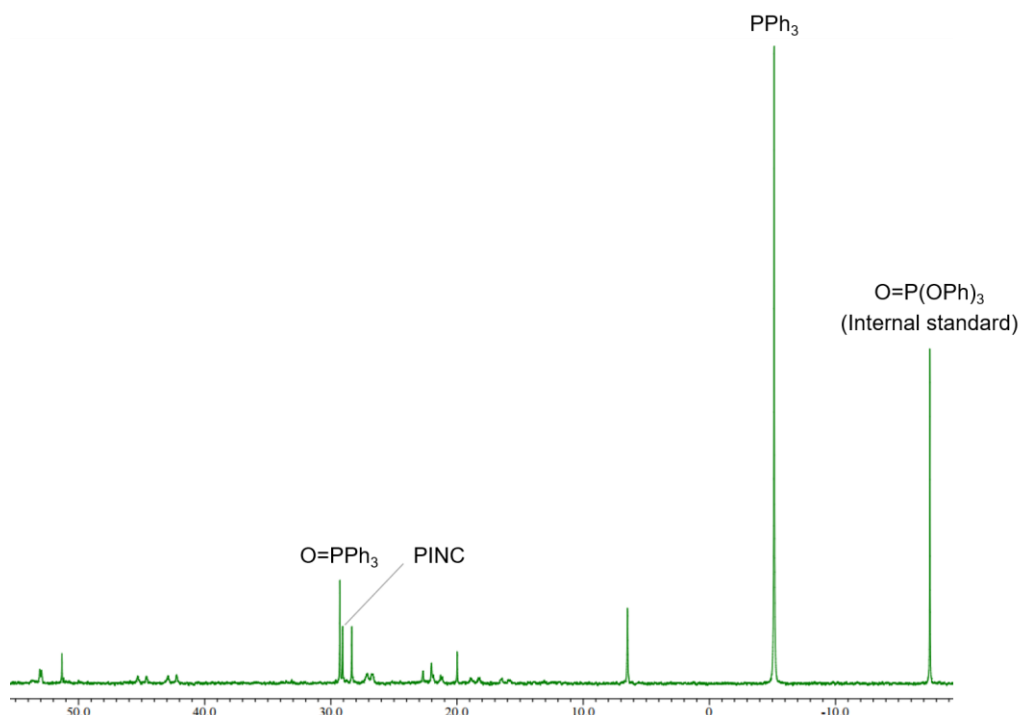
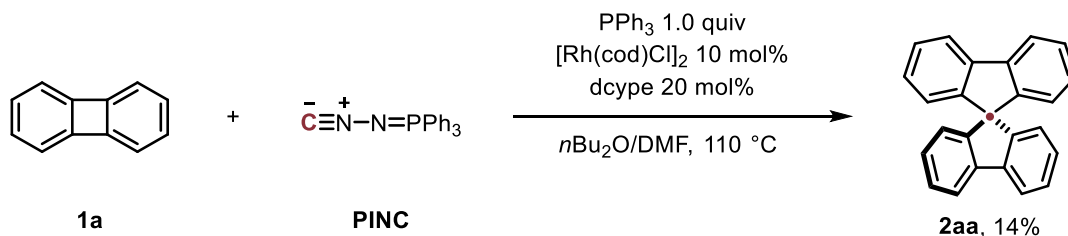


Figure S2. ^{31}P NMR spectrum of the crude reaction mixture after the standard reaction.

Effect of PPh_3 under the standard reaction conditions

To examine the effect of PPh_3 on the overall catalytic reaction, the standard reaction was performed in the presence of PPh_3 (1.0 equiv relative to PINC).

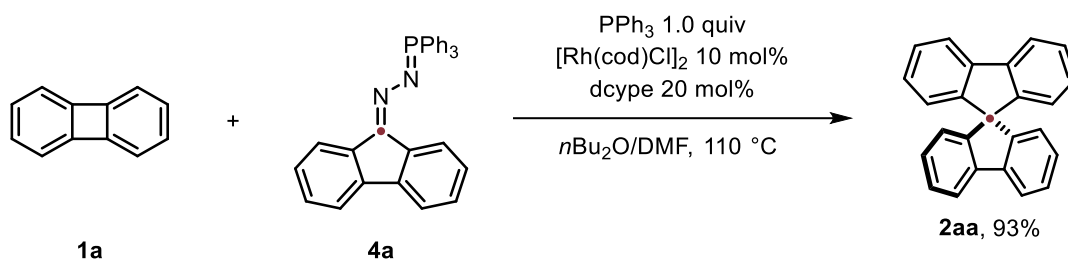


In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with $[\text{Rh}(\text{cod})\text{Cl}]_2$ (5.4 mg, 0.011 mmol), dcype (8.1 mg, 0.019 mmol), **1a** (37.7 mg, 0.25 mmol), PPh_3 (25.6 mg, 0.098 mmol), $n\text{Bu}_2\text{O}$ (0.6 mL) and DMF (0.1 mL) and heated to 90 $^\circ\text{C}$ using an oil bath. A solution of PINC (29.6 mg, 0.10 mmol) in DMF (0.5 mL) was added dropwise over 1 h (0.5 mL/h) using a syringe pump. After completion of the addition, the reaction mixture was stirred at 90 $^\circ\text{C}$ for 1.5 h and then heated to 110 $^\circ\text{C}$ and stirred for 24 h. The crude was analyzed by ^1H NMR using 1,3,5-trimethoxybenzene as an internal standard. Spirobifluorene **2aa** was obtained in 14% NMR yield.

The substantial decrease in yield upon addition of PPh_3 from the outset indicates that PPh_3 can interfere with the catalytic reaction when present during the initial stage.

Effect of PPh₃ on the second carbon-atom-transfer step

Because free PPh₃ is expected to be generated primarily upon conversion of the phosphazine intermediate at elevated temperature, the effect of PPh₃ on the second carbon-atom-transfer step was examined independently using isolated phosphazine **4a**.

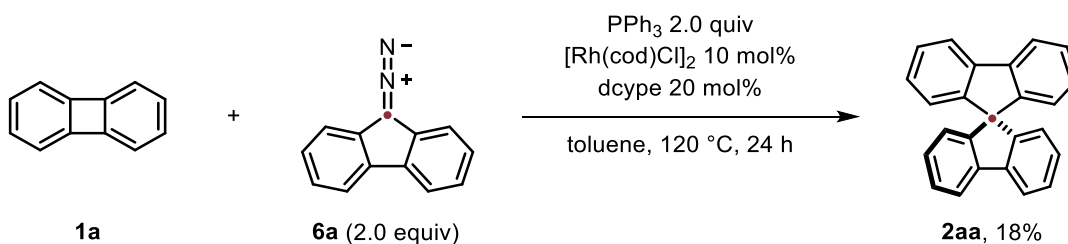


In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with [Rh(cod)Cl]₂ (5.6 mg, 0.011 mmol), dcype (9.1 mg, 0.022 mmol), **1a** (18.5 mg, 0.12 mmol), **4a** (42.6 mg, 0.094 mmol), PPh₃ (25.5 mg, 0.097 mmol), *n*Bu₂O (0.6 mL) and DMF (0.6 mL) and heated to 110 °C using an oil bath for 24 h. The crude was analyzed by ¹H NMR using 1,3,5-trimethoxybenzene as an internal standard. Spirobifluorene **2aa** was obtained in 93% NMR yield.

This yield is comparable to that obtained in the absence of added PPh₃, indicating that PPh₃ does not substantially inhibit the second carbon-atom-transfer step under these conditions. Thus, although PPh₃ can interfere with the reaction when present from the outset, its accumulation at the stage at which it is generated during the actual reaction is unlikely to significantly suppress catalytic turnover.

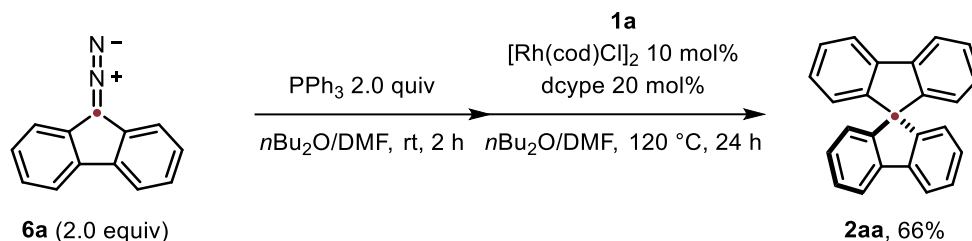
Reactions of biphenylene with diazo compound in the presence of PPh₃

To examine whether independently prepared diazo compound **6a** can enter the present carbon-atom-transfer pathway, its reaction was investigated in the presence of PPh₃.



In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with [Rh(cod)Cl]₂ (5.1 mg, 0.010 mmol), dcype (8.4 mg, 0.020 mmol), **1a** (16.5 mg, 0.11 mmol), **6a** (36.8 mg, 0.19 mmol), PPh₃ (50.8 mg, 0.19 mmol) and toluene (1 mL) and heated to 120 °C using an aluminum block and stirred for 24 h. The crude was analyzed by ¹H NMR using 1,3,5-trimethoxybenzene as an internal standard. Spirobifluorene **2aa** was obtained in 18% NMR yield.

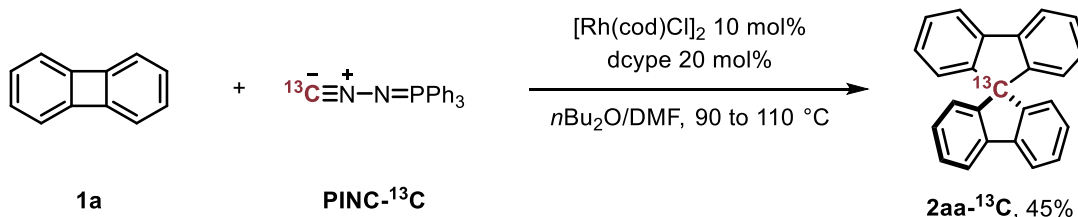
The effect of premixing **6a** with PPh₃ was then examined.



In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with **6a** (36.8 mg, 0.19 mmol), PPh₃ (50.8 mg, 0.19 mmol), *n*Bu₂O (0.6 mL) and DMF (0.6 mL), and stirred at room temperature for 2 h. [Rh(cod)Cl]₂ (5.1 mg, 0.010 mmol), dcype (8.4 mg, 0.020 mmol) and **1a** (14.1 mg, 0.09 mmol) were then added to the resulting mixture, and the mixture was heated to 120 °C for 24 h using an aluminum block. The crude was analyzed by ¹H NMR using 1,3,5-trimethoxybenzene as an internal standard. Spirobifluorene **2aa** was obtained in 66% NMR yield.

Together with the independently observed reactivity of phosphazine **4a**, these results are consistent with formation of a phosphazine intermediate from diazo compound **6a** and PPh₃. They further demonstrate that an independently prepared diazo compound can provide a complementary entry to the present spirofusion reaction.

XIII. ¹³C-Labeling Experiment



In a nitrogen-filled glovebox, a 5 mL screw-capped vial equipped with a magnetic stir bar was charged with [Rh(cod)Cl]₂ (5.9 mg, 0.012 mmol), dcype (8.5 mg, 0.02 mmol), **1a** (37.4 mg, 0.25 mmol), *n*Bu₂O (0.6 mL) and DMF (0.1 mL) and heated to 90 °C using an oil bath. A solution of PINC-¹³C (29.4 mg, 0.10 mmol) in DMF (0.5 mL) was added dropwise over 1 h (0.5 mL/h) using a syringe pump. After completion of the addition, the reaction mixture was stirred at 90 °C for 1.5 h and then heated to 110 °C and stirred for 24 h. The reaction mixture was cooled to room temperature and purified by flash column chromatography on silica gel to afford spirobifluorene **2aa-¹³C** as a white solid (13.7 mg, 45%).

9,9'-Spiro[fluorene]-9-¹³C (2aa-¹³C).

^1H NMR (CDCl_3 , 400 MHz) δ : 7.85 (d, $J = 7.6$ Hz, 4H), 7.37 (t, $J = 7.4$ Hz, 4H), 7.11 (t, $J = 7.6$ Hz, 4H), 6.74 (dt, $J = 7.5$, 1.2 Hz, 4H).

^{13}C NMR (CDCl_3 , 101 MHz) δ : 148.7 (d, $J = 42.9$ Hz), 141.8 (d, $J = 4.8$ Hz), 127.8 (d, $J = 3.4$ Hz), 127.7, 124.0 (d, $J = 2.9$ Hz), 120.0 (d, $J = 2.4$ Hz), 65.9.

HRMS (DART+, $[\text{M}+\text{H}]^+$) Calcd for $^{12}\text{C}_{24}^{13}\text{CH}_{17}$: 318.1358. Found: 318.1370.

XIV. Differential Scanning Calorimetry Analysis

Differential scanning calorimetry (DSC) analysis of PINC was performed to evaluate its thermal stability. The measurement was carried out on a Rigaku ThermoPlus EVO2 DSCvesta instrument under a nitrogen atmosphere. A sample of PINC was placed in a sealed aluminum pan and heated from 25 °C to 300 °C at a rate of 5 °C/min.

The DSC thermogram showed an exothermic event with a peak at 168 °C. The enthalpy change associated with this event was determined to be 459.5 J/g. These results suggest that PINC exhibits high thermal stability under the measurement conditions, with an exothermic thermal event occurring at elevated temperature.

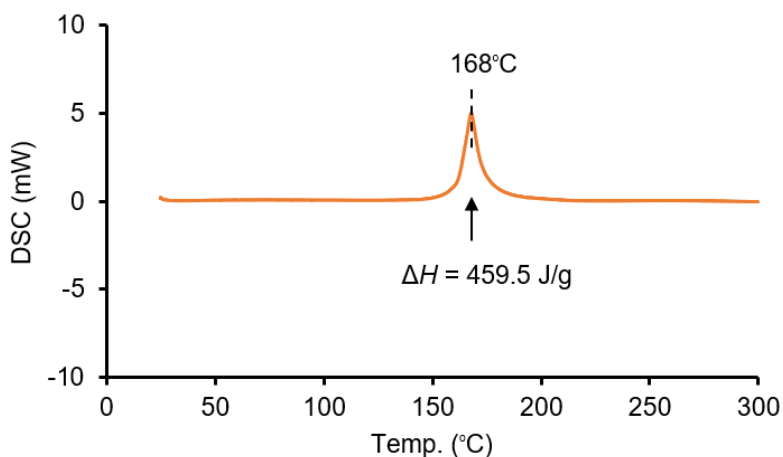


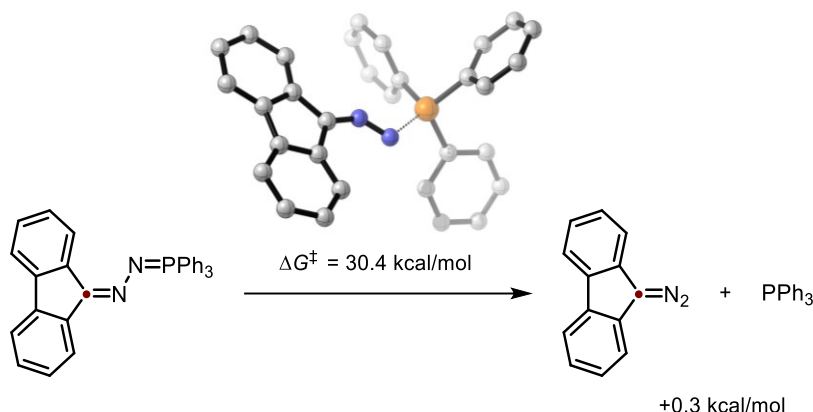
Figure S3. DSC thermogram of PINC.

XV. Computational Details

Calculations were performed with the Gaussian 09 (G09RevD.01) program¹⁰. Geometry optimizations and frequency calculations for all reported structures were carried out using M06 density functional. The LANL2DZ basis set with the associated effective core potential (ECP) was employed for Rh, and the 6-31G* basis set was used for all other atoms. Single-point energy calculations were subsequently performed at the M06/def2-TZVP level of theory on the optimized geometries. All reported minima were confirmed by the absence of imaginary frequencies, whereas each transition state (TS) exhibited

one imaginary frequency. Intrinsic reaction coordinate (IRC) calculations were performed to confirm that each TS connects the corresponding reactants and products. Reported energy values correspond to Gibbs free energies calculated at 298.15 K and 1 atm.

XVI. Relative Gibbs Free Energies



The relative energies of the phosphazine and diazoalkane were estimated by DFT calculations. Solvent effects were taken into account using the SMD continuum model with toluene as the solvent. The free energy of the diazoalkane is 0.3 kcal/mol higher than that of the phosphazine, and the activation barrier for PPh₃ dissociation is 30.4 kcal/mol. These results are consistent with the requirement for heating in this SCAD reaction and suggest that the diazoalkane is generated gradually from the phosphazine under the reaction conditions.

XVII. Cartesian Coordinates of the Optimized Geometries

SM							
Cl	1.28852800	0.15505100	3.32479900	C	3.68746000	-3.95404300	-0.98452000
P	-1.63711800	0.07707000	-0.18030300	C	2.74820900	1.32526800	-0.20314300
P	1.33546000	0.12022000	-0.34631200	C	3.81241500	0.86691500	0.79852800
C	0.45669000	0.63920600	-1.90402500	C	3.38813900	1.76041200	-1.52744600
C	-0.93723700	0.02902700	-1.91234200	C	4.85503800	1.95711200	1.01915800
C	-2.71456200	-1.44236800	-0.10505900	C	4.43214500	2.84812400	-1.28627700
C	-3.56878400	-1.43691100	1.16516300	C	5.49362600	2.38916200	-0.29453000
C	-3.55022400	-1.81679100	-1.33276000	H	1.02753100	0.37186900	-2.80518000
C	-4.26573200	-2.77916400	1.36309700	H	0.39805000	1.73675600	-1.86927400
C	-4.23162300	-3.16709400	-1.11936600	H	-1.60186700	0.51319900	-2.64246400
C	-5.09207300	-3.15519600	0.13874400	H	-0.87758300	-1.03317900	-2.19409500
C	-2.72703500	1.59053900	-0.10009500	H	-1.94772200	-2.23193800	0.02276600
C	-1.86448200	2.83938000	-0.32229000	H	-4.33421700	-0.64433700	1.08966100
C	-3.96800200	1.62870400	-0.99192800	H	-2.94497700	-1.19304500	2.03934400
C	-2.66589100	4.11697200	-0.10110900	H	-4.32479400	-1.05688700	-1.51632500
C	-4.75670300	2.92278600	-0.79321000	H	-2.92684500	-1.84741200	-2.23821100
C	-3.88900500	4.15578700	-1.00734000	H	-4.89590000	-2.74923000	2.26265200
C	1.94733700	-1.59016700	-0.76141900	H	-3.50331600	-3.55578000	1.54089200
C	3.00949400	-1.69335100	-1.85948600	H	-4.83524100	-3.42772000	-2.00019500
C	2.36962200	-2.38268800	0.47965400	H	-3.46115600	-3.95086000	-1.02417400
C	3.27167200	-3.15576700	-2.21405100	H	-5.57438200	-4.13175300	0.28411500
C	2.64347800	-3.83908500	0.12005500	H	-5.90525400	-2.41980700	0.01128500
				H	-3.05833100	1.60456100	0.95561300

H	-1.49305200	2.83880000	-1.36396400	C	3.67746400	1.58553000	-2.05207700
H	-0.98148700	2.80232100	0.33476100	C	4.82092400	2.89601500	0.31666600
H	-3.66549400	1.54264300	-2.05107800	C	4.42089200	2.91597700	-2.15661300
H	-4.62244100	0.77317000	-0.77901900	C	5.46059400	3.06734700	-1.05451500
H	-2.02805000	4.99537300	-0.27143000	H	-0.13233200	3.50800500	2.37767100
H	-2.98758200	4.16349300	0.95268400	H	-1.28154200	5.58172600	1.51861900
H	-5.62740400	2.93599200	-1.46390200	H	-3.56019000	5.50425700	0.63761500
H	-5.15568000	2.93853200	0.23520700	H	-4.86017100	3.37100600	0.56723600
H	-4.47274700	5.07022100	-0.83276600	H	-5.11506000	-0.29375200	1.52420100
H	-3.55955000	4.19089200	-2.06013100	H	-4.09516700	-2.32126700	2.58931300
H	1.02075500	-2.06502200	-1.14412800	H	-1.81512000	-2.28512800	3.46468200
H	3.95104800	-1.24461500	-1.50000400	H	-0.44079100	-0.19230100	3.43421400
H	2.71582600	-1.13247800	-2.76022200	H	2.18081900	-0.78456300	-2.83851200
H	3.28020600	-1.93548700	0.91241400	H	0.99762300	0.51892200	-2.65753900
H	1.59470500	-2.30033500	1.25538100	H	-0.25742100	-1.58207500	-3.13121100
H	4.03981100	-3.22042000	-2.99767500	H	0.58680000	-2.40711700	-1.82177200
H	2.35241400	-3.59327000	-2.64006300	H	-2.72875000	-2.00920600	0.26399800
H	2.96283100	-4.39167500	1.01415700	H	-2.20488700	-3.29699400	-2.46258600
H	1.70441500	-4.31041200	-0.21885000	H	-3.54298000	-2.20608900	-2.06591500
H	3.85864200	-5.00658000	-1.25043900	H	-0.42086400	-3.81410200	-0.60611800
H	4.65044200	-3.56459100	-0.61219400	H	-0.55427500	-2.98783900	0.95250200
H	2.24021100	2.20663300	0.23337200	H	-4.27737600	-4.57417200	-1.95741000
H	4.31663200	-0.03167400	0.40243700	H	-4.41479300	-3.77318300	-0.39043600
H	3.34066800	0.58407100	1.75063900	H	-1.32158400	-5.37121800	1.08359000
H	3.87361100	0.89749300	-2.01061100	H	-2.64523300	-4.25972500	1.44270400
H	2.63027500	2.12991400	-2.23253600	H	-3.42600700	-6.03881200	-0.11568400
H	5.61846200	1.60262700	1.72511400	H	-2.13682500	-5.63372200	-1.25031400
H	4.37048800	2.82518100	1.49626600	H	-3.12176200	0.20532400	-1.32478100
H	4.89048300	3.14212700	-2.24132300	H	-0.72786200	1.91703900	-2.18070400
H	3.92989500	3.74679400	-0.89000700	H	-1.54446900	2.03137700	-0.62988100
H	6.23277200	3.18501600	-0.12684100	H	-1.35514300	0.15980500	-3.83517800
H	6.04432700	1.53584700	-0.72737600	H	-2.59196000	-1.04743200	-3.49574600
Rh	-0.02096400	0.11487000	1.37198600	H	-2.39841300	3.76111200	-2.19756700
IM1A				H	-3.67619700	2.63161200	-1.76023900
Cl	1.41403800	1.27113800	2.58559600	H	-3.48182500	0.67935300	-5.02005000
C	-1.87561200	2.31709700	1.93424800	H	-4.33738000	0.74917700	-3.47820200
C	-1.15119800	3.48080300	1.99642100	H	-3.73525900	3.04734100	-4.21195000
C	-1.80787100	4.62834700	1.50421200	H	-2.04017900	2.57895300	-4.35417700
C	-3.10343600	4.58574400	1.00353300	H	2.17526900	-2.37341400	-0.33040200
C	-3.84272800	3.38550200	0.95479900	H	4.89091800	-1.01310900	-0.71762500
C	-3.19447700	2.26831500	1.41961600	H	3.91683200	-1.72348100	-2.00571000
C	-3.26240500	0.80396900	1.69996200	H	3.89277300	-0.93360700	1.74005500
C	-4.07063200	-0.28480500	1.83125600	H	2.27934400	-1.57941200	1.99128600
C	-3.49098800	-1.42164500	2.46814200	H	5.68136000	-3.30076700	-1.23143300
C	-2.20488400	-1.40313300	2.95725300	H	4.06888000	-3.95499400	-0.93815200
C	-1.36815900	-0.24760700	2.86940300	H	4.05467500	-3.18209600	2.76484200
C	-1.90925000	0.83619600	2.19437800	H	3.08791500	-3.87898500	1.46302600
P	-1.01546800	-0.84447200	-0.87344700	H	5.51324500	-4.30085000	1.05813600
P	1.90041300	-0.04580300	-0.47513800	H	5.83930900	-2.56718400	1.14249900
C	1.34993100	-0.42501500	-2.21517000	H	2.31506700	2.27388900	-0.53345100
C	0.21027800	-1.42767500	-2.15020900	H	4.82999700	0.74825200	0.31549700
C	-2.02904200	-2.36218100	-0.51199400	H	3.62916700	1.45533900	1.41269300
C	-2.86525000	-2.96115300	-1.64277600	H	4.38945600	0.75753600	-2.21441100
C	-1.14523600	-3.43340200	0.13640300	H	2.93323100	1.52290700	-2.85748600
C	-3.68837400	-4.14413300	-1.13496100	H	5.57709200	2.97320100	1.11018600
C	-1.97607400	-4.60889800	0.63795700	H	4.09985800	3.71171800	0.49352100
C	-2.81120200	-5.20725400	-0.48761100	H	4.88682200	3.00630200	-3.14842700
C	-2.14226100	0.31403300	-1.83274900	H	3.68894900	3.73781700	-2.07862700
C	-1.70657500	1.77818600	-1.68549100	H	5.96405100	4.04125200	-1.13393100
C	-2.32081100	0.00206400	-3.32290300	Rh	6.24143000	2.29846800	-1.18743400
C	-2.72678200	2.71891700	-2.31721900		0.07612900	0.10700200	0.86519800
C	-3.35824700	0.92606300	-3.95577900	IM1B			
C	-2.96627200	2.38835200	-3.78480000	Cl	1.63664400	1.68453100	2.37170200
C	2.89896200	-1.57308000	-0.07996800	P	-0.62971600	-0.28842600	-1.27851900
C	4.14963400	-1.79989400	-0.93271200	P	2.22465200	0.33378200	-0.57881500
C	3.20234400	-1.72649800	1.41219000	C	1.82697400	0.48614800	-2.38613100
C	4.77151700	-3.16164300	-0.63039500	C	0.61927800	-0.38851400	-2.68365000
C	3.82463500	-3.08933500	1.69445300	C	-0.95207600	-2.11253700	-0.96842500
C	5.07725500	-3.31175700	0.85506000	C	-2.02434100	-2.33599000	0.09173900
C	3.02588000	1.43683600	-0.67077600	C	-1.13815700	-3.08762600	-2.13506100
C	4.09117200	1.56112500	0.42521300	C	-2.01174300	-3.77757100	0.59012900

C	-1.07315600	-4.52412100	-1.61870700	C	-1.79525100	0.27903900	2.71453800
C	-2.13834400	-4.77317300	-0.55657800	C	-3.07299400	-0.27987600	2.49648600
C	-2.11889300	0.48829100	-2.09557200	C	-3.45301600	-1.44290400	3.16227900
C	-1.70764600	1.87751400	-2.60219000	H	-2.83910000	-2.94331200	4.57264000
C	-2.80217200	-0.32468500	-3.19487800	H	-0.60987400	-1.94276000	4.96087400
C	-2.86559700	2.62316700	-3.25523700	H	0.08853700	0.12402900	3.75079800
C	-3.95592900	0.44853300	-3.82943800	H	-4.43706400	-1.88101200	2.99245300
C	-3.49519500	1.79571800	-4.36808200	C	-1.66431200	1.45936300	1.81857700
C	2.78769000	-1.43995000	-0.44323000	C	-2.98022300	1.61975900	1.15777000
C	4.02876600	-1.85265900	-1.23626500	C	-3.46854500	2.63819700	0.35119300
C	2.84477700	-1.93694800	1.00444500	C	-4.77466500	2.54039900	-0.12141600
C	4.20614300	-3.36923100	-1.18583700	C	-5.56811100	1.43259800	0.19003200
C	3.03442000	-3.44966200	1.03826900	C	-5.08548000	0.42593800	1.01929700
C	4.27089800	-3.87118300	0.25214500	C	-3.79674900	0.53586900	1.53556200
C	3.66810600	1.48811100	-0.31268400	H	-2.84243500	3.49194200	0.08649100
C	4.59479200	1.06859700	0.83424100	H	-5.17992100	3.33352600	-0.74834200
C	4.49359100	1.80038800	-1.56566700	H	-6.58017900	1.36791300	-0.20573500
C	5.60260300	2.17338200	1.13202000	H	-5.71732800	-0.42059700	1.28767700
C	5.52085000	2.89163100	-1.26975600	N	-1.17336500	2.61827800	2.29941800
C	6.42528200	2.51655200	-0.10321100	N	-0.77052000	3.61564200	2.63022800
H	2.67738000	0.23787800	-3.03730600	TS1A ($\nu_i = -268.99 \text{ cm}^{-1}$)			
H	1.58507500	1.54717500	-2.54716700	Cl	1.62696400	-0.59302900	2.82135600
H	0.15194500	-0.11901500	-3.64046200	C	-1.38108500	0.59649500	2.24876100
H	0.94245500	-1.43281500	-2.78918200	C	-0.79190500	1.69215700	2.85922900
H	0.00571600	-2.38384400	-0.48322300	C	-1.61483400	2.81278500	3.09391600
H	-3.02231600	-2.09059700	-0.31791900	C	-2.97464300	2.79656800	2.81846200
H	-1.84616100	-1.65819300	0.93426600	C	-3.59854700	1.62168400	2.35958300
H	-2.11638600	-2.93067200	-2.61446600	C	-2.78794300	0.54076700	2.09584400
H	-0.38224200	-2.94041000	-2.91996700	C	-2.89340800	-0.91499800	1.94264500
H	-2.81078300	-3.92281100	1.33171300	C	-3.85475000	-1.89748700	2.01645200
H	-1.06116300	-3.95156800	1.12491500	C	-3.41058100	-3.22671600	2.13820200
H	-1.18542300	-5.23218000	-2.45208700	C	-2.06103500	-3.51251800	2.28205400
H	-0.07223400	-4.70435000	-1.18629600	C	-1.08159100	-2.49849100	2.27721400
H	-2.07829700	-5.80515400	-0.18323700	C	-1.51101800	-1.20742300	2.01898100
H	-3.13407300	-4.66533800	-1.02050100	P	-1.08951300	0.05662600	-1.01430900
H	-2.84259300	0.63106900	-1.27378000	P	1.98199300	-0.02255700	-0.49565900
H	-0.90400600	1.77063200	-3.35241200	C	1.37381600	0.51149400	-2.17163600
H	-1.27799300	2.45960500	-1.77188100	C	0.05773400	-0.18974600	-2.45908200
H	-2.07137200	-0.59159900	-3.97896800	C	-2.55048100	-1.09189500	-1.37684800
H	-3.18151700	-1.26917700	-2.78316300	C	-3.92756400	-0.44575700	-1.17511600
H	-2.51579200	3.59237200	-3.63849800	C	-2.50233300	-1.78897400	-2.74205700
H	-3.63218600	2.83898300	-2.49406000	C	-5.04731000	-1.47210600	-1.32011700
H	-4.41621800	-0.15453200	-4.62502000	C	-3.62654300	-2.81244700	-2.87677900
H	-4.73653400	0.61191200	-3.06651000	C	-4.99024700	-2.16869000	-2.67244500
H	-4.33494900	2.33687900	-4.82625900	C	-1.76458000	1.78320400	-1.26499600
H	-2.75269300	1.63348100	-5.16899200	C	-0.91334100	2.88193700	-0.62058700
H	1.93951600	-1.97378000	-0.91016900	C	-2.08522300	2.15722900	-2.71434800
H	4.92696400	-1.36971100	-0.81818300	C	-1.65691700	4.21305100	-0.66325800
H	3.95179100	-1.52051700	-2.28320700	C	-2.83281900	3.48727200	-2.76907900
H	3.67894100	-1.45140900	1.53628600	C	-2.03698900	4.59618000	-2.08926900
H	1.92558200	-1.63830900	1.53422400	C	2.84262400	-1.62388000	-0.92944500
H	5.10703800	-3.66402200	-1.74248300	C	4.05159400	-1.50959800	-1.86487100
H	3.35132300	-3.84663500	-1.69750400	C	3.17905800	-2.49914000	0.28107700
H	3.09965200	-3.79982900	2.07780600	C	4.52205000	-2.89262100	-2.30894700
H	2.14283100	-3.93615600	0.60134400	C	3.65876700	-3.87568700	-0.16805400
H	4.38999100	-4.96358800	0.27198700	C	4.85307700	-3.77120400	-1.10955300
H	5.16689100	-3.44931900	0.73906200	C	3.23233900	1.28874900	-0.03042500
H	3.16128700	2.41517100	0.00844400	C	4.26442100	0.80036100	0.99196100
H	5.14440300	0.15444300	0.55098300	C	3.93309000	1.98303500	-1.20483000
H	4.00655100	0.84372800	1.73117000	C	5.13346500	1.95476000	1.47872600
H	5.01629900	0.88928500	-1.90608900	C	4.80890600	3.13178600	-0.70862000
H	3.85289300	2.12564500	-2.39650300	C	5.82755700	2.65586000	0.31893200
H	6.25687200	1.87020100	1.96131700	H	0.26510800	1.70144300	3.11437400
H	5.05404100	3.06607300	1.47684100	H	-1.16383400	3.71643300	3.50282300
H	6.11407800	3.10083200	-2.17161400	H	-3.57519100	3.68182600	3.02228100
H	4.98394200	3.82373000	-1.02535000	H	-4.68344300	1.55736900	2.27675900
H	7.13180900	3.33088600	0.11097000	H	-4.91832500	-1.65742700	2.02004800
H	7.03453900	1.64025700	-0.38587000	H	-4.13879000	-4.03576400	2.17318100
Rh	0.31561600	0.74635000	0.52529600	H	-1.74457000	-4.54570700	2.41985800
C	-2.55795600	-2.03362600	4.04447400	H	-0.03387400	-2.72590500	2.45758300
C	-1.29776600	-1.46795800	4.26342600	H	2.11958700	0.31264200	-2.95420600
C	-0.90085900	-0.30848100	3.60461800				

H	1.22479800	1.59989700	-2.14459400	C	4.50806100	-1.60185100	3.05636100
H	-0.38608100	0.14710900	-3.40552900	C	3.22648400	1.26876400	-1.35450300
H	0.22504300	-1.27182200	-2.55211300	C	3.90736500	2.09205600	-0.25466000
H	-2.44089400	-1.87247600	-0.60342800	C	4.26422000	0.75912900	-2.35906500
H	-4.07951900	0.34937200	-1.92518200	C	4.67403600	3.26076300	-0.86336700
H	-3.99122100	0.03508100	-0.18916100	C	5.05168900	1.92463100	-2.95422000
H	-2.59975000	-1.04153900	-3.54888700	C	5.70601000	2.77532800	-1.87361000
H	-1.53783800	-2.29150600	-2.89313800	H	2.98056000	-1.75050000	-2.24177600
H	-6.02113200	-0.98305700	-1.17375100	H	1.60072700	-0.84352600	-2.89010100
H	-4.94769600	-2.22520500	-0.52063100	H	0.70658400	-3.04038700	-2.37895900
H	-3.56766200	-3.30276800	-3.85884200	H	1.57485900	-3.12376500	-0.85858200
H	-3.48176900	-3.60230400	-2.12029600	H	0.04244000	-2.12167500	1.65674000
H	-5.78917300	-2.91836500	-2.75775900	H	-2.67884400	-3.24160600	0.83321900
H	-5.16639900	-1.42874100	-3.47227300	H	-2.36916000	-1.63493100	1.50299000
H	-2.71362800	1.76395300	-0.69987900	H	-0.57157500	-4.80469100	0.31169000
H	0.04394700	2.98778300	-1.16289900	H	1.03083600	-4.17632800	0.69554600
H	-0.66048200	2.60972200	0.41300400	H	-3.13958200	-3.22616200	3.26157400
H	-1.14230600	2.25392000	-3.28121500	H	-1.51332600	-2.62799600	3.59841900
H	-2.67001800	1.37134000	-3.21666900	H	0.25995300	-5.75430500	2.43782000
H	-1.04653700	5.00191400	-0.20102800	H	0.52216400	-4.13741400	3.09402000
H	-2.56805600	4.12432100	-0.04670500	H	-1.61065900	-5.08937000	3.96226900
H	-3.05567800	3.75490000	-3.81183900	H	-2.19376000	-5.32571300	2.31346100
H	-3.80588100	3.36910900	-2.26139800	H	-2.77088500	-2.01895100	-1.17544600
H	-2.60529300	5.53682900	-2.10006800	H	-0.89130400	-1.71681400	-3.56676300
H	-1.11611600	4.78203300	-2.66884200	H	-1.78006700	-0.41397800	-2.78018700
H	2.04231500	-2.15107300	-1.48612400	H	-1.03324700	-4.15556600	-2.49665400
H	4.87811800	-1.00664100	-1.33505300	H	-2.04324900	-4.36642200	-1.06658200
H	3.82423500	-0.89341300	-2.74765600	H	-2.95420000	-1.23701200	-4.84379200
H	3.96890200	-2.01734200	0.87913500	H	-3.94341100	-1.49333400	-3.40562000
H	2.30856200	-2.57420800	0.94638200	H	-3.19273100	-5.18295400	-3.11413200
H	5.39164200	-2.79739300	-2.97465900	H	-4.07758400	-3.85322600	-2.36468700
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H	3.91106700	-4.48634200	0.70982400	H	-2.19978600	-3.60940500	-4.77444700
H	2.83469600	-4.39768500	-0.68491500	H	2.17676800	-1.80097600	0.83054600
H	5.17784300	-4.76770000	-1.44043700	H	4.96797400	-0.61788700	0.47518800
H	5.70420100	-3.32784300	-0.56505800	H	4.33743900	-2.02496600	-0.38700800
H	2.59769600	2.04015200	0.47825200	H	3.32879200	0.73398100	2.06375700
H	4.91267000	0.04595300	0.51448000	H	1.65642300	0.19582500	2.17633900
H	3.75985300	0.31158500	1.83510000	H	5.67479100	-2.71757300	1.60298700
H	4.56237000	1.25452700	-1.74251000	H	3.99216700	-2.32653000	1.74373800
H	3.20616600	2.36714100	-1.93419800	H	3.00643000	-0.51282500	4.18367800
H	5.86927400	1.58435300	2.20588100	H	2.38894900	-1.91092000	3.29901700
H	4.49949300	2.67760600	2.01922800	H	4.78206600	-2.25768800	3.89479600
H	5.30882500	3.61437300	-1.56063700	H	5.21966300	-0.75850400	3.07349100
H	4.16316500	3.89937200	-0.24906000	H	2.53956100	1.95301800	-1.88339000
H	6.43421200	3.49955800	0.67699500	H	4.61766400	1.45358000	0.29874200
H	6.52579900	1.95040700	-0.16409500	H	3.15600800	2.45760800	0.45648100
Rh	0.13476600	-0.25052200	0.89974200	H	4.96073500	0.06387800	-1.85847000
				H	3.78627600	0.19585800	-3.17281100
				H	5.15701600	3.84655200	-0.06872200
				H	3.95439600	3.93585700	-1.35637500
				H	5.80432600	1.54583200	-3.66087200
				H	4.36135900	2.55460100	-3.54037600
				H	6.23960400	3.62346800	-2.32574000
				H	6.46649700	2.17037700	-1.34941700
				Rh	-0.15337400	0.51420000	-0.25412400
				C	-3.34037700	5.11667300	-1.18597100
				C	-3.05710900	4.12765800	-2.12832400
				C	-2.61504200	2.87094400	-1.72168700
				C	-2.47783200	2.62549200	-0.36683100
				C	-2.77674600	3.61325000	0.58609600
				C	-3.19908600	4.87064500	0.17812600
				H	-3.67200700	6.09765500	-1.52273400
				H	-3.16749200	4.34649000	-3.18889300
				H	-2.35501100	2.09947800	-2.44699800
				H	-3.41050400	5.65286100	0.90678900
				C	-1.97664000	1.38356300	0.31604200
				C	-2.09528400	1.72894000	1.77272500
				C	-1.76727200	0.96676800	2.88228400
				C	-1.90463100	1.53187200	4.14916400
				C	-2.34192700	2.84816500	4.29226100
				C	-2.65299200	3.62454400	3.17813100
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Cl	0.59152600	2.83512300	0.09167100				
P	-0.44870700	-1.72015500	-0.62757900				
P	2.05188800	-0.01466200	-0.68894400				
C	1.99374300	-1.33713900	-1.98873800				
C	1.04455600	-2.43462200	-1.52753300				
C	-0.57516600	-2.72369400	0.96302900				
C	-2.00804700	-2.67396700	1.50155600				
C	-0.02305600	-4.15223600	1.01030100				
C	-2.09997000	-3.25747200	2.90698400				
C	-0.12738800	-4.72589800	2.42242200				
C	-1.55789300	-4.68021600	2.94391300				
C	-1.85151800	-2.29848400	-1.71617000				
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C	-1.95341700	-3.79886700	-2.00318600				
C	-3.01478100	-1.81238600	-3.90940200				
C	-3.14861800	-4.10479900	-2.90455300				
C	-3.09183900	-3.30590200	-4.19953000				
C	2.83765400	-0.91747700	0.74285000				
C	4.25597500	-1.45669300	0.55306800				
C	2.69200800	-0.16479500	2.06863900				
C	4.64909100	-2.34383800	1.73243600				
C	3.09374400	-1.06108900	3.23530400				

C	-2.53473100	3.05783200	1.91661600	H	5.76385700	0.72810200	2.78384100
H	-1.38196300	-0.04551700	2.75749400	H	2.24614100	2.51981700	0.07798100
H	-1.65234400	0.94772700	5.03251600	H	-0.73630000	3.06550600	0.45839600
H	-2.43150000	3.27882400	5.28842600	H	0.02050500	2.51272900	-1.04229400
H	-2.97734100	4.65800700	3.29717700	H	0.65755800	3.18247400	2.61342300
N	-3.35440200	0.41606900	0.05363100	H	2.37631100	2.77423300	2.58241400
N	-4.05501600	-0.33120900	-0.39062700	H	-0.26724800	4.99500800	-1.02397900
IM2A				H	1.44194700	4.55851200	-1.08456300
Cl	-1.09879100	-0.74130000	-2.94935200	H	2.04387700	5.24862800	2.61283500
C	1.80234900	-0.16254700	-2.03725400	H	2.85435000	4.72677800	1.13485000
C	2.15569300	0.90431000	-2.85699200	H	1.07400300	6.37061300	0.58885600
C	3.35351100	0.87211400	-3.57309200	H	-0.12649100	5.38268200	1.42024300
C	4.19586200	-0.23407400	-3.48431500	H	-2.23696900	-1.97371300	1.78615700
C	3.84069500	-1.31438300	-2.68477600	H	-4.99444300	-0.86089700	1.10226700
C	2.64764300	-1.28288900	-1.95945800	H	-4.11687700	-0.53695000	2.60081900
C	2.16398200	-2.31151300	-1.04580500	H	-3.85843800	-2.16896400	-0.80251300
C	2.82377300	-3.49672500	-0.71251100	H	-2.21244600	-2.74672800	-0.60768300
C	2.29729200	-4.36285000	0.24030800	H	-5.74305300	-2.39625300	2.90565200
C	1.09469200	-4.05519700	0.86552200	H	-4.08980500	-2.97096300	3.13079200
C	0.41762800	-2.87661100	0.54053300	H	-3.85371500	-4.60164800	-0.28810500
C	0.94417900	-2.00630000	-0.40380200	H	-2.94214500	-4.30812500	1.19283100
P	1.13433500	0.61083100	0.90740300	H	-5.36544700	-4.57108500	1.71759900
P	-1.98964300	-0.04600000	0.45273100	H	-5.76626900	-3.27932100	0.58456700
C	-1.41429000	0.72069700	2.06164100	H	-2.48743200	1.93150800	-0.71951800
C	0.03046300	0.34090400	2.37114400	H	-4.78031200	-0.07058700	-0.92602900
C	2.79732500	-0.05180000	1.41963100	H	-3.42186500	0.05727000	-2.06277400
C	3.95661400	0.60955600	0.66481200	H	-4.78115600	1.34937500	1.22337400
C	3.09724400	-0.10911000	2.92005600	H	-3.44094800	2.44856300	1.55208800
C	5.24543400	-0.17221100	0.89727600	H	-5.42439400	1.30784900	-2.88223500
C	4.39059500	-0.88957400	3.15046300	H	-4.06507300	2.39135300	-2.59622700
C	5.55917000	-0.28044500	2.38466000	H	-5.40620200	3.70033700	0.70982400
C	1.33415400	2.44606300	0.69768500	H	-4.04834800	3.83517600	-0.40998000
C	0.20534500	3.08618500	-0.11832200	H	-6.15139200	3.38154800	-1.66182600
C	1.56838200	3.22833100	1.98993600	Rh	-6.43070100	1.92914200	-0.69964400
C	0.54479800	4.53685500	-0.44273600		0.09303200	-0.25812500	-0.92660700
C	1.89585200	4.68715400	1.67988100	IM2B			
C	0.80571900	5.33320400	0.83138100	Cl	-1.14386300	-1.02098100	-2.78595100
C	-2.94165700	-1.53509300	1.05089100	P	0.60928900	0.52545800	1.31109100
C	-4.25136700	-1.28072700	1.80039500	P	-2.35728000	0.03015300	0.31444400
C	-3.14837700	-2.56924300	-0.06083100	C	-2.08853400	0.95209200	1.91589000
C	-4.79786300	-2.58541200	2.37723500	C	-0.76972100	0.53693000	2.55395700
C	-3.69725600	-3.86974000	0.51580800	C	1.95794900	-0.46327900	2.14535600
C	-4.99118100	-3.63215300	1.28625900	C	3.34097600	-0.12364000	1.58393300
C	-3.18258000	1.21540100	-0.23878600	C	2.00202200	-0.48771000	3.67628900
C	-4.04597800	0.62927400	-1.36148900	C	4.37331900	-1.14521700	2.04719000
C	-4.04618500	2.01473400	0.74230800	C	3.04613200	-1.49529700	4.15651700
C	-4.79646700	1.73883800	-2.09053500	C	4.42319400	-1.20781700	3.56953100
C	-4.78758200	3.12746400	0.00433200	C	1.24486100	2.27146200	1.19832300
C	-5.63942000	2.56795600	-1.12894800	C	0.29084500	3.16860300	0.40283700
H	1.49203200	1.76598900	-2.95934000	C	1.63418600	2.96198000	2.50624500
H	3.62520400	1.71236600	-4.21191700	C	0.94488600	4.51192800	0.10002200
H	5.12729400	-0.25748200	-4.04801900	C	2.27638000	4.32044500	2.22768600
H	4.49944400	-2.18266400	-2.62770500	C	1.36996600	5.21160400	1.38688000
H	3.76772400	-3.74130200	-1.20130300	C	-3.15217900	-1.54880900	0.91457800
H	2.82757200	-5.27960800	0.49288100	C	-4.54282400	-1.44269900	1.54262800
H	0.67315700	-4.72925200	1.61062200	C	-3.11360500	-2.64944800	-0.15064100
H	-0.52007700	-2.64745800	1.04375300	C	-4.98519000	-2.78563600	2.11935700
H	-2.07618600	0.43661000	2.89298800	C	-3.56792200	-3.98441800	0.42891200
H	-1.49387700	1.81192400	1.96492000	C	-4.95232000	-3.87731100	1.05666500
H	0.40526300	0.87825800	3.25452700	C	-3.60847100	1.09873100	-0.56786600
H	0.10907800	-0.73549800	2.59276100	C	-4.26760600	0.36554800	-1.74142800
H	2.74321600	-1.09724100	1.07245800	C	-4.66472200	1.80818800	0.28586600
H	4.09546300	1.64294200	1.03102200	C	-5.09993200	1.32570100	-2.58440200
H	3.74032000	0.67063000	-0.41125300	C	-5.48536800	2.77095400	-0.56975600
H	3.20247700	0.90941600	3.33352900	C	-6.14133900	2.05070600	-1.74114300
H	2.27723600	-0.59177700	3.46993800	H	-2.92540900	0.80567900	2.61420800
H	6.07522000	0.30468100	0.35737900	H	-2.06922700	2.02258600	1.66632200
H	5.13044500	-1.18191700	0.46656300	H	-0.52129000	1.15894400	3.42713200
H	4.61462400	-0.93900000	4.22538500	H	-0.84245800	-0.50072200	2.91604600
H	4.23497800	-1.92848900	2.81145300	H	1.72045100	-1.49139500	1.81355000
H	6.47178400	-0.87049900	2.54718300	H	3.64419500	0.87967200	1.93146900

H	3.31693900	-0.07848100	0.48698100	C	-3.04497400	0.14085700	-0.02365300
H	2.25444200	0.51186900	4.06770100	C	-2.58151400	-0.29549700	-1.33972200
H	1.02098000	-0.74751500	4.09768300	C	-3.41019200	-0.50574800	-2.44213900
H	5.36149800	-0.89687200	1.63498200	C	-2.87177900	-0.79238900	-3.69294500
H	4.10446700	-2.13418000	1.63663800	C	-1.49225200	-0.87173300	-3.83960200
H	3.08760100	-1.49815700	5.25490800	C	-0.66023800	-0.68724300	-2.73146800
H	2.72779100	-2.50716200	3.85350900	C	-1.17530000	-0.41103100	-1.46686500
H	5.14646300	-1.96440700	3.90444100	P	0.08305500	2.11673400	-0.58718000
H	4.78408000	-0.23889200	3.95617800	P	2.31812100	-0.31204700	-0.64634900
H	2.15582300	2.15331700	0.58110100	C	2.56114600	1.24317300	-1.66834600
H	-0.62085600	3.35135900	0.99885900	C	1.28860000	2.01569600	-1.99136600
H	-0.03421700	2.65273000	-0.51475400	C	-1.45424900	2.80266900	-1.41647900
H	0.72979700	3.10555800	3.12372300	C	-2.43584400	3.48548400	-0.45464700
H	2.32338300	2.34351500	3.09861900	C	-1.27028300	3.63506100	-2.69302600
H	0.25965300	5.14836600	-0.47722000	C	-3.78268500	3.68645800	-1.14251800
H	1.83129400	4.34567700	-0.53687400	C	-2.62765100	3.83352600	-3.36631700
H	2.53528100	4.81675200	3.17365700	C	-3.63007400	4.49228500	-2.42632700
H	3.22635800	4.15663700	1.69067200	C	0.68921300	3.48567300	0.53222200
H	1.87101200	6.16383200	1.16335500	C	2.06266600	3.21791800	1.15509400
H	0.46910400	5.46381900	1.97226200	C	0.70429100	4.88679800	-0.09169300
H	-2.44806300	-1.85587600	1.71546500	C	2.38259500	4.25401100	2.22738800
H	-5.26785100	-1.13304800	0.77094600	C	1.01922500	5.94107100	0.96917100
H	-4.56855200	-0.66926400	2.32566000	C	2.34643700	5.66797400	1.66378700
H	-3.77217900	-2.37395600	-0.99088200	C	2.81158700	-1.64725200	-1.86966200
H	-2.10443000	-2.72242500	-0.58033800	C	4.25144200	-1.69618700	-2.38429800
H	-5.99063100	-2.69559300	2.55501000	C	2.39825200	-3.03584500	-1.38440500
H	-4.30953200	-3.06332400	2.94681700	C	4.36906900	-2.70736100	-3.52438200
H	-3.55639100	-4.75555700	-0.35368600	C	2.49879600	-4.05703300	-2.51110800
H	-2.84698700	-4.31066600	1.19920200	C	3.90992100	-4.09466000	-3.08812300
H	-5.26162800	-4.84080000	1.48608800	C	3.71638400	-0.11193600	0.58516300
H	-5.68682800	-3.63510800	0.26946000	C	3.87493200	-1.31685700	1.50984400
H	-2.95037500	1.87902600	-1.00083100	C	5.09047400	0.36655800	0.10587000
H	-4.92893700	-0.42538900	-1.34545200	C	4.75449600	-0.95964200	2.70466900
H	-3.50267000	-0.12979700	-2.35522300	C	5.94264600	0.76140400	1.31042600
H	-5.34293300	1.06486800	0.73498800	C	6.10782800	-0.41285400	2.26809000
H	-4.20286900	2.35518900	1.12004000	H	-1.54156300	1.10915900	2.87876900
H	-5.57963200	0.78052100	-3.40904600	H	-3.90957100	1.55076500	3.48227100
H	-4.42739700	2.06540100	-3.05064600	H	-5.72864900	1.05032400	1.86266500
H	-6.24090600	3.27425400	0.05061700	H	-5.17771900	0.16122300	-0.37961100
H	-4.82067300	3.56196000	-0.95748500	H	-4.49241400	-0.42220800	-2.32908700
H	-6.71577200	2.75917900	-2.35482500	H	-3.52788600	-0.94330400	-4.54886100
H	-6.86698200	1.31599000	-1.35062900	H	-1.05383400	-1.08112200	-4.81548500
Rh	-0.14592300	-0.28725900	-0.69350600	H	0.41711100	-0.77240700	-2.87562200
C	4.46164400	1.78311400	-3.43005300	H	3.09080500	0.99049900	-2.59891100
C	3.22893900	2.37563800	-3.17118700	H	3.23772700	1.89186800	-1.10096300
C	2.23170200	1.66417000	-2.50065500	H	1.53608500	3.02573400	-2.35080700
C	2.49360100	0.36285800	-2.09584400	H	0.73282500	1.51552300	-2.79645800
C	3.74185500	-0.23906200	-2.37997600	H	-1.94830000	1.88098900	-1.75262100
C	4.73073200	0.46503000	-3.03974500	H	-2.04993800	4.46894900	-0.13952600
H	5.23013300	2.35092100	-3.95252100	H	-2.56596300	2.89045500	0.45760000
H	3.04105200	3.39668300	-3.49865700	H	-0.82293500	4.61808400	-2.47362600
H	1.25262000	2.10064400	-2.30119400	H	-0.59506100	3.13042800	-3.39672300
H	5.69728000	0.01182500	-3.25960100	H	-4.48598000	4.17407100	-0.45247300
C	1.62105200	-0.56943700	-1.37026300	H	-4.21141800	2.69642600	-1.37501600
C	2.41649200	-1.80244900	-1.28297200	H	-2.50770900	4.42672300	-4.28427700
C	2.06948200	-3.02595900	-0.72686900	H	-3.01089300	2.84497400	-3.67490600
C	3.01126200	-4.05856000	-0.73000000	H	-4.60168600	4.61504000	-2.92575400
C	4.27333300	-3.85876200	-1.28279400	H	-3.27628700	5.50813700	-2.17709600
C	4.62843500	-2.63109500	-1.85657800	H	-0.05437900	3.46949100	1.35201700
C	3.69404100	-1.61347300	-1.85944600	H	2.83750400	3.27359400	0.36805400
H	1.06983600	-3.15918000	-0.31101100	H	2.08485100	2.21668600	1.59639100
H	2.75731600	-5.02745100	-0.30420500	H	1.47531600	4.92235600	-0.88213500
H	4.99635100	-4.67302600	-1.27550000	H	-0.24719900	5.13356000	-0.57370500
H	5.61721000	-2.49303000	-2.29402000	H	3.36438500	4.03866200	2.67278900
				H	1.64470300	4.15364300	3.04108100
				H	1.01826800	6.94137800	0.51301200
TS2A ($\nu_1 = -477.76 \text{ cm}^{-1}$)				H	0.20747500	5.93745700	1.71646100
Cl	0.98712000	0.30143600	2.55323700	H	2.52591400	6.41049400	2.45418600
C	-2.01916200	0.39624900	0.90418600	H	3.16470100	5.78599900	0.93253700
C	-2.33606400	0.91547200	2.15733300	H	2.17480900	-1.41278600	-2.74342600
C	-3.66787300	1.15200600	2.49689500	H	4.91931400	-2.00677800	-1.56452900
C	-4.68919400	0.87229100	1.58999500	H	4.60024000	-0.70635900	-2.71490900
C	-4.37784000	0.37101500	0.33290300				

H	3.05093400	-3.34434500	-0.54848900	C	4.39550300	0.46726400	-3.32417400
H	1.37766300	-3.00049300	-0.98088500	C	5.17854400	1.77393200	-3.28222500
H	5.40469500	-2.74392500	-3.89090200	C	-1.01178500	1.73483600	2.69025500
H	3.74990000	-2.36801300	-4.37223700	C	-0.67587900	2.96254700	3.53927500
H	2.19809700	-5.05262800	-2.15528900	C	-2.48521800	1.37050500	2.88217700
H	1.78262300	-3.77843700	-3.30501700	C	-0.98597000	2.69416100	5.01176000
H	3.96536200	-4.79945100	-3.92936500	C	-2.78105300	1.06279000	4.34492100
H	4.60114900	-4.47461200	-2.31673100	C	-2.43122400	2.25807300	5.22392200
H	3.29524800	0.68591700	1.21882900	C	-1.68492100	2.85537000	-0.12081500
H	4.31855800	-2.16657000	0.95939300	C	-3.13871000	2.39370700	-0.22569700
H	2.88676600	-1.61879800	1.87391800	C	-1.64982600	4.36209900	0.15456400
H	5.60636300	-0.43806400	-0.43924900	C	-3.80536300	3.09511800	-1.40527300
H	5.01944500	1.21518300	-0.58892000	C	-2.33942600	5.09799300	-0.99458500
H	4.88346700	-1.83688100	3.35414900	C	-3.76616300	4.60753600	-1.21257300
H	4.22043600	-0.20192300	3.30127900	H	1.46017800	-0.41021800	-2.34315000
H	6.92303500	1.12958300	0.97520300	H	0.87781200	-1.23981700	-4.56594500
H	5.45245400	1.59972000	1.83603500	H	-0.39126000	-3.33767600	-4.87710200
H	6.70517300	-0.11780900	3.14241200	H	-1.07626900	-4.70949200	-2.89745700
H	6.67497500	-1.21077900	1.75747800	H	-1.11717700	-5.64365500	0.22422400
Rh	-0.13212100	-0.11319700	0.27352100	H	-0.52531100	-5.58922900	2.65621400
C	-3.50077400	-2.40356600	4.32989100	H	0.74344700	-3.69091200	3.58563600
C	-2.22158900	-1.92046600	4.59825300	H	1.40206600	-1.77384100	2.18230000
C	-1.27521500	-1.79372400	3.58353800	H	0.90103200	3.73503100	1.41414600
C	-1.62672000	-2.17824200	2.29657800	H	1.16641700	3.05979200	-0.21253700
C	-2.89561200	-2.72998100	2.04212100	H	3.11313900	2.59113100	1.39907400
C	-3.84873900	-2.81495700	3.04571900	H	2.01328300	1.66053400	2.42386100
H	-4.23155500	-2.47528600	5.13407700	H	3.09831300	-0.60998000	2.36648500
H	-1.95923400	-1.62323300	5.61202100	H	4.60934800	-1.79031500	-0.01318000
H	-0.29254000	-1.36893200	3.78002300	H	3.07916800	-2.41812000	0.58918800
H	-4.84109900	-3.21562800	2.84099300	H	5.55024500	0.38906400	0.84598000
C	-1.67869200	-2.94006700	0.07114600	H	4.74056900	1.27420200	2.14059800
C	-1.41967800	-3.38049200	-1.21995800	H	4.98468700	-3.67868300	1.56663000
C	-2.42303400	-4.03542200	-1.92786600	H	4.12033500	-2.80437900	2.83255500
C	-3.68156400	-4.22901100	-1.36057900	H	6.69064700	0.00642000	3.02524900
C	-3.94636800	-3.80905000	-0.06059500	H	5.18031200	-0.55675900	3.73993000
C	-2.93261700	-3.18847900	0.65713900	H	6.58125500	-2.49967100	3.11211900
H	-0.45858600	-3.19608700	-1.69366700	H	6.70969800	-1.90801100	1.45502100
H	-2.22812900	-4.37302800	-2.94407700	H	2.36937100	1.32215000	-1.81209800
H	-4.46324000	-4.71928200	-1.93876700	H	4.97643300	2.20356500	-0.49481500
H	-4.92566600	-3.97351400	0.38784500	H	3.48395100	3.15559500	-0.59629900
C	-0.87273900	-2.07503300	0.99549100	H	5.00951400	-0.18262900	-1.36613700
N	0.50155000	-3.11482400	1.43661700	H	3.53617200	-0.96843700	-1.94378900
N	1.44572000	-3.49269000	1.88183500	H	5.01049900	3.76492900	-2.43900000
TS2B ($\nu_1 = -278.74 \text{ cm}^{-1}$)				H	3.48220100	3.08402700	-3.02074400
Cl	0.53122900	2.52735700	-2.78820100	H	4.96130300	-0.30886900	-3.85946800
C	0.48704000	-2.08130700	-1.33292700	H	3.45414500	0.62296800	-3.87893900
C	0.93934700	-1.35967800	-2.42203800	H	5.39055200	2.12857600	-4.30063900
C	0.58417600	-1.83467900	-3.70165100	H	6.15711000	1.58986300	-2.80369800
C	-0.14261800	-3.00125700	-3.87204800	H	-0.40894800	0.88565500	3.06888300
C	-0.54991300	-3.76553600	-2.76441500	H	-1.26368500	3.82640600	3.18252000
C	-0.23435900	-3.28247100	-1.51615400	H	0.38195900	3.24174900	3.43704100
C	-0.28370100	-3.68391200	-0.10953700	H	-3.10219200	2.22946000	2.57283800
C	-0.62460300	-4.77428400	0.65708400	H	-2.77289200	0.52994000	2.23602300
C	-0.26774200	-4.74757200	2.01538100	H	-0.75918700	3.58657000	5.61194500
C	0.45240200	-3.68384300	2.53576900	H	-0.31223200	1.89777200	5.37238500
C	0.82608400	-2.58297300	1.73894300	H	-3.83826100	0.78846800	4.46838000
C	0.40234000	-2.56537700	0.41973800	H	-2.19031400	0.18378700	4.65829200
P	2.41489700	0.45512200	0.37230800	H	-2.61030100	2.02936300	6.28384300
P	-0.53220200	1.80741400	0.88133500	H	-3.10150200	3.09600300	4.96772000
C	1.02524700	2.79984300	0.85236200	H	-1.20696900	2.70771400	-1.11178500
C	2.19486700	1.98937500	1.38669100	H	-3.68996100	2.65447400	0.69241000
C	3.65490800	-0.47811700	1.41572100	H	-3.21269400	1.30441500	-0.33615800
C	3.98788100	-1.87939200	0.89027300	H	-2.15723300	4.58616500	1.11172300
C	4.94902300	0.26336000	1.76236300	H	-0.61909400	4.73013400	0.23909700
C	4.75865600	-2.67064300	1.94101800	H	-4.84089200	2.74285700	-1.52018500
C	5.75361400	-0.52128900	2.79746700	H	-3.27011500	2.82611500	-2.33150500
C	6.04138400	-1.94462600	2.33210000	H	-2.32877000	6.18132800	-0.80709700
C	3.24595300	1.06734500	-1.18406900	H	-1.74662200	4.92262400	-1.90712300
C	4.06031500	2.36213700	-1.09188800	H	-4.21750800	5.11877200	-2.07456900
C	4.06493600	-0.00431000	-1.91104600	H	-4.38110000	4.87237300	-0.33416900
C	4.42126100	2.83843500	-2.49850600	Rh	-0.00341100	-0.35042400	0.06614100
				C	-1.83381100	-0.79928300	-0.31845700

C	-2.77468000	-1.61243300	0.46180400	H	0.32446900	3.26663900	0.92011500
C	-2.46011100	-0.66619800	-1.63473600	H	2.31591200	2.55617600	2.21691200
C	-2.70038800	-2.01955200	1.78722000	H	1.51090800	1.06332000	2.70790900
C	-3.85194700	-2.02655100	-0.35747400	H	2.87848200	-1.04099500	1.54129900
C	-2.02376000	0.05596200	-2.73931800	H	5.09256300	-0.23460600	-0.38931100
C	-3.65496600	-1.42469900	-1.68511200	H	3.73155400	-1.27342500	-0.80781200
C	-3.70280900	-2.84692000	2.29709700	H	5.11207800	0.99253100	1.91748000
H	-1.85510400	-1.71007900	2.40343600	H	3.77426600	0.73064500	3.03906600
C	-4.83828100	-2.85221000	0.14349500	H	5.71206300	-2.61860300	-0.12495800
C	-2.79166400	0.00171300	-3.90841300	H	4.35714300	-2.86770100	0.98127600
H	-1.12280200	0.67940700	-2.69408300	H	5.76133700	-0.61295900	3.70184500
C	-4.40150700	-1.48293200	-2.84131300	H	4.38380100	-1.64521700	3.29392600
C	-4.75306800	-3.25785900	1.48207400	H	6.47130900	-2.53889100	2.27270000
H	-3.65911400	-3.17807700	3.33283600	H	6.74844500	-1.00094500	1.45253500
H	-5.66755000	-3.18397600	-0.48078300	H	3.11629700	1.67470800	-1.63911600
C	-3.95374400	-0.75748900	-3.95851300	H	2.21868800	3.97674600	0.16424900
H	-2.47109700	0.57123700	-4.77874900	H	1.21034500	3.20757100	-1.09434900
H	-5.31985500	-2.06759100	-2.89535000	H	4.44328000	3.05702400	0.76358300
H	-5.52496800	-3.90831000	1.89087800	H	5.12435800	1.67307100	-0.09162700
H	-4.53764800	-0.78617900	-4.87756500	H	2.24366800	5.27329900	-1.96154200
				H	2.84155400	3.85692000	-2.82541500
IM3				H	6.14095700	3.75165100	-0.92214100
Cl	0.00765600	1.42882300	-2.32207400	H	5.23094400	2.94070500	-2.19707600
C	1.32848100	-1.62640100	-1.55896900	H	4.74789500	5.36647000	-2.25479500
C	1.84334400	-1.38615900	-2.82974700	H	4.27723100	5.34192900	-0.55412300
C	2.59894800	-2.36370800	-3.48031300	H	-1.73368700	-0.28373700	2.59571500
C	2.84396000	-3.58864200	-2.86640000	H	-2.30124400	2.54324400	3.61073000
C	2.36321300	-3.82477200	-1.58404400	H	-0.87141800	1.57903600	3.99566900
C	1.61976100	-2.84620300	-0.91757800	H	-4.07617000	1.53083300	1.91054500
C	1.25100900	-2.88930300	0.49821200	H	-3.72712800	-0.04054900	1.18104200
C	1.62315500	-3.90875500	1.38003100	H	-2.55971400	1.41712400	5.80154500
C	1.45199100	-3.76649900	2.75245200	H	-2.24409200	-0.15471700	5.06334000
C	0.92775100	-2.58047000	3.25473900	H	-5.39927400	-0.24476200	3.00386300
C	0.52379300	-1.57263700	2.37639400	H	-3.93083700	-1.13763700	3.39489700
C	0.63161900	-1.71640800	0.99071700	H	-4.69264900	0.17013800	5.37756600
P	2.19459600	0.87858500	0.40392900	H	-4.63178200	1.66123200	4.43374900
P	-1.09449700	1.33877000	0.95403400	H	-1.31270800	2.98487500	-0.67042500
C	0.22037500	2.46584200	1.66491700	H	-3.98610900	1.56822800	-0.32140000
C	1.57651900	1.80562600	1.89813800	H	-2.71685700	1.19367200	-1.50817900
C	3.50696400	-0.25006300	1.10665200	H	-3.44140400	3.44158900	1.49824700
C	4.35577500	-0.93879800	0.03010000	H	-1.86169100	4.22569400	1.44978200
C	4.38219400	0.24368600	2.26248700	H	-4.49781900	2.64565600	-2.48363500
C	5.09888200	-2.12294000	0.64112300	H	-2.91427300	3.42364600	-2.50068700
C	5.12611000	-0.94701000	2.86875500	H	-3.62598700	5.67660600	0.46395900
C	5.95797800	-1.67865300	1.81996700	H	-2.39619500	5.25795800	-0.73183000
C	3.06389700	2.16335700	-0.64832300	H	-4.66837200	5.02731600	-1.71778200
C	2.23961800	3.44786800	-0.80588800	H	-5.13076400	3.90988200	-0.43175700
C	4.48335100	2.55204100	-0.21865500	Rh	0.14852200	-0.33163100	-0.45024000
C	2.85975600	4.37005400	-1.84922500	C	-1.44332000	-1.34964100	-1.03730300
C	5.12375000	3.48660500	-1.24451200	C	-2.45273800	-2.07782600	-0.23377400
C	4.28945000	4.73802600	-1.47814200	C	-1.99914400	-1.36696000	-2.39631400
C	-2.11903200	0.73431400	2.42242300	C	-2.42101700	-2.56260000	1.07050700
C	-1.93749200	1.50771200	3.73139700	C	-3.62378500	-2.27796700	-1.00626400
C	-3.60622900	0.55288600	2.09886600	C	-1.44076800	-0.98081600	-3.61288500
C	-2.69121400	0.83741400	4.87699100	C	-3.33829700	-1.83023300	-2.36926100
C	-4.33639600	-0.12124800	3.25662700	C	-3.55210300	-3.19224100	1.59905600
C	-4.16832600	0.66613000	4.54881700	H	-1.51997000	-2.48277900	1.67038200
C	-2.09405600	2.59887000	0.00955200	C	-4.75610800	-2.85874600	-0.47373500
C	-3.16197400	2.00051100	-0.91018200	C	-2.22633300	-1.02592000	-4.76838000
C	-2.64273100	3.77929100	0.81632500	H	-0.41009100	-0.65671300	-3.66487100
C	-3.72191400	3.07625700	-1.83506500	C	-4.12175200	-1.85257100	-3.50150400
C	-3.21472700	4.84137200	-0.12114300	C	-4.71401600	-3.31518600	0.84919400
C	-4.27693700	4.25365900	-1.04207800	H	-3.51708800	-3.58649600	2.61327200
H	1.67393700	-0.42058300	-3.30935400	H	-5.65768800	-2.98377300	-1.07271300
H	3.00128700	-2.16276100	-4.47334400	C	-3.54983200	-1.43773800	-4.71300800
H	3.42427400	-4.35419400	-3.37951800	H	-1.79216200	-0.72539000	-5.71951800
H	2.59103700	-4.77090300	-1.09057600	H	-5.15597800	-2.19366200	-3.46674500
H	2.08771100	-4.81589300	0.99086700	H	-5.59251500	-3.78967300	1.28368200
H	1.75367100	-4.56668400	3.42646200	H	-4.15038200	-1.45160900	-5.62135800
H	0.82286700	-2.43550200	4.32993300				
H	0.12016400	-0.65631000	2.80798900	TS3 ($v_i = -171.01 \text{ cm}^{-1}$)			
H	-0.13199000	2.94815800	2.58595000	C	2.53463500	1.29305000	-0.43620200

O	2.56667800	2.45248100	-0.03893200	C	3.39514400	1.48428300	-0.82008600
C	1.24842800	0.98689400	-1.16471400	C	2.93734200	2.94583000	-0.91306000
Rh	-0.37332100	0.27855200	-0.29583800	C	4.90417300	1.46321700	-0.55793300
O	-0.19719600	-1.55658800	-1.26960900	C	3.66675500	3.67210300	-2.03686400
C	-1.05700200	-2.48170200	-1.05022600	C	5.65820900	2.19930200	-1.66477000
O	-2.03968200	-2.41749700	-0.26038500	C	5.17399600	3.63357000	-1.82578300
Rh	-2.36145200	-0.66764300	0.80285300	C	-1.89540600	1.54660200	2.23994500
O	-3.47543700	0.08799500	-0.77337200	C	-1.82618800	2.39509900	3.51124200
C	-2.89101600	0.71682600	-1.70256500	C	-3.31297300	1.54767600	1.66023100
O	-1.63522300	0.94581000	-1.79486100	C	-2.84523900	1.90135000	4.53660000
O	0.73882200	-0.45992600	1.29601500	C	-4.31455800	1.03964000	2.69239500
C	0.14283800	-1.10183900	2.23005100	C	-4.25620200	1.87837200	3.96287200
O	-1.09450400	-1.34950600	2.30028200	C	-1.10948700	3.30359200	-0.10588800
O	-0.75696800	1.99995100	0.78143500	C	-2.20294100	3.02852700	-1.14102900
C	-1.75167800	2.05054500	1.58420700	C	-1.41222800	4.58568500	0.67446700
O	-2.58377900	1.12417100	1.80653400	C	-2.31096500	4.20771900	-2.10253100
C	-1.93436800	3.36097700	2.31706900	C	-1.54304400	5.76873100	-0.28483100
H	-0.99859000	3.64252300	2.80868200	C	-2.59710600	5.50436900	-1.35366300
H	-2.17487700	4.14845800	1.59494300	H	0.45856500	-1.34863000	-3.30825000
H	-2.73783500	3.27732200	3.05026600	H	1.19928300	-3.55421500	-4.16274200
C	1.02468600	-1.58365500	3.36176400	H	1.44159100	-5.47631800	-2.60403400
H	1.95239100	-2.00186900	2.96244300	H	1.03179000	-5.17942400	-0.19327100
H	1.29052600	-0.72989800	3.99550100	H	0.61728800	-4.75691800	1.81666700
H	0.49778900	-2.32471900	3.96487200	H	0.58574300	-4.06396400	4.18707000
C	-3.74485100	1.28216700	-2.81689200	H	0.37878000	-1.64029900	4.75055200
H	-3.81726400	2.36885000	-2.69514100	H	0.12748000	0.01538500	2.99862800
H	-3.27431100	1.08877900	-3.78459100	H	0.69672300	2.94796900	2.74249100
H	-4.74633900	0.85042000	-2.78517400	H	1.22202900	3.39407600	1.13023100
C	-0.85950000	-3.75950200	-1.83682300	H	3.05500100	2.13935000	2.04218100
H	-1.01152800	-3.55508600	-2.90215800	H	2.00425700	0.89070400	2.70226000
H	0.16704300	-4.11765700	-1.71416200	H	2.56341500	-1.51507000	1.52300000
H	-1.56588000	-4.52224900	-1.50658600	H	4.55195700	-1.38992100	-0.78770800
Cl	1.31611200	1.42541400	-2.81804000	H	2.90683800	-2.02048900	-0.89234500
C	3.56768300	0.26085700	-0.25495800	H	5.31484100	-0.20247100	1.47797300
C	4.80664000	0.54907800	0.37436800	H	4.13960400	-0.10086300	2.79074900
C	3.29989000	-1.03051700	-0.74440100	H	4.56464700	-3.84798000	-0.49193900
C	5.73662400	-0.49155700	0.47225200	H	3.40872200	-3.71555700	0.83602400
C	4.24390300	-2.04452500	-0.63147000	H	5.79174900	-1.93005400	3.18193400
H	2.33507300	-1.24555700	-1.19676500	H	4.14627000	-2.55810500	3.04345800
C	5.46843100	-1.76899200	-0.02136600	H	5.73182600	-3.96327300	1.72931400
H	6.69343600	-0.29267900	0.94830800	H	6.24678300	-2.54645900	0.81164000
H	4.02642400	-3.03828100	-1.01130000	H	3.19372300	1.01448400	-1.79908600
H	6.21847300	-2.54983400	0.07379300	H	3.16176500	3.45736400	0.04077300
C	5.15384400	1.90709000	0.93280100	H	1.85688900	2.99429500	-1.08660300
H	5.11341400	2.68474100	0.16323400	H	5.11690900	1.94584500	0.41336000
H	4.44569000	2.21535500	1.70851600	H	5.28710300	0.43835400	-0.48823900
H	6.16044100	1.89211800	1.36210900	H	3.31210400	4.71048700	-2.10423200
TS3 ($\nu_i = -731.94 \text{ cm}^{-1}$)				H	3.40540700	3.18917500	-2.99306600
Cl	0.49355300	1.28640100	-2.40173000	H	6.73800600	2.17368500	-1.45916000
C	0.31766600	-2.00785700	-1.26176500	H	5.50697900	1.65781000	-2.61366300
C	0.56680300	-2.19091200	-2.62512500	H	5.69872400	4.12643500	-2.65651500
C	0.98510200	-3.42571600	-3.10236900	H	5.42535300	4.20380600	-0.91450000
C	1.12852400	-4.50422600	-2.22546000	H	-1.70446100	0.50625000	2.54392500
C	0.88458800	-4.33820600	-0.87117300	H	-2.02016200	3.45485800	3.27429400
C	0.48957100	-3.08987500	-0.37372100	H	-0.82168900	2.35137800	3.95799200
C	0.36743800	-2.75920600	1.04037800	H	-3.59830400	2.57121500	1.36781000
C	0.49573900	-3.70254000	2.06642300	H	-3.35412300	0.93045700	0.74931200
C	0.48428100	-3.31882700	3.39995500	H	-2.80298700	2.52593200	5.44020400
C	0.36653500	-1.96836200	3.71118100	H	-2.56392800	0.88005700	4.84788300
C	0.22004800	-1.02608100	2.69381300	H	-5.32766000	1.04917900	2.26707900
C	0.18001000	-1.38468100	1.34010500	H	-4.08701500	-0.01380500	2.93170300
P	2.32091800	0.49206400	0.35063500	H	-4.96881500	1.50197900	4.71001700
P	-0.59229500	1.83023200	0.91620900	H	-4.56559400	2.91130200	3.72698900
C	0.93885700	2.53561200	1.75433600	H	-0.18602300	3.47177500	-0.69004700
C	2.12825800	1.57653000	1.85393600	H	-3.17493500	2.88530600	-0.64544900
C	3.32630900	-0.95402400	0.96007700	H	-1.96992600	2.10921400	-1.69238100
C	3.74826200	-1.86429800	-0.20060800	H	-2.35924200	4.46925600	1.22928500
C	4.47234000	-0.72863200	1.95021900	H	-0.63420400	4.79332300	1.42518000
C	4.24880800	-3.20012400	0.33832500	H	-3.09463100	4.01376700	-2.84824900
C	4.96212100	-2.07814400	2.47575100	H	-1.36363800	4.29732000	-2.66032600
C	5.38524100	-2.99773700	1.33428300	H	-1.77979600	6.68420100	0.27643000
				H	-0.56774600	5.94132000	-0.77062000

H	-2.65477500	6.35292700	-2.04995600	H	1.85064000	-5.17068600	2.14953600
H	-3.58652600	5.42877600	-0.86969900	H	0.94832500	-3.43934600	3.68905700
Rh	0.01900400	-0.14914900	-0.29191200	H	0.10924700	-1.31330900	2.82394600
C	-1.68820900	-1.07080000	-0.90481000	H	0.15039100	1.95838400	3.23436100
C	-2.59060900	-1.93887200	-0.09558700	H	0.69504500	2.82749000	1.81122100
C	-2.32110800	-1.10986900	-2.25660400	H	2.62759000	1.65568900	2.71425700
C	-2.67727500	-2.15040700	1.27947200	H	1.75373800	0.11836400	2.76722400
C	-3.55286800	-2.56287400	-0.92422300	H	2.92490700	-1.63573800	0.88827300
C	-2.05512000	-0.38551300	-3.41620200	H	5.06419600	-0.24226800	-0.78606400
C	-3.38258700	-2.04342500	-2.27604000	H	3.66224500	-1.10585100	-1.41729100
C	-3.64316400	-3.01801300	1.79521400	H	5.20856400	0.13030000	1.88123800
H	-2.01161500	-1.64304600	1.96740200	H	3.91719700	-0.55901700	2.86653300
C	-4.50753000	-3.42500900	-0.42290600	H	5.70201900	-2.56876300	-1.34299100
C	-2.81229300	-0.62275900	-4.56624800	H	4.42449100	-3.19396800	-0.28987200
H	-1.26255400	0.35864200	-3.42215400	H	5.96875400	-1.97280200	2.92621600
C	-4.12360900	-2.29120500	-3.41436500	H	4.58348000	-2.84096500	2.25746500
C	-4.53808700	-3.66446100	0.95391300	H	6.61903100	-3.25875500	0.88304900
H	-3.69050400	-3.17983200	2.87071400	H	6.82411600	-1.52458700	0.62866200
H	-5.23714900	-3.89593900	-1.08093400	H	3.32781300	1.84370600	-1.27523200
C	-3.82404800	-1.57358000	-4.57559500	H	2.40530300	3.67650600	0.98800900
H	-2.59725400	-0.05143500	-5.46754300	H	1.43589200	3.22841300	-0.44842700
H	-4.93471400	-3.01895500	-3.40806800	H	4.60556700	2.58539600	1.42398300
H	-5.28264400	-4.34249800	1.36836000	H	5.29560600	1.42852800	0.28652300
H	-4.39609700	-1.75315900	-5.48467900	H	2.52109100	5.42091400	-0.78305100
IM4				H	3.13317700	4.22623000	-1.92713000
Cl	0.50385400	1.63018100	-2.20433000	H	6.36262600	3.62681000	0.00409300
C	-0.24337900	-1.91568400	-2.20415100	H	5.49203500	3.15162500	-1.45529600
C	-0.19033300	-1.80198300	-3.61424900	H	5.03347300	5.53302800	-0.95846200
C	0.89423700	-2.20585900	-4.36018900	H	4.50269400	5.11897500	0.67257500
C	2.01215100	-2.75581600	-3.72855400	H	-1.81314100	-0.85742500	2.00532100
C	1.99285500	-2.91254400	-2.36028300	H	-2.04691600	1.48878100	3.96382500
C	0.89505300	-2.51365700	-1.57168800	H	-0.79060800	0.24633400	4.01467900
C	0.95127500	-2.79900200	-0.11853800	H	-3.77128700	1.48031400	2.00912700
C	1.45756700	-3.99906700	0.38164900	H	-3.64362800	0.23318700	0.75687700
C	1.46714800	-4.23105900	1.75560900	H	-2.59941000	-0.30146100	5.60108000
C	0.96379100	-3.26090600	2.61412700	H	-2.47905900	-1.52358600	4.32913000
C	0.47825900	-2.05043900	2.11003300	H	-5.45559200	-0.29975600	2.36364600
C	0.48325200	-1.79387600	0.74074300	H	-4.18900000	-1.52465300	2.40041800
P	2.34007900	0.60153700	0.48997000	H	-4.86546600	-0.92492500	4.72398800
P	-0.81342900	1.10573300	1.10855700	H	-4.50596600	0.77472400	4.41029500
C	0.52661500	1.82136100	2.21316300	H	-0.65225900	3.12825400	-0.01926200
C	1.84612700	1.06346200	2.21531100	H	-3.56952000	2.25728700	-0.11688700
C	3.58262700	-0.76628100	0.72574500	H	-2.33839900	1.91624800	-1.34245200
C	4.35695200	-1.05732500	-0.56369200	H	-2.86687400	3.34967300	2.09454500
C	4.50368100	-0.71200200	1.94881600	H	-1.18166600	3.78192000	2.39238000
C	5.13763100	-2.36055600	-0.42271900	H	-3.66132800	3.93072800	-1.93409000
C	5.29049200	-2.01661000	2.06218900	H	-1.95509600	4.31568800	-1.69966400
C	6.06744900	-2.31331400	0.78465700	H	-2.49295700	5.78724600	1.78203500
C	3.25990700	2.07987800	-0.19787600	H	-1.24422000	5.45806300	0.57761600
C	2.45511300	3.38012100	-0.07565800	H	-3.38119800	6.01973500	-0.55357200
C	4.66991500	2.32601200	0.35179300	H	-4.21378900	4.74376900	0.33714100
C	3.12212300	4.50377000	-0.86000600	Rh	0.22732200	-0.18319500	-0.46627400
C	5.35578000	3.46259900	-0.40589800	C	-1.43465400	-1.40071900	-1.47212800
C	4.54164500	4.74842900	-0.36651800	C	-2.31013800	-2.28663200	-0.62717400
C	-2.02961000	0.20342400	2.21541900	C	-2.42064800	-0.53866300	-2.19934200
C	-1.83342800	0.43335600	3.71714200	C	-2.06799800	-3.43399300	0.13476100
C	-3.49454700	0.42875800	1.82818700	C	-3.65555400	-1.87100200	-0.75730400
C	-2.75548800	-0.47306200	4.52663300	C	-2.27235900	0.40222500	-3.22385500
C	-4.40865800	-0.47394100	2.65176000	C	-3.71951000	-0.77996500	-1.70788400
C	-4.21293100	-0.25618900	4.14572300	C	-3.11726700	-4.08632400	0.77891200
C	-1.53701800	2.71495400	0.49968000	H	-1.07472900	-3.85624300	0.22843800
C	-2.63106900	2.62337200	-0.56034000	C	-4.70330400	-2.52170000	-0.11597300
C	-1.94344400	3.70042700	1.60415900	C	-3.38550500	1.09140200	-3.69832300
C	-2.87146300	3.99908800	-1.17292200	H	-1.29220000	0.64494700	-3.62033400
C	-2.19326500	5.08007300	0.99523200	C	-4.82687400	-0.07187900	-2.16171000
C	-3.24339800	5.02441100	-0.10788300	C	-4.43105800	-3.63574300	0.66747700
H	-1.06462600	-1.42098000	-4.13182700	H	-2.89708900	-4.97650000	1.36662100
H	0.86725800	-2.10745000	-5.44383400	H	-5.72737400	-2.16946300	-0.24725700
H	2.87957200	-3.06965000	-4.30635900	C	-4.65583200	0.87425800	-3.16495400
H	2.84848500	-3.36002000	-1.85455700	H	-3.25032100	1.82736100	-4.48988000
H	1.81253000	-4.76581600	-0.30873900	H	-5.81646400	-0.27315200	-1.74947500
				H	-5.23826800	-4.16299000	1.17391900

H	-5.51086400	1.43364700	-3.54195300	H	-2.34143400	4.78309800	2.61120100
TS4 ($v_i = -193.81 \text{ cm}^{-1}$)				H	-3.58333100	3.53243400	2.70112200
Cl	-1.98431700	-0.74192300	2.13989200	H	-5.38043000	4.68455200	-0.45327300
C	0.24711700	-3.09363700	1.65721100	H	-5.43852700	3.47113000	0.82781200
C	0.54716300	-3.59465300	2.92035100	H	-4.54171100	5.61031400	1.72113200
C	-0.29415500	-4.52597200	3.52071300	H	-3.28702300	5.62756300	0.48100400
C	-1.44100300	-4.96111100	2.86232600	H	2.44493600	-0.27529700	-1.71695900
C	-1.73618400	-4.48219600	1.59290500	H	2.36619500	2.21680900	-3.49606300
C	-0.89213900	-3.55436700	0.98891800	H	1.36764300	0.77430500	-3.72965900
C	-1.01230600	-3.03026200	-0.36505200	H	3.90739500	2.37406900	-1.37684300
C	-1.67514800	-3.73800000	-1.37429200	H	3.94816500	0.99992200	-0.26207900
C	-1.54090000	-3.38569500	-2.71082000	H	3.34807200	0.68188500	-5.19906900
C	-0.66596900	-2.35538100	-3.04327700	H	3.41452000	-0.61775900	-4.00044400
C	-0.00173300	-1.64628600	-2.04514700	H	5.93409500	1.05027500	-1.76324600
C	-0.24245000	-1.88814100	-0.68435800	H	4.98023000	-0.41615400	-2.00081300
P	-2.09616400	0.88345200	-0.52738100	H	5.63934000	0.51020800	-4.19674500
P	0.98462800	1.41407000	-0.81400400	H	4.89489300	2.06147800	-3.80018600
C	-0.21126800	2.28053100	-1.98458500	H	0.44265600	3.21735700	0.50417900
C	-1.49254300	1.49363600	-2.17195400	H	3.31868000	2.51489400	1.17271800
C	-3.43538600	-0.36680200	-0.94788100	H	1.87778400	1.88006000	1.97516100
C	-4.63108500	-0.35466800	0.01158600	H	3.01767300	3.99880000	-0.93437600
C	-3.92944800	-0.34369500	-2.40023400	H	1.40296200	4.31939800	-1.56511500
C	-5.52170300	-1.56476200	-0.25023400	H	2.80885700	3.83267800	3.20324900
C	-4.85756300	-1.52862300	-2.66589200	H	1.16946100	4.14352000	2.62610500
C	-6.02288800	-1.57538300	-1.68750000	H	2.27071100	6.28171700	-0.31612700
C	-2.99936800	2.28313000	0.30721600	H	0.84283000	5.61838500	0.48307400
C	-2.11671500	3.18782600	1.16556800	H	2.61191300	6.12087300	2.16171100
C	-3.88353300	3.12378800	-0.61691300	H	3.75574900	5.10182200	1.28623800
C	-2.97914600	4.12984500	1.99843200	Rh	-0.28329300	-0.08809500	0.46508600
C	-4.75118400	4.07218300	0.20795800	C	1.09202300	-2.06946400	0.96569100
C	-3.90033500	4.95960000	1.11061200	C	2.24367500	-2.54623700	0.13693200
C	2.46535200	0.82274600	-1.84262700	C	1.73244000	-1.06770000	1.87941200
C	2.33672600	1.12326400	-3.33892000	C	2.29684900	-3.54451200	-0.83445400
C	3.83343400	1.27795800	-1.32106000	C	3.41666300	-1.84350200	0.47563900
C	3.47168600	0.47790900	-4.12615100	C	1.23942200	-0.46267200	3.04668000
C	4.97235400	0.67547400	-2.14280600	C	3.11257400	-0.94446100	1.57389500
C	4.82163700	0.97369800	-3.62762700	C	3.50430800	-3.81061500	-1.47040800
C	1.45308200	2.95000600	0.15324300	H	1.40544100	-4.11330200	-1.09739800
C	2.26911700	2.74013100	1.41946300	C	4.62736100	-2.12279200	-0.15596100
C	1.97029900	4.15885600	-0.63631800	C	2.10734400	0.27587000	3.84952700
C	2.21172200	3.98890200	2.29292200	H	0.20108700	-0.60474100	3.33992200
C	1.89988100	5.40920900	0.24031500	C	3.96404600	-0.19202700	2.37575300
C	2.68704400	5.22219600	1.53358600	C	4.66334700	-3.10267800	-1.13943500
H	1.44092100	-3.25056900	3.44076000	H	3.54912800	-4.58964400	-2.22983800
H	-0.05509900	-4.90973400	4.51122500	H	5.53355700	-1.58031300	0.11884400
H	-2.10879500	-5.67482200	3.34204300	C	3.45497700	0.42295800	3.51598100
H	-2.64262600	-4.80827700	1.08242500	H	1.72292400	0.73765100	4.75803000
H	-2.25361900	-4.62171700	-1.10245000	H	5.02731700	-0.12537100	2.14002800
H	-2.06043800	-3.94717100	-3.48551300	H	5.60078700	-3.33045400	-1.64509000
H	-0.48915200	-2.09474400	-4.08739300	H	4.11394900	1.00278800	4.16115200
H	0.69445200	-0.87171100	-2.35207400	Pro			
H	0.25794100	2.51841600	-2.94632100	C	-2.28998100	-0.50822400	-0.52610200
H	-0.44054400	3.24419600	-1.50791200	C	-0.96072100	-0.81737700	-0.84591500
H	-2.25711500	2.07714800	-2.70383400	C	0.00000000	0.00002900	-0.00002600
H	-1.29522100	0.59053900	-2.76677400	C	-0.96072600	0.81743500	0.84585800
H	-2.91339000	-1.32547900	-0.79733300	C	-2.28998400	0.50822500	0.52608800
H	-5.22509000	0.56503000	-0.13890700	C	0.96076600	0.84587600	-0.81740100
H	-4.28345100	-0.36675600	1.05122700	C	2.29001200	0.52604500	-0.50819700
H	-4.46819200	0.59904600	-2.60418500	C	2.28995400	-0.52614600	0.50825100
H	-3.08956400	-0.39466000	-3.10620100	C	0.96068100	-0.84589800	0.81741100
H	-6.36388900	-1.57054400	0.45573400	C	-3.33681500	-1.14417100	-1.18522200
H	-4.93671700	-2.48020000	-0.05037100	C	-3.03700400	-2.08877200	-2.16240000
H	-5.22100300	-1.48925500	-3.70300100	C	-1.71259900	-2.39363000	-2.47726900
H	-4.26606500	-2.45541600	-2.57390800	C	-0.66235400	-1.75673100	-1.81779700
H	-6.64730400	-2.45950600	-1.87933000	C	-0.66236400	1.75685000	1.81768300
H	-6.66899900	-0.69499300	-1.84925200	C	-1.71261400	2.39373700	2.47715700
H	-3.65469100	1.74216200	1.01007300	C	-3.03701700	2.08881600	2.16233800
H	-1.46359700	3.80022600	0.51616300	C	-3.33682300	1.14416300	1.18521000
H	-1.46425900	2.57529000	1.80789400	C	3.33676500	-1.18528400	1.14422000
H	-3.24667700	3.71620300	-1.29795300	C	3.03691700	-2.16242100	2.08884900
H	-4.51465800	2.48595800	-1.25403500	C	1.71249900	-2.47722700	2.39371700

C	0.66227800	-1.81773300	1.75680200	H	-3.84495700	2.59551800	2.68771400
C	0.66243900	1.81774700	-1.75677800	H	-4.37284700	0.90867800	0.94186500
C	1.71271300	2.47720300	-2.39364500	H	4.37279800	-0.94194400	0.90876700
C	3.03710400	2.16232400	-2.08873100	H	3.84483500	-2.68780900	2.59557300
C	3.33687300	1.18515300	-1.14410900	H	1.49788600	-3.24446000	3.13566700
H	-4.37284200	-0.90872900	-0.94184300	H	-0.37524000	-2.05999400	1.99031200
H	-3.84493900	-2.59548100	-2.68777500	H	-0.37507000	2.06004100	-1.99029100
H	-1.49802200	-3.13555300	-3.24453800	H	1.49817900	3.24446900	-3.13558500
H	0.37516100	-1.99021600	-2.06009600	H	3.84506000	2.68768900	-2.59541700
H	0.37514900	1.99038500	2.05994000	H	4.37289100	0.94177000	-0.90863400
H	-1.49804400	3.13570400	3.24438700				

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