Supporting Information

Palladium-Catalyzed [3+2] Annulation of Alkynes with Concomitant Aromatic Ring Expansion: A Concise Approach to (Pseudo)azulenes

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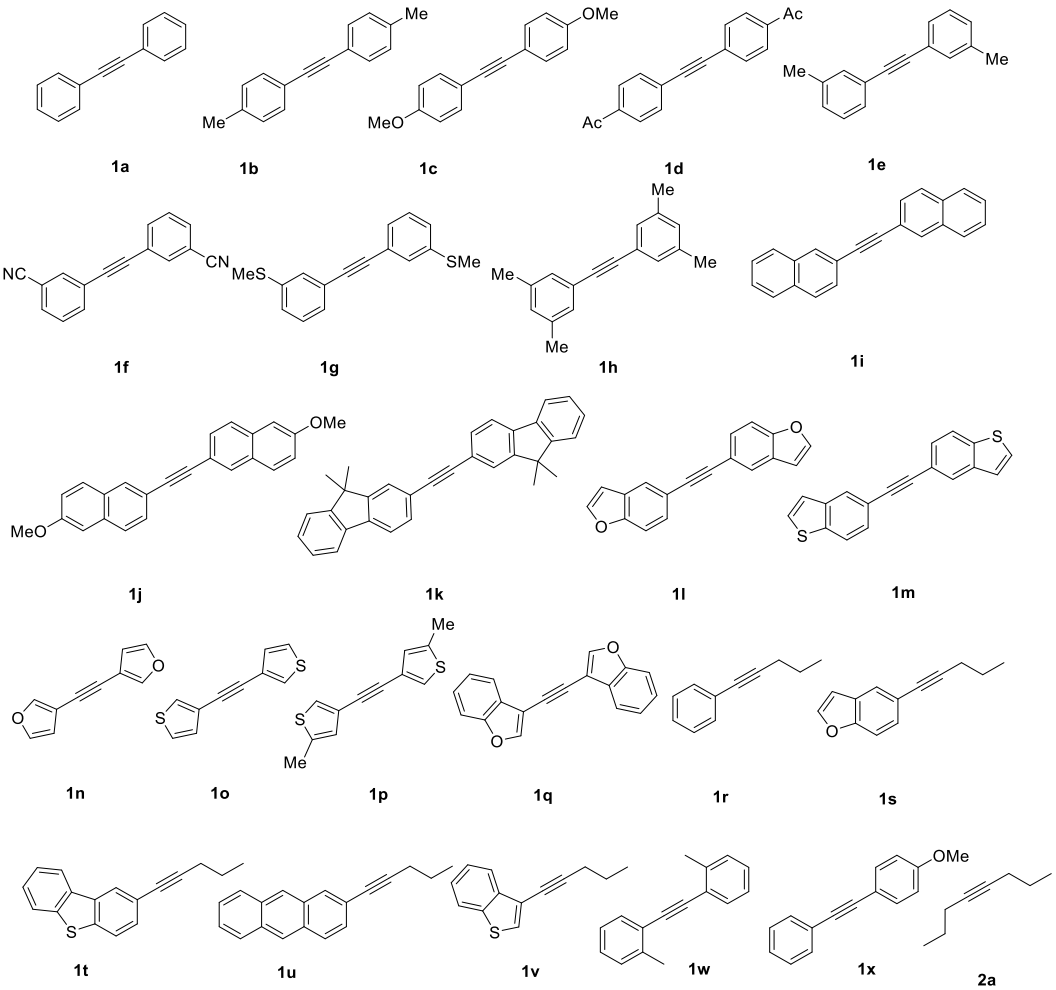
Content

I. General remarks

NMR spectra were recorded on an Agilent 400-MR DD2 spectrometer. The ^{1}H NMR (400 MHz) chemical shifts were recorded relative to $CDCl_3$ as the internal reference ($CDCl_3$: $\delta = 7.26$ ppm). The ^{13}C NMR (100 MHz) chemical shifts were given using $CDCl_3$ as the internal standard ($CDCl_3$: $\delta = 77.16$ ppm). X-Ray single-crystal diffraction data were obtained on an Agilent Technologies Gemini plus single crystal diffraction. High-resolution mass spectra (HRMS) were obtained with a Shimadzu LCMS-IT-TOF (ESI). Unless otherwise noted, all reagents were obtained from commercial suppliers. $Pd(acac)_2$ was prepared according to the literature procedures.[1] The boron reagents, Pd-catalyst and the synthetic aryl alkynes were dried with P_2O_5 in vacuum oven and stored in glovebox. The solvents were purified using an Innovative Technology PS-MD-5 Solvent Purification System, and the 2-methyltetrahydrofuran was redistilled with sodium silk and stored with molecular sieve in glovebox.

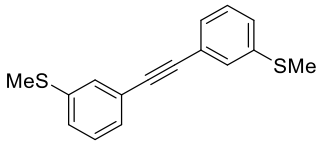
II. Preparation of the alkynes

List of alkyne substrates



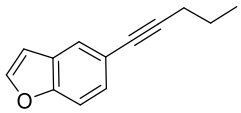
Compound **1a** was purchased from Energy Chemical, and compounds **1r** and **2a** were purchased from Tokyo Chemical Industry (TCI) without further purification. Compounds **1b**[2], **1c**[2], **1d**[3], **1e**[2], **1f**[3], **1g**[2], **1h**[2],

1i[2], **1j**[2], **1k**[2], **1l**[3], **1m**[3], **1n**[3], **1o**[3], **1p**[3], **1q**[3], **1s**[4], **1t**[4], **1u**[4], **1v**[4] and **1w**[2] were prepared according to the literature. The ^{1}H NMR and ^{13}C NMR data were in accordance with the reported data. The following compounds have not been reported.



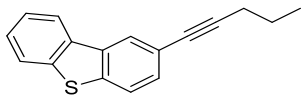
1,2-Bis(3-(methylthio)phenyl)ethyne (1g)

The titled compound was synthesized according to the literature.[2] 3-Bromothioanisole (538.0 μL, 2 mmol) and propiolic acid (123.1 μL, 4 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether/ dichloromethane = 10:1) afforded **1g** as a white solid (329.4 mg, 61% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.40 (s, 2H), 7.31 – 7.28 (m, 3H), 7.24 – 7.21 (m, 3H), 2.50 (s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 139.1, 129.2, 128.8, 128.3, 126.7, 123.9, 89.4, 15.8.



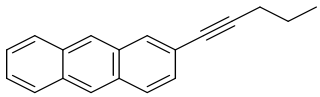
5-(Pent-1-yn-1-yl)benzofuran (1s)

The titled compound was synthesized according to the literature.[4] 5-Bromobenzofuran (250.5 μL, 2 mmol) and 1-pentyne (236.6 μL, 2.4 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **1s** as brownness oil (239.2 mg, 65% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.66 (s, 1H), 7.61 (d, J = 2.4 Hz, 1H), 7.42 – 7.40 (m, 1H), 7.36 – 7.33 (m, 1H), 6.72 – 6.71 (m, 1H), 2.40 (t, J = 7.2 Hz, 2H), 1.70 – 1.60 (m, 2H), 1.07 (t, J = 7.6 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 154.3, 145.7, 128.1, 127.6, 124.6, 118.7, 111.4, 106.6, 88.8, 81.0, 22.4, 21.5, 13.7.



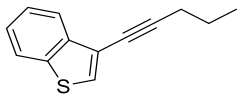
2-(Pent-1-yn-1-yl)dibenzo[b,d]thiophene (1t)

The titled compound was synthesized according to the literature.[4] 2-Bromodibenzothiophene (526.3 mg, 2 mmol) and 1-pentyne (236.6 μL, 2.4 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **1t** as white solid (210.0 mg, 42% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.01 (s, 1H), 7.92 (d, J = 7.6 Hz, 1H), 7.56 (d, J = 8.4 Hz, 1H), 7.52 – 7.44 (m, 3H), 7.34 (t, J = 7.6 Hz, 1H), 2.43 (t, J = 7.2 Hz, 2H), 1.72 – 1.63 (m, 2H), 1.09 (t, J = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 156.7, 155.5, 130.9, 127.6, 124.5, 124.0, 123.9, 123.1, 120.9, 118.8, 111.9, 111.7, 89.3, 80.8, 22.5, 21.6, 13.8.



2-(Pent-1-yn-1-yl)anthracene (1u)

The titled compound was synthesized according to the literature.[4] 2-Bromoanthracene (514.3 mg, 2 mmol) and 1-pentyne (236.6 μL, 2.4 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **1s** as a yellow solid (384.5. mg, 79% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.35 (d, J = 8.8 Hz, 2H), 8.08 (s, 1H), 8.01 – 7.96 (m, 2H), 7.91 (d, J = 8.8 Hz, 1H), 7.48 – 7.44 (m, 2H), 7.42 (dd, J = 8.8, 1.2 Hz, 1H), 2.47 (t, J = 7.2 Hz, 2H), 1.70 (h, J = 7.2 Hz, 2H), 1.11 (t, J = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 132.14, 132.05, 131.4, 131.3, 130.6, 128.34, 128.30, 128.25, 128.17, 126.3, 126.1, 125.74, 125.72, 121.0, 91.5, 81.5, 22.4, 21.7, 13.8.

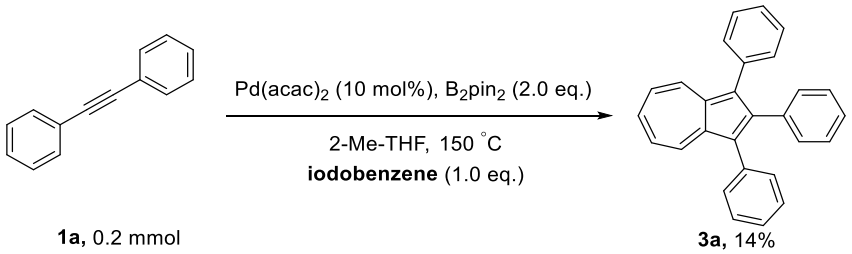


3-(Pent-1-yn-1-yl)benzo[b]thiophene (1v)

The titled compound was synthesized according to the literature.[4] 3-Bromo-1-benzothiophene (462.2 mg, 2 mmol) and 1-pentyne (236.6 μL, 2.4 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **1s** as brownness oil (256.1 mg, 64% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.94 (d, J = 8.0 Hz, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.51 (s, 1H), 7.46 – 7.36 (m, 2H), 2.49 (t, J = 7.2 Hz, 2H), 1.71 (h, J = 7.2 Hz, 2H), 1.11 (t, J = 7.6 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 139.6 138.9, 128.6, 125.0, 124.6, 123.2, 122.7, 119.2, 93.0, 74.4, 22.5, 21.7, 13.8.

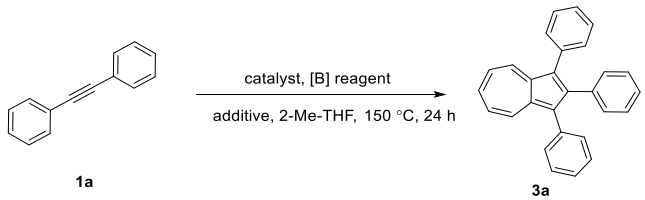
III. Optimization of the reaction conditions

Reaction discovery



A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with alkyne **1a** (0.2 mmol, 1.0 equiv), iodobenzene (0.2 mmol, 1.0 equiv), $Pd(acac)_2$ (10.0 mol%), B_2pin_2 (2.0 equiv) and 2-Me-THF (1.0 mL) under N_2 The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether) to provide the 1,2,3-triphenylazulene **3a** (5.1 mg, 14%).

Condition optimization:

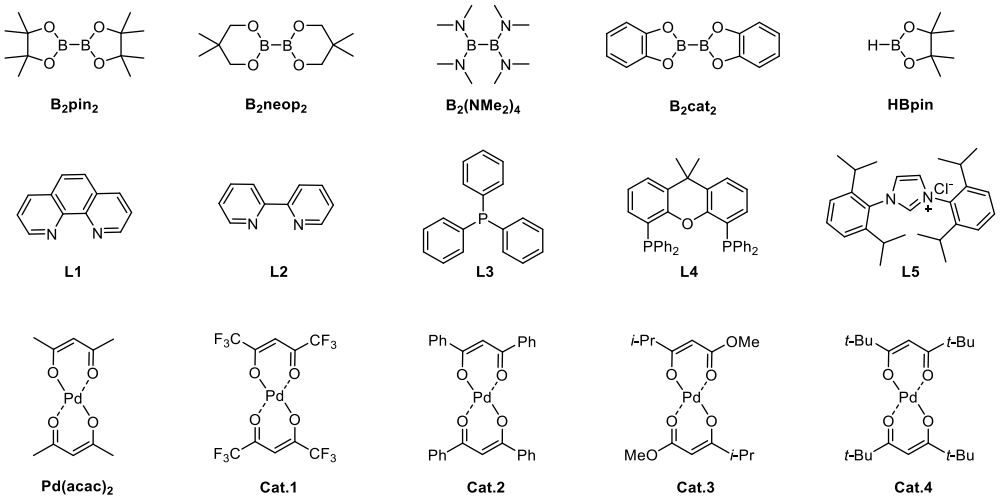


A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with alkyne **1a** (0.2 mmol, 1.0 equiv), catalyst (10.0 mol%), [B] reagent (2.0 equiv), additive (3.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel to provide the desired product **3a**.

Table S1. Optimization of the reaction conditions[a]

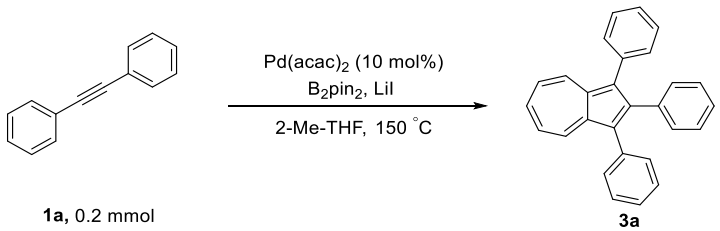
Entry	Catalyst (10 mol%)	[B] (2.0 equiv)	Additive (3.0 equiv)	Yield (%)
1	$Pd(acac)_2$	B_2pin_2	KI	12
2	$Pd(acac)_2$	B_2pin_2	Cs_2CO_3	n.d.
3	$Pd(acac)_2$	B_2pin_2	KO^tBu	n.d.
4	$Pd(acac)_2$	B_2pin_2	LiO^tBu	n.d.
5	$Pd(acac)_2$	B_2pin_2	K_3PO_4	n.d.
6	$Pd(acac)_2$	B_2pin_2	LiBr	n.d.
7	$Pd(acac)_2$	B_2pin_2	LiCl	n.d.
8	$Pd(acac)_2$	B_2pin_2	I_2	12
9	$Pd(acac)_2$	B_2pin_2	Bu_4NI, TMSI, NiI_2 or CuI	n.d.
10	**$Pd(acac)_2$**	**B_2pin_2**	**LiI**	**62**
11	$Pd(CH_3CN)Cl_2$	B_2pin_2	LiI	21
12	$PdCl_2$	B_2pin_2	LiI	trace
13	$Pd(OAc)_2$	B_2pin_2	LiI	n.d.
14	$Pd(PPh_3)_2Cl_2$	B_2pin_2	LiI	n.d.
15	$Pd(allyl)Cl_2$	B_2pin_2	LiI	n.d.
16	Cat. **1**	B_2pin_2	LiI	51
17	Cat. **2**	B_2pin_2	LiI	46
18	Cat. **3**	B_2pin_2	LiI	42
19	Cat. **4**	B_2pin_2	LiI	Trace
20	$PdCl_2$+**L1**, **L2**, **L3**, **L4** or **L5**	B_2pin_2	LiI	n.d.
21	$Cu(acac)_2$ $Ni(acac)_2$ or $Fe(acac)_3$	B_2pin_2	LiI	n.d.

22	$Pd(acac)_2$	B_2neop_2	LiI	12
23	$Pd(acac)_2$	$B_2(NMe_2)_4$, B_2cat_2 or HBpin	LiI	n.d.
24[b]	$Pd(acac)_2$	B_2pin_2	LiI	52
25[c]	$Pd(acac)_2$	B_2pin_2	LiI	28
26[d]	$Pd(acac)_2$	B_2pin_2	LiI	50
27	-	B_2pin_2	LiI	n.d.
28	$Pd(acac)_2$	-	LiI	n.d.
29	$Pd(acac)_2$	B_2pin_2	-	n.d.



[a]Reaction conditions: **1a** (0.2 mmol), catalyst (10 mol %), boron reagent [B] (2.0 equiv), additive (3.0 equiv) in 2-Me-THF (1 mL) at 150 °C under N_2 for 24 h. [b]THF was used as the solvent. [c]1,4-Dioxane was used as the solvent. [d]CH_3CN was used as the solvent. TMSI = iodotrimethylsilane. n.d. = not detected.

Table S2. The effect of the equivalents of B_2pin_2 and LiI on the reaction[a]



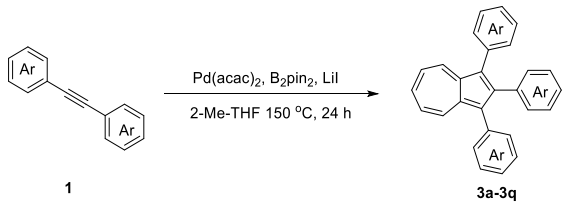
Entry	B_2pin_2 (equiv)	LiI (equiv)	Yield (%)
1	0	3.0	0
2	0.2	3.0	30
3	0.5	3.0	46

4	1.0	3.0	54
5	2.0	0	0
6	2.0	0.2	15
7	2.0	0.5	32
8	2.0	1.0	44

[a]Reaction conditions: **1a** (0.2 mmol), $Pd(acac)_2$ (10 mol %), LiI and B_2pin_2 in 2-Me-THF (1 mL) at 150 °C under N_2 for 24 h.

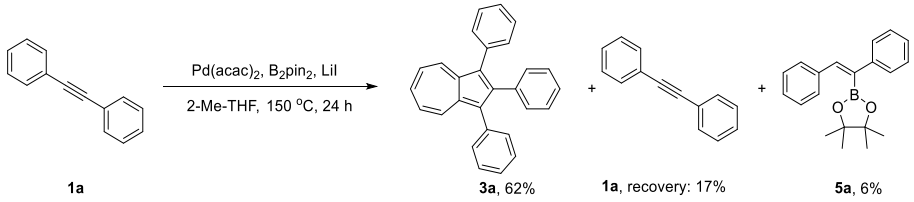
IV. General procedure for the annulation of alkynes to synthesize (pseudo)azulenes

General procedure I: the homo annulation to synthesize 3a-3q



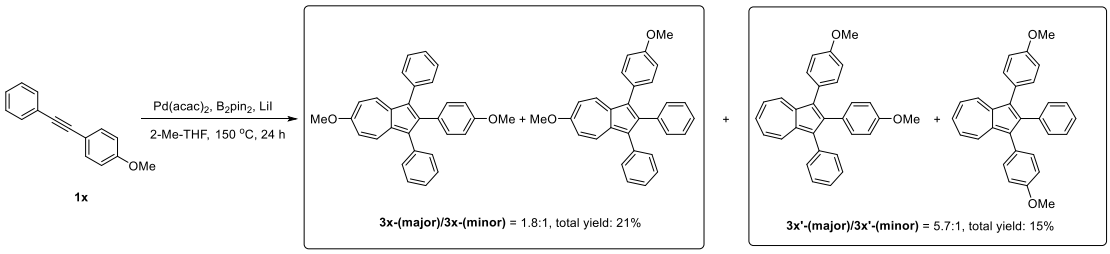
A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with alkyne **1** (0.2 mmol, 1.0 equiv), $Pd(acac)_2$ (10.0 mol%), B_2pin_2 (2.0 equiv), LiI (3.0 equiv) and 2-Me-THF (1.0 mL) under N_2 The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel to provide the desired product.

Scheme S1 Homo-annulation of 1a



A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with 1,2-diphenylethyne **1a** (0.2 mmol, 35.6 mg), $Pd(acac)_2$ (10.0 mol%), B_2pin_2 (2.0 equiv), LiI (3.0 equiv) and 2-Me-THF (1.0 mL) under N_2 The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether) to provide **1a** (6.0 mg, substrate recovery: 17%) and **3a** (22.1 mg, 62% yield). Then the eluent was changed to petroleum ether/dichloromethane (5:1) to provide **5a** (3.7 mg, 6%).

Scheme S2. Homo-annulation of 1x



A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with 1-methoxy-4-(phenylethynyl)benzene **1x** (0.2 mmol, 41.6 mg), $Pd(acac)_2$ (10.0 mol%), B_2pin_2 (2.0 equiv), LiI (3.0 equiv) and 2-Me-THF (1.0 mL) under N_2 The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/dichloromethane = 8:1) to provide the unseparated mixture of **3x-(major)** and **3x-(minor)** (8.7 mg, **3x-(major)**: **3x-(minor)** = 1.8:1, total yield: 21%), and the unseparated mixture of **3x'-(major)** and **3x'-(minor)** (6.3 mg, **3x'-(major)**: **3x'-(minor)** = 5.7:1, total yield: 15%). HRMS (ESI^+) m/z, **3x-(major)** and **3x-(minor)**: $[M+H]^+$ calcd for $C_{30}H_{25}O_2^+$ 417.1849; found 417.1849; **3x'-(major)** and **3x'-(minor)**: $[M+H]^+$ calcd for $C_{30}H_{25}O_2^+$ 417.1849; found 417.1847.

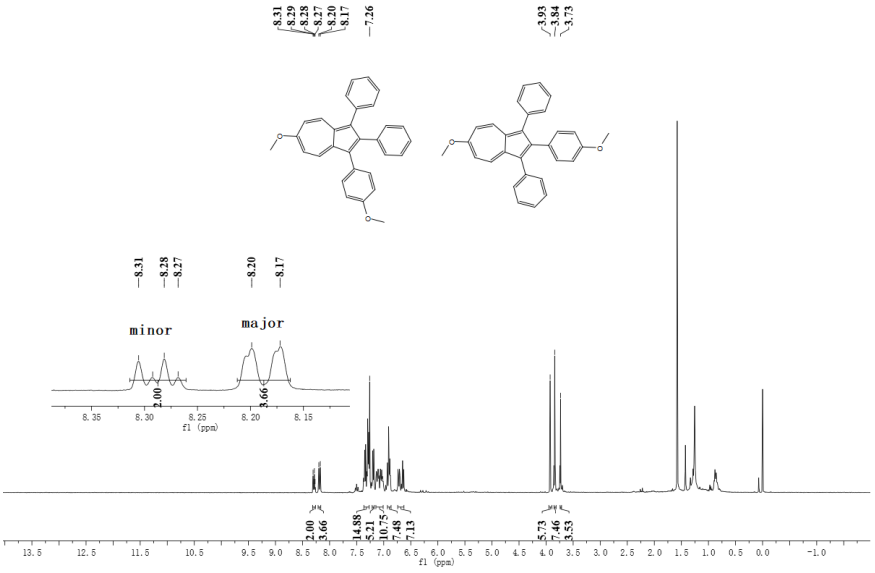


Figure S1. Copy of ^1H NMR spectrum of mixture **3x-(major)** and **3x-(minor)**.

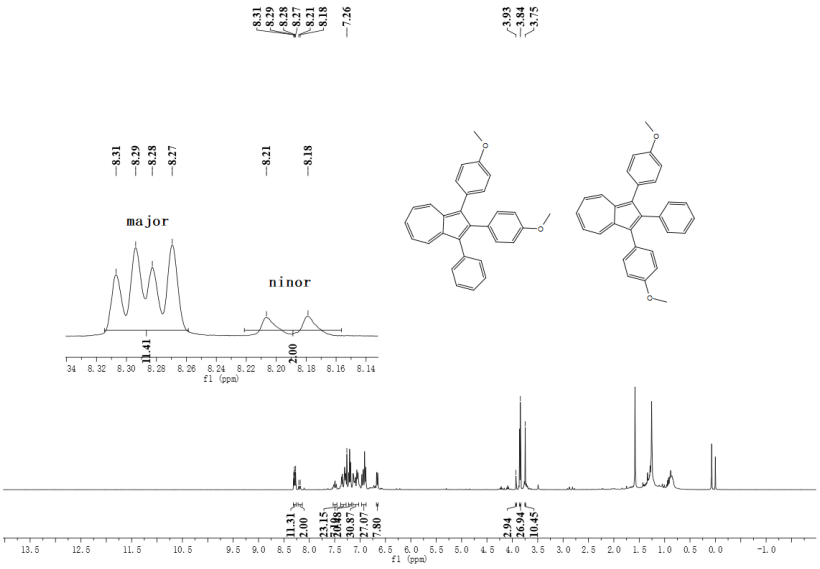
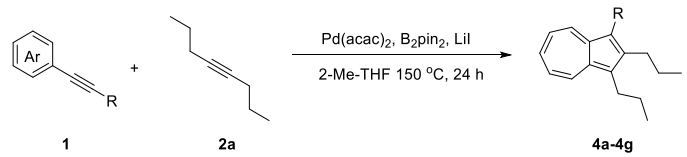


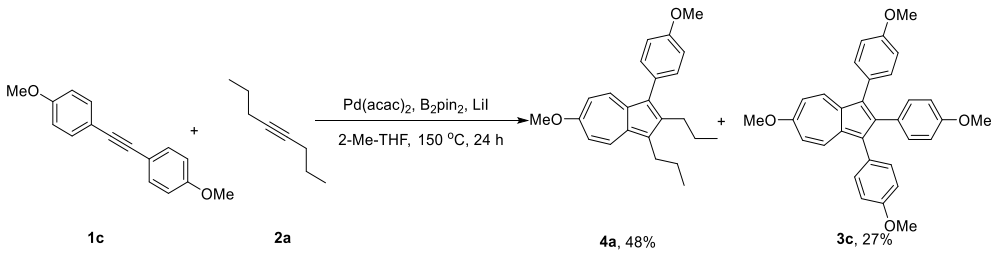
Figure S2. Copy of ^{1}H NMR spectrum of the mixture of **3x'-(major)** and **3x'-(minor)**.

General procedure II: the cross annulation to synthesize for 4a-4g



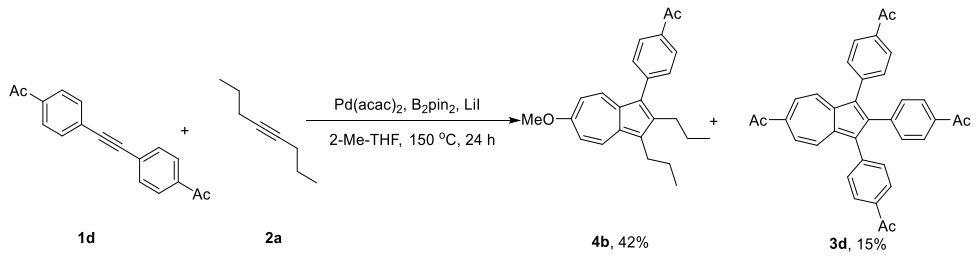
A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with alkyne **1** (0.1 mmol, 1.0 equiv), 4-octyne **2a** (0.3 mmol, 3 equiv), $Pd(acac)_2$ (20.0 mol%), B_2pin_2 (4.0 equiv), LiI (6.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h or 48 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel to provide the desired product.

Scheme S3. Cross-annulation of 1c and 2a



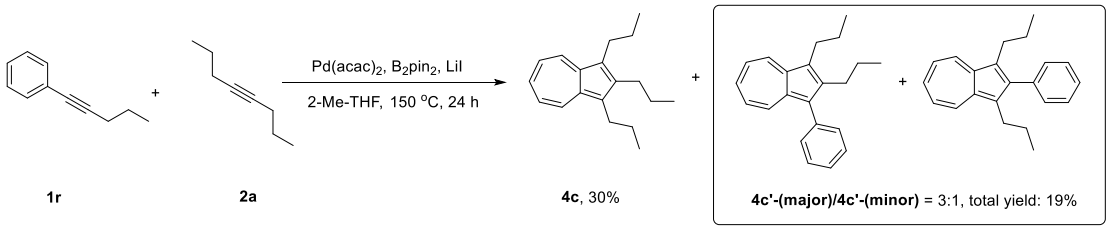
A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with 1,2-bis(4-methoxyphenyl)ethyne **1c** (0.1 mmol, 23.8 mg), 4-octyne **2a** (0.3 mmol, 3 equiv), $Pd(acac)_2$ (20.0 mol%), B_2pin_2 (4.0 equiv), LiI (6.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 8:1) to afforded **4a** (16.6 mg, 48% yield) and **3c** (6.4 mg, 27% yield).

Scheme S4. Cross-annulation of 1d and 2a



A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with 1,2-bis(4-acetylphenyl)ethyne **1d** (0.1 mmol, 26.2 mg), 4-octyne **2a** (0.3 mmol, 3 equiv), $Pd(acac)_2$ (20.0 mol%), B_2pin_2 (4.0 equiv), LiI (6.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 8:1) to afforded **4b** (15.6 mg, 42% yield) and **3d** (3.9 mg, 15% yield).

Scheme S5. Cross-annulation of 1r and 2a



A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with pent-1-yn-1-ylbenzene **1r** (0.1 mmol, 16.0 μL), 4-octyne **2a** (0.3 mmol, 3 equiv), $Pd(acac)_2$ (20.0 mol%), B_2pin_2 (4.0 equiv), LiI (6.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether) to afforded **4c** (7.5 mg, 30% yield) and the unseparated mixture of **4c'-(major)** and **4c'-(minor)** (2.7 mg, **4c'-(major)**:**4c'-(minor)** = 3:1, total yield: 19%). HRMS (ESI^+) (**4c'-(major)** and **4c'-(minor)**) m/z: $[M+H]^+$ calcd for $C_{22}H_{25}^+$ 289.1951; found 289.1951.

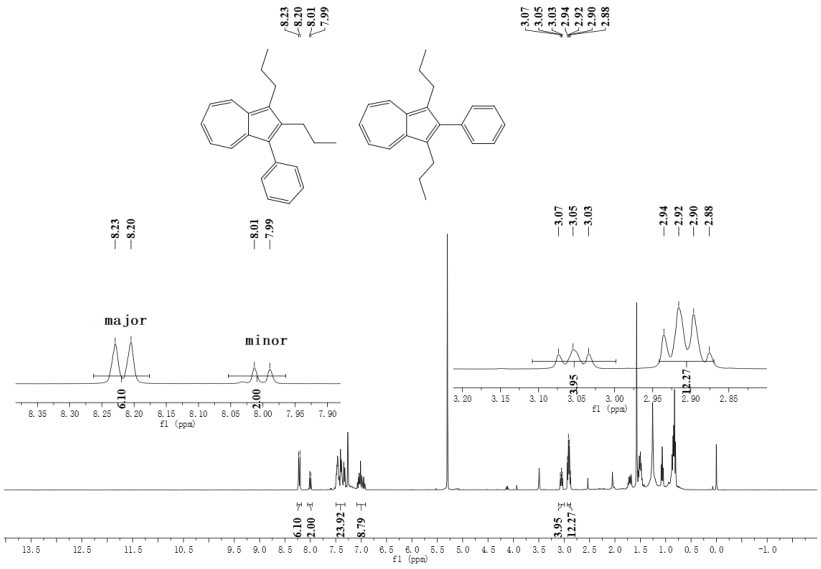
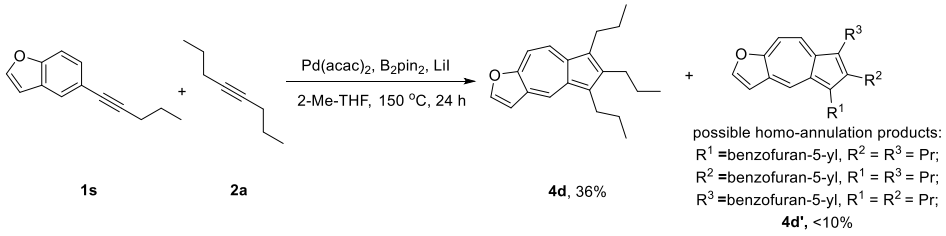


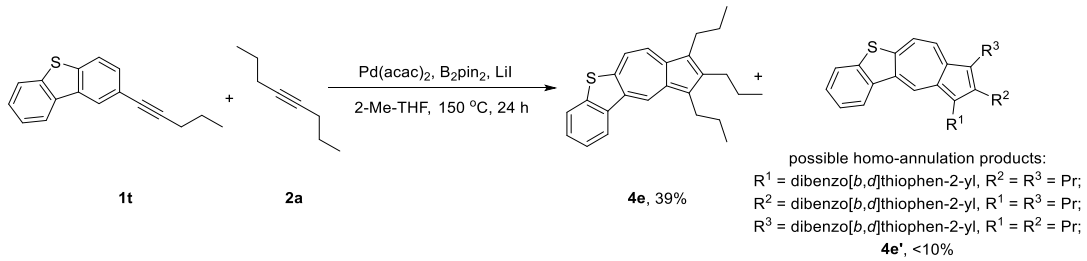
Figure S3. Copy of ^{1}H NMR spectrum of the mixture of **4c'-(major)** and **4c'-(minor)**.

Scheme S6. Cross-annulation of 1s and 2a



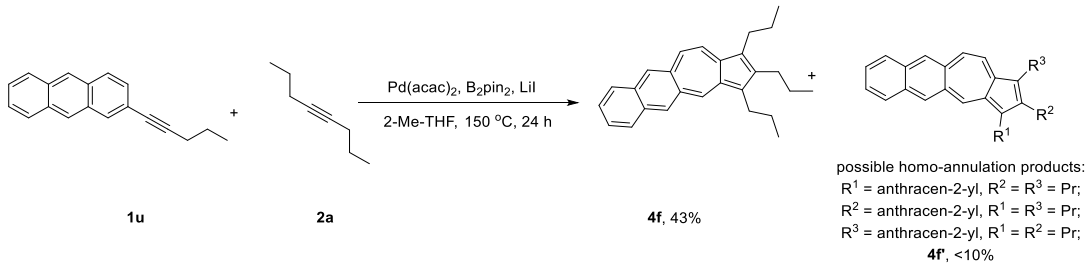
A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with 5-(pent-1-yn-1-yl)benzofuran **1s** (0.1 mmol, 18.4 mg), 4-octyne **2a** (0.3 mmol, 3 equiv), $Pd(acac)_2$ (20.0 mol%), B_2pin_2 (4.0 equiv), LiI (6.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 ºC for 48 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether) to afforded **4d** (10.5 mg, 36% yield). The homo-annulation products **4d'** (less than 10% yield) could not be completely purified owing to the unseparated uncertain impurities, the corresponding molecular weight peak of **4d'** was detected by high resolution mass spectrometry (HRMS) analysis. HRMS (ESI^+) for **4d'**, m/z: $[M+H]^+$ calcd for $C_{26}H_{25}O_2^+$ 369.1849; found 369.1847.

Scheme S7. Cross-annulation of 1t and 2a



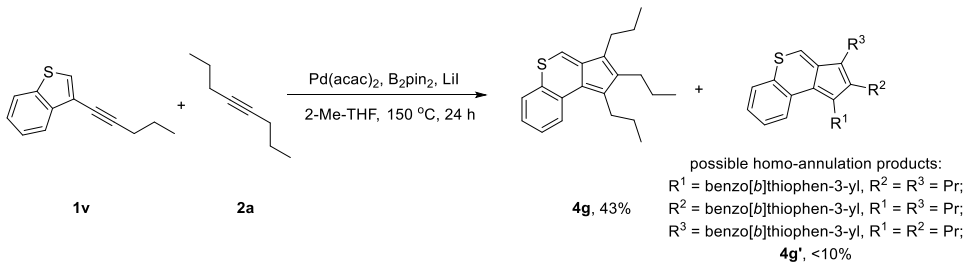
A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with 2-(pent-1-yn-1-yl)dibenzo[*b,d*]thiophene **1t** (0.1 mmol, 25.0 mg), 4-octyne **2a** (0.3 mmol, 3 equiv), $Pd(acac)_2$ (20.0 mol%), B_2pin_2 (4.0 equiv), LiI (6.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether) to afforded **4e** (15.6 mg, 39% yield). The homo-annulation products **4e'** (less than 10% yield) could not be completely purified owing to the unseparated uncertain impurities, the corresponding molecular weight peak of **4e'** was detected by high resolution mass spectrometry (HRMS) analysis. HRMS (ESI^+) for **4e'**, m/z: $[M+H]^+$ calcd for $C_{34}H_{29}S_2^+$ 501.1705; found 501.1707.

Scheme S8. Cross-annulation of 1u and 2a



A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with 2-(pent-1-yn-1-yl)anthracene **1u** (0.1 mmol, 24.4 mg), 4-octyne **2a** (0.3 mmol, 3 equiv), $Pd(acac)_2$ (20.0 mol%), B_2pin_2 (4.0 equiv), LiI (6.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 48 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether) to afforded **4f** (15.1 mg, 43% yield). The homo-annulation products **4f'** (less than 10% yield) could not be completely purified owing to the unseparated uncertain impurities, the corresponding molecular weight peak of **4f'** was detected by high resolution mass spectrometry (HRMS) analysis. HRMS (ESI^+) for **4f'**, m/z: $[M+H]^+$ calcd for $C_{38}H_{33}^+$ 489.2577; found 489.2577.

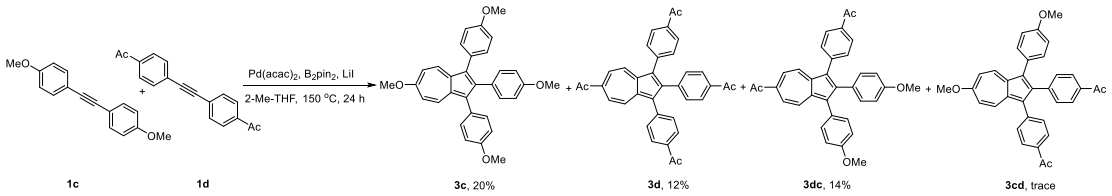
Scheme S9. Cross-annulation of 1v and 2a



A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with 3-(pent-1-yn-1-yl)benzo[*b*]thiophene **1v** (0.1 mmol, 20.0 mg), 4-octyne **2a** (0.3 mmol, 3 equiv), $Pd(acac)_2$ (20.0 mol%), B_2pin_2 (4.0 equiv), LiI (6.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 48 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by

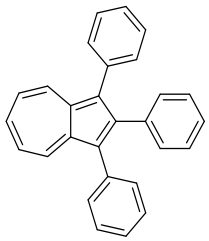
column chromatography on silica gel (petroleum ether) to afforded **4g** (9.2 mg, 30% yield). The homo-annulation products **4g'** (less than 10% yield) could not be completely purified owing to the unseparated uncertain impurities, the corresponding molecular weight peak of **4g'** was detected by high resolution mass spectrometry (HRMS) analysis. HRMS (ESI^+) for **4g'** m/z: $[M+H]^+$ calcd for $C_{26}H_{25}S_2^+$ 401.1392; found 401.1390.

Scheme S10. Competition experiment between 1c and 1d



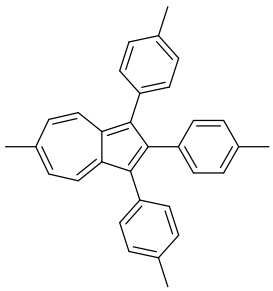
The competition experiment between 1c and 1d: A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with 1,2-bis(4-methoxyphenyl)ethyne **1c** (0.1 mmol, 23.8 mg), 1,2-bis(4-acetylphenyl)ethyne **1d** (0.1 mmol, 26.2 mg), $Pd(acac)_2$ (20.0 mol%), B_2pin_2 (4.0 equiv), LiI (6.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/dichloromethane = 4:1) to afforded **3c** (4.8 mg, 20% yield), **3d** (3.1 mg, 12%) and **3dc** (7.1 mg, 14%). Only trace amounts of across-annulation product **3cd** were detected.

V. Preparation and characterization of the described substances



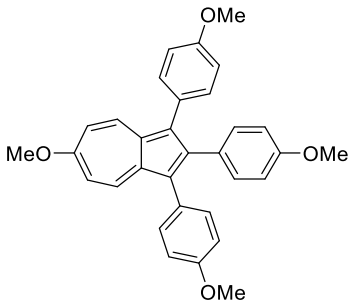
1,2,3-Triphenylazulene (3a)

Following the general procedure I. 1,2-Diphenylethyne (35.6mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **3a** as a blue solid (22.1 mg, 62% yield). When 1,2-diphenylethyne (356.2 mg, 2.0 mmol) was used, **3a** was obtained in 48% yield (171.0 mg). ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.36 (d, J = 9.6 Hz, 2H), 7.55 (t, J = 9.6 Hz, 1H), 7.39 – 7.35 (m, 4H), 7.32 – 7.30 (m, 6H), 7.14 – 7.10 (m, 5H), 7.06 – 7.04 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 148.1, 138.2, 137.4, 136.5, 136.4, 136.0, 131.7, 131.5, 129.1, 128.2, 127.7, 126.7, 126.4, 123.9. HRMS (ESI^+) m/z: $[M+H]^+$ calcd for $C_{28}H_{21}^+$ 357.1638; found 357.1634.



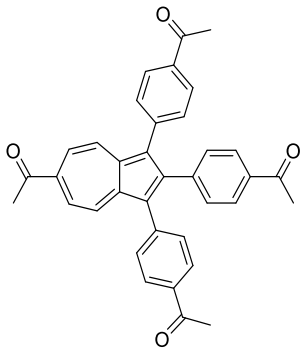
6-Methyl-1,2,3-tri-*p*-tolylazulene (3b)

Following the general procedure I. 1,2-Di-*p*-tolylethyne (41.2 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **3b** as a blue solid (28.9 mg, 70% yield). M.p.: ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.16 (d, J = 8 Hz, 2H), 7.16 (s, 8H), 6.97 (d, J = 12 Hz, 2H), 6.92 (s, 4H), 2.58 (s, 3H), 2.39 (s, 6H), 2.27 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 149.5, 146.5, 136.02, 135.99, 135.7, 134.9, 133.7, 133.6, 131.5, 131.4, 129.0, 128.9, 128.5, 125.1, 28.0, 21.4. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{32}H_{29}^+$ 413.2264; found 413.2264.



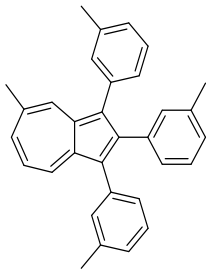
6-Methoxy-1,2,3-tris(4-methoxyphenyl)azulene (3c)

Following the general procedure I. 1,2-Bis(4-methoxyphenyl)ethyne (47.6 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether / ethyl acetate = 5:1) afforded **3c** as a purple blue solid (34.9 mg, 73% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.14 (dt, J = 11.2, 1.2 Hz, 2H), 7.21 – 7.18 (m, 4H), 7.96 – 6.88 (m, 6H), 6.69 – 6.65 (m, 4H), 3.92 (s, 3H), 3.84 (s, 6H), 3.75 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 167.4, 158.1, 158.0, 143.5, 134.9, 133.1, 132.6, 129.6, 129.3, 129.1, 113.7, 113.2, 110.4, 56.0, 55.4, 55.2. HRMS (ESI$^+$) m/z: $[M+Na]^+$ calcd for $C_{32}H_{28}O_4Na^+$ 499.1880; found 499.1882.



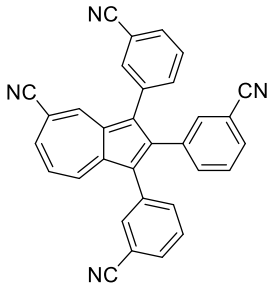
1,1',1''-((6-Acetylazulene-1,2,3-triyl)tris(benzene-4,1-diyl))tris(ethan-1-one) (3d)

Following the general procedure I. 1,1'-(Ethyne-1,2-diylbis(4,1-phenylene))bis(ethan-1-one) (52.4 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) afforded **3d** as a bluish green solid (23.5 mg, 45% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.43 (d, J = 10.8 Hz, 2H), 8.98 – 7.95 (m, 4H), 7.85 (d, J = 10.8 Hz, 2H), 7.76 – 7.73 (m, 2H), 7.36 – 7.33 (m, 4H), 7.11 – 7.09 (m, 2H), 2.75 (s, 3H), 2.64 (s, 6H), 2.56 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 200.1, 197.96, 197.92, 149.6, 144.4, 140.4, 140.2, 140.0, 136.0, 135.6, 135.3, 131.7, 131.5, 129.2, 128.6, 128.2, 124.2, 29.5, 26.82, 26.76. HRMS (ESI$^+$) m/z: $[M+Na]^+$ calcd for $C_{36}H_{28}O_4Na^+$547.1880; found 547.1880.



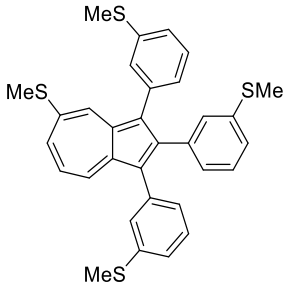
5-Methyl-1,2,3-tri-*m*-tolylazulene (3e)

Following the general procedure I. 1,2-Di-*m*-tolylethyne (41.2 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **3e** as a blue solid (25.6 mg, 62% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.24 – 8.22 (m, 2H), 7.44 (d, J = 10.4 Hz, 1H), 7.26 – 7.20 (m, 2H), 7.13 – 7.03 (m, 6H), 7.02 – 6.97 (m, 2H), 6.95 – 6.92 (m, 1H), 6.83 – 6.82 (m, 2H), 2.56 (s, 3H), 2.34 (s, 6H), 2.11 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 148.4, 138.9, 137.5, 137.44, 137.36, 137.1, 136.82, 136.77, 136.60, 136.55, 136.5, 134.1, 132.9, 132.5, 132.33, 132.29, 129.0, 128.8, 128.6, 128.1, 127.93, 127.92, 127.4, 127.3, 126.9, 122.9, 26.9, 21.69, 21.66, 21.5. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{32}H_{29}^+$ 413.2264; found 413.2261.



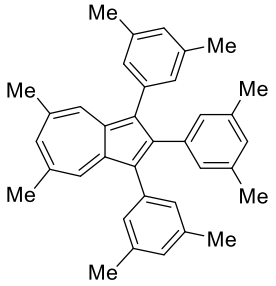
3,3',3''-(5-Cyanoazulene-1,2,3-triyl)tribenzonitrile (3f)

Following the general procedure I. 3,3'-(Ethyne-1,2-diyl)dibenzonitrile (45.6 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (dichloromethane/ethyl acetate = 8:1) afforded **3f** as a blue solid (19.6 mg, 43% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.36 (d, J = 1.2 Hz, 1H), 8.33 (d, J = 9.6 Hz, 1H), 7.89 (d, J = 10.8 Hz, 1H), 7.74 – 7.69 (m, 2H), 7.61 – 7.47 (m, 6H), 7.42 (d, J = 8.0 Hz, 1H), 7.36 – 7.28 (m, 2H), 7.20 – 7.17 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 147.4, 141.7, 139.5, 138.8, 137.8, 135.9, 135.60, 135.57, 135.5, 135.3, 135.12, 135.05, 134.4, 134.3, 134.0, 131.9, 131.8, 131.6, 131.5, 131.2, 130.0, 129.8, 129.6, 125.1, 121.0, 118.4, 118.3, 118.1 113.4, 113.3, 113.0, 108.6. HRMS (ESI$^+$) m/z: $[M+Na]^+$ calcd for $C_{32}H_{16}N_4Na^+$ 479.1267; found 479.1263.



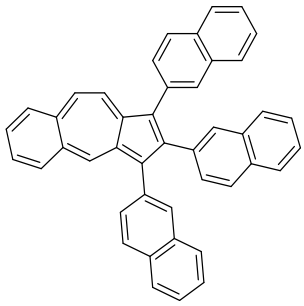
((5-(Methylthio)azulene-1,2,3-triyl)tris(benzene-3,1-diyl))tris(methylsulfane) (3g)

Following the general procedure I. 1,2-Bis(3-(methylthio)phenyl)ethyne (54.0 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) afforded **3g** as a blue solid (27.5 mg, 51% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.43 (d, J = 2.0 Hz, 1H), 8.21 (d, J = 9.6 Hz, 1H), 7.61 (dd, J = 10.4, 1.6 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.22 – 7.18 (m, 2H), 7.11 – 7.01 (m, 7H), 6.91 – 6.89 (m, 1H), 6.80 (dt, J = 7.2, 1.6 Hz, 1H), 2.54 (s, 3H), 2.304 (s, 3H), 2.301 (s, 3H),2.06 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 148.4, 138.44, 138.38, 137.83, 137.75, 137.4, 136.8, 136.6, 136.6, 136.24, 136.19, 134.4, 134.1, 129.7, 129.51, 129.47, 128.73, 128.70, 128.4, 128.3, 128.24, 128.21, 128.0, 126.1, 125.2, 125.1, 123.3, 18.8, 16.0, 15.9, 15.8. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{32}H_{29}S_4^+$ 541.1147; found 541.1143.



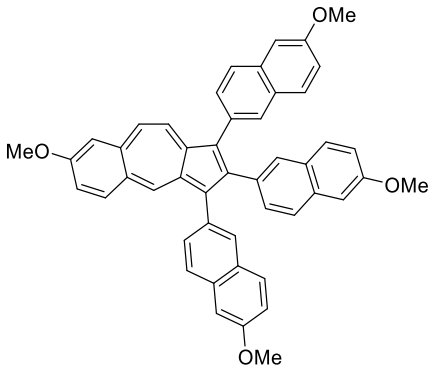
1,2,3-Tris(3,5-dimethylphenyl)-5,7-dimethylazulene (3h)

Following the general procedure I. 1,2-Bis(3,5-dimethylphenyl)ethyne (46.8 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **3h** as a blue solid (19.7 mg, 42% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.12 (d, J = 1.2 Hz, 2H), 7.35 (s, 1H), 6.91 (s, 2H), 6.88 (s, 4H), 6.72 (s, 1H), 6.61 (s, 2H), 2.52 (s, 3H), 2.28 (s, 6H), 2.07 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 148.7, 140.0, 137.1, 136.7, 136.53, 136.46, 136.3, 135.5, 131.6, 129.7, 129.4, 128.0, 127.6, 126.9, 27.4, 21.6, 21.4. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{36}H_{37}^+$ 469.2890; found 469.2885.



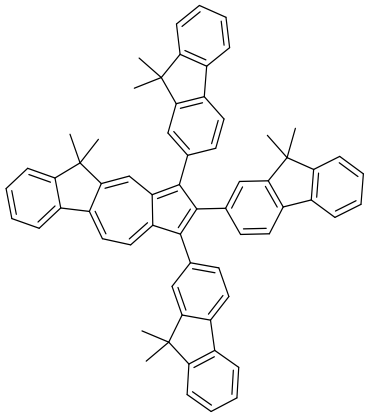
1,2,3-Tri(naphthalen-2-yl)benzo[*f*]azulene (3i)

Following the general procedure I. 1,2-Di(naphthalen-2-yl)ethyne (55.6 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **3i** as a dark green solid (42.3 mg, 76% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.47 (s, 1H), 8.01 – 7.96 (m, 3H), 7.87 – 7.78 (m, 6H), 7.74 (d, J = 8.4 Hz, 1H), 7.68 (d, J = 8.4 Hz, 2H), 7.62 – 7.59 (m, 1H), 7.56 – 7.35 (m, 10H), 7.30 – 7.28 (m, 1H), 7.25 – 7.18 (m, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 145.4, 141.5, 141.3, 139.3, 135.8, 134.9, 133.81, 133.78, 133.7, 133.6, 133.5, 133.2, 132.8, 132.44, 132.40, 132.3, 132.2, 131.2, 130.8, 130.6, 130.30, 130.26, 130.2, 129.6, 129.4, 129.2, 128.4, 128.3, 128.22, 128.15, 127.88, 127.87, 127.8, 127.63, 127.60, 127.3, 127.0, 126.8, 126.7, 126.13, 126.08, 125.93, 125.91, 125.7. HRMS (ESI$^+$) m/z: $[M+Na]^+$ calcd for $C_{44}H_{28}Na^+$ 579.2083; found 579.2082.



7-Methoxy-1,2,3-tris(6-methoxynaphthalen-2-yl)benzo[f]azulene (3j)

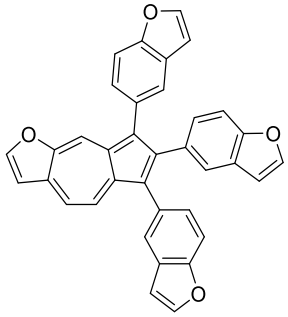
Following the general procedure I. 1,2-Bis(6-methoxynaphthalen-2-yl)ethyne (67.6 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether/ethyl acetate = 6:1) afforded **3j** as a dark green solid (55.4 mg, 82% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.19 (s, 1H), 7.74 (d, J = 11.6 Hz, 1H), 7.69 (d, J = 13.6 Hz, 2H), 7.56 – 7.52 (m, 3H), 7.43 (d, J = 8.4 Hz, 1H), 7.37 (d, J = 8.4 Hz, 1H), 7.18 (d, J = 8.4 Hz, 1H), 7.11 (d, J = 9.2 Hz, 2H), 7.04 (d, J = 15.6 Hz, 1H), 7.00 – 6.91 (m, 8H), 6.85 (dd, J = 8.8, 2.8 Hz, 1H), 6.78 – 6.73 (m, 2H), 3.75 (s, 6H), 3.73 (s, 3H), 3.65 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 160.9, 157.8, 157.7, 144.2, 144.1, 141.5, 140.9, 138.9, 137.9, 134.8, 133.40, 133.3, 133.20, 131.88, 131.78, 131.7, 131.2, 130.9, 130.5, 130.3, 130.1, 129.94, 129.85, 129.7, 129.64, 129.59, 129.4, 129.1, 129.0, 128.7, 126.9, 126.6, 126.4, 126.0, 125.7, 118.81, 118.77, 118.4, 115.7, 114.0, 105.9, 105.6, 55.6, 55.50, 55.48, 55.4. HRMS (ESI$^+$) m/z: [M+H]$^+$ calcd for $C_{48}H_{37}O_4^+$ 677.2686; found 677.2688.



1,2,3-Tris(9,9-dimethyl-9*H*-fluoren-2-yl)-5,5-dimethyl-5*H*-benzo[*a*]cyclopenta[*f*]azulene (3k)

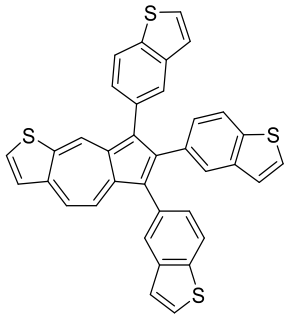
Following the general procedure I. 1,2-Bis(9,9-dimethyl-9*H*-fluoren-2-yl)ethyne (82.0 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether/dichloromethane = 30:1) afforded **3k** as a dark green solid (49.9 mg, 61% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.65 (s, 1H), 8.58 (d, J = 10.4 Hz, 1H), 7.93 – 7.91 (m, 1H), 7.75 – 7.72 (m, 5H), 7.58 (d, J = 6.8 Hz, 1H), 7.50 – 7.47 (m, 2H), 7.45 – 7.39 (m, 6H), 7.36 – 7.29 (m, 7H), 7.25 – 7.21 (m, 2H), 7.14 (d, J = 0.8 Hz, 1H), 7.06 (dd, J = 7.6, 1.2 Hz, 1H), 1.57 (s, 3H), 1.43 (s, 3H), 1.42 (s, 6H), 1.34 (s, 6H), 1.12 (s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 154.05, 154.02, 153.95, 153.9, 153.7, 153.6, 153.1, 147.9, 147.7, 147.5, 140.9,

139.44, 139.40, 139.3, 137.4, 137.3, 137.2, 136.1, 136.0, 135.69, 135.68, 135.6, 134.8, 131.0, 130.5, 130.4, 130.3, 129.45, 129.43, 128.9, 127.6, 127.12, 127.08, 127.05, 127.0, 126.9, 126.32, 126.29, 126.25, 123.0, 122.8, 122.7, 122.6, 121.3, 120.02, 120.00, 119.9, 119.7, 119.3, 115.8, 49.5, 46.9, 46.8, 46.5, 27.3, 27.24, 27.22, 27.1, 27.0. HRMS (ESI$^+$) m/z: [M+H]$^+$ calcd for $C_{64}H_{53}^+$ 821.4142; found 821.4139.



6,7,8-Tri(benzofuran-5-yl)azuleno[*5,6-b*]furan (3l)

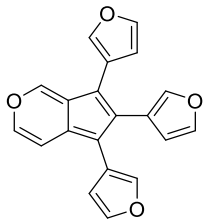
Following the general procedure I. 1,2-Di(benzofuran-5-yl)ethyne (51.6 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **3l** as a purple solid (40.8 mg, 79% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.50 (s, 1H), 8.23 (d, J = 11.2 Hz, 1H), 7.65 (dd, J = 6.8, 2.0 Hz, 2H), 7.61 (d, J = 2.0 Hz, 3H), 7.48 (d, J = 2.0 Hz, 1H), 7.45 (dd, J = 10.4, 8.4 Hz, 2H), 7.33 (dd, J = 11.2, 0.8 Hz, 1H), 7.25 – 7.15 (m, 4H), 6.98 (dd, J = 8.4, 1.6 Hz, 1H), 6.88 (dd, J = 2.0, 0.8 Hz, 1H), 6.76 (ddd, J = 7.6, 2.0, 0.8 Hz, 2H), 6.51 (dd, J = 2.0, 0.8 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 159.2, 154.05, 154.04, 153.9, 145.4, 145.3, 145.2, 144.8, 143.1, 137.4, 132.0, 131.5, 131.4, 131.3, 130.5, 129.5, 129.1, 128.7, 128.2, 127.54, 127.52, 127.0, 124.3, 124.1, 123.8, 123.4, 112.4, 111.17 (2C), 110.7, 110.0, 107.01, 106.99, 106.95. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{36}H_{20}O_4Na^+$ 539.1254; found 539.1256.



6,7,8-Tris(benzo[*b*]thiophen-5-yl)azuleno[*5,6-b*]thiophene (3m)

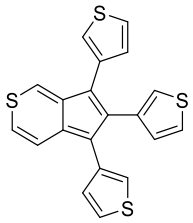
Following the general procedure I. 1,2-Bis(benzo[*b*]thiophen-5-yl)ethyne (58.0 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **3m** as a dark green solid (43.6 mg, 75% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.62 (s, 1H), 8.09 (d, J = 11.2 Hz, 1H), 7.89 (d, J = 4.2 Hz, 2H), 7.79 (dd, J = 15.6, 8.4 Hz, 2H), 7.55 (d, J = 8.4 Hz, 1H), 7.5 – 7.45 (m, 4H), 7.41 (d, J = 5.6 Hz, 1H), 7.38 – 7.32 (m, 3H), 7.28 (d, J = 5.6 Hz, 1H), 7.24 (d, J = 8.0 Hz, 1H), 7.17 (d, J = 7.2

Hz, 1H), 7.06 – 7.02 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 149.2, 145.7, 139.89, 139.85, 139.4, 138.23, 138.15, 138.1, 135.1, 133.3, 132.7, 132.63, 132.59, 132.2, 131.7, 131.4, 129.6, 128.7, 128.1, 127.94, 127.88, 126.74, 126.65, 126.6, 126.5, 126.0, 124.5, 124.4, 124.34, 124.26, 122.33, 122.28, 121.9, 117.7. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{36}H_{20}S_4Na^+$ 603.0340; found 603.0338.



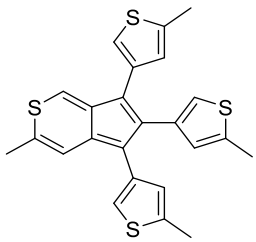
5,6,7-Tri(furan-3-yl)cyclopenta[*c*]pyran (3n)

Following the general procedure I. 1,2-Di(furan-3-yl)ethyne (31.6 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether/dichloromethane = 10:1) afforded **3n** as an orange solid (19.9 mg, 63% yield). When 1,2-di(furan-3-yl)ethyne (316.1 mg, 2.0 mmol) was used, **3n** was obtained in 54% yield (170.6 mg). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.08 (s, 1H), 7.28 – 7.26 (m, 2H), 7.26 – 7.22 (m, 3H), 7.14 (s, 1H), 7.08 (s, 1H), 6.97 – 6.95 (m, 1H), 6.21 – 6.17 (m, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 146.6, 143.0, 142.7, 142.5, 141.5, 140.1, 139.8, 139.5, 136.2, 126.2, 121.9, 120.3, 119.9, 119.6, 114.9, 113.5, 112.2, 111.7, 111.6, 108.6. HRMS (ESI$^+$) m/z: [M+H]$^+$ calcd for $C_{20}H_{13}O_4^+$ 317.0808; found 317.0809.



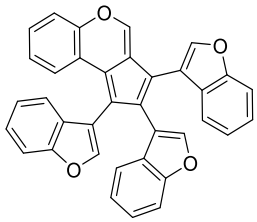
5,6,7-Tri(thiophen-3-yl)cyclopenta[*c*]thiopyran (3o)

Following the general procedure I. 1,2-Di(thiophen-3-yl)ethyne (38.0 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **3o** as a dark red solid (27.4 mg, 72% yield). When 1,2-di(thiophen-3-yl)ethyne (380.0 mg, 2.0 mmol) was used, **3o** was obtained in 63% yield (239.4 mg). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.45 (d, J = 2.8 Hz, 1H), 8.05 (d, J = 9.6 Hz, 1H), 7.33 – 7.29 (m, 2H), 7.17 – 7.14 (m, 3H), 6.96 – 6.90 (m, 4H), 6.79 (d, J = 4.8 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 139.1, 136.5, 136.3, 135.9, 135.6, 130.9, 129.73, 129.67, 129.5, 125.2, 125.0, 124.8, 124.3, 124.2, 123.5, 123.2, 122.7, 122.5, 117.5, 113.6. HRMS (ESI$^+$) m/z: [M+H]$^+$ calcd for $C_{20}H_{13}S_4^+$ 380.9895; found 380.9890.



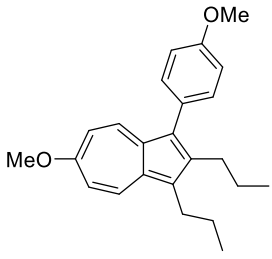
3-Methyl-5,6,7-tris(5-methylthiophen-3-yl)cyclopenta[*c*]thiopyran (3p)

Following the general procedure I. 1,2-Bis(5-methylthiophen-3-yl)ethyne (43.6 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **3p** as a dark red solid (33.3 mg, 76% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.24 (s, 1H), 7.69 (s, 1H), 6.84 (dd, J = 10.0, 1.6 Hz, 2H), 6.69 (d, J = 1.2 Hz, 1H), 6.61 – 6.60 (m, 2H), 6.46 – 6.45 (m, 1H), 2.51 (d, J = 1.2 Hz, 3H), 2.48 (d, J = 1.2 Hz, 3H), 2.46 (d, J = 1.2 Hz, 3H), 2.39 (d, J = 1.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 140.0, 139.0, 138.6, 137.9, 136.6, 136.5, 136.0, 135.5, 130.1, 128.1, 127.9, 127.8, 125.7, 125.5, 122.8, 122.7, 121.6, 120.4, 120.3, 117.1, 22.2, 15.5, 15.40, 15.36. HRMS (ESI$^+$) m/z: [M+H]$^+$ calcd for $C_{24}H_{21}S_4^+$ 437.0521; found 437.0521.



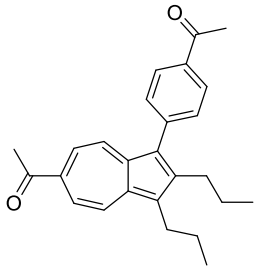
1,2,3-Tri(benzofuran-3-yl)cyclopenta[*c*]chromene (3q)

Following the general procedure I. 1,2-Di(benzofuran-3-yl)ethyne (51.6 mg, 0.2 mmol) was used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **3q** as an orange solid (44.4 mg, 86% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.35 (s, 1H), 7.66 (dd, J = 8.4, 1.6 Hz, 1H), 7.59 (dd, J = 8.4, 1.2 Hz, 1H), 7.55 – 7.53 (m, 1H), 7.52 (s, 1H), 7.49 – 7.47 (m, 2H), 7.40 (d, J = 8.0 Hz, 1H), 7.36 – 7.25 (m, 6H), 7.17 – 7.07 (m, 4H), 6.89 (d, J = 7.2 Hz, 1H), 6.82 – 6.78 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 155.43, 155.39, 155.0, 149.1, 147.0, 143.7, 143.5, 143.0, 135.9, 127.9, 127.8, 127.2, 126.8, 125.53, 125.47, 125.0, 124.6, 124.6, 124.1, 123.0, 122.9, 122.5, 122.0, 121.4, 121.0, 120.9, 118.1, 117.8, 116.7, 116.4, 115.6, 115.5, 111.8, 111.7, 111.3. HRMS (ESI$^+$) m/z: [M+H]$^+$ calcd for $C_{36}H_{21}O_4^+$ 517.1434; found 517.1445.



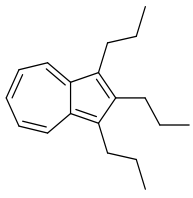
6-Methoxy-1-(4-methoxyphenyl)-2,3-dipropylazulene (4a)

Following the general procedure II. 1,2-Bis(4-methoxyphenyl)ethyne (23.8 mg, 0.1 mmol) and 4-octyene (44.0 μL, 0.3 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether/ethyl acetate = 8:1) afforded **4a** as a purple oil (16.6 mg, 48% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.07 (d, *J* = 10.8 Hz, 1H), 7.85 (d, *J* = 10.7 Hz, 1H), 7.31 (d, *J* = 8.8 Hz, 2H), 7.01 (d, *J* = 8.8 Hz, 2H), 6.67 (dd, *J* = 10.8, 2.8 Hz, 1H), 6.56 (dd, *J* = 10.8, 2.4 Hz, 1H), 3.89 (s, 6H), 3.00 – 2.96 (m, 2H), 2.83 – 2.79 (m, 2H), 1.71 – 1.66 (m, 2H), 1.51 – 1.45 (m, 2H), 1.05 (t, *J* = 7.2 Hz, 3H), 0.86 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 166.13, 158.27, 146.56, 133.01, 132.93, 132.01, 131.96, 131.58, 130.45, 129.75, 129.61, 125.95, 113.67, 110.16, 108.74, 108.67, 55.88, 55.42, 29.64, 27.91, 25.75, 24.58, 14.87, 14.81. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{24}H_{29}O_2^+$ 349.2162; found 349.2163.



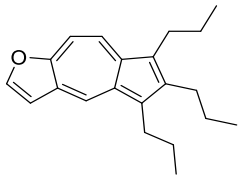
1-(4-(6-Acetyl-2,3-dipropylazulen-1-yl)phenyl)ethan-1-one (4b)

Following the general procedure II. 1,1'-(Ethyne-1,2-diylbis(4,1-phenylene))bis(ethan-1-one) (26.2 mg, 0.1 mmol) and 4-octyene (44.0 μL, 0.3 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether/ethyl acetate = 8:1) afforded **4b** as a blue oil (15.6 mg, 42% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.32 (d, *J* = 10.0 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 2H), 8.06 (d, *J* = 10.4 Hz, 1H), 7.77 (dd, *J* = 10.4, 1.2 Hz, 1H), 7.67 (dd, *J* = 10.0, 1.2 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 2H), 3.08 – 3.04 (m, 2H), 2.95 – 2.91 (m, 2H), 2.72 (s, 3H), 2.70 (s, 3H), 1.74 – 1.68 (m, 2H), 1.51 – 1.46 (m, 2H), 1.06 (t, *J* = 7.2 Hz, 3H), 0.86 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 200.8, 198.2, 155.1, 142.2, 142.0, 138.2, 137.8, 135.5, 131.7, 131.2, 131.1, 130.1, 129.3, 128.5, 122.3, 121.2, 30.1, 27.70, 27.65, 27.1, 26.9, 25.5, 24.3, 14.7. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{26}H_{29}O_2^+$ 373.2162; found 373.2163.



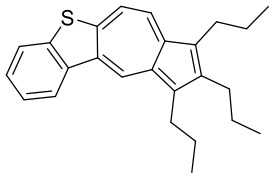
1,2,3-Tripropylazulene (4c)

Following the general procedure II. 1-Phenyl-1-pentyne (16.0 μL, 0.1 mmol) and 4-octyene (44.0 μL, 0.3 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **4c** as a blue oil (7.5 mg, 30% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* (ppm) 8.10 (d, *J* = 9.2 Hz, 2H), 7.38 (t, *J* = 10.0 Hz, 1H), 6.95 (t, *J* = 10.0 Hz, 1H), 3.00 – 2.96 (m, 4H), 2.90 – 2.86 (m, 2H), 1.67 – 1.59 (m, 6H), 1.07 – 1.00 (m, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* (ppm) 151.3, 135.9, 135.6, 131.4, 128.2, 120.6, 30.0, 27.9, 25.6, 24.7, 15.1, 14.8. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{19}H_{27}^+$ 255.2107; found 255.2112.



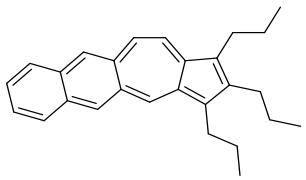
5,6,7-Tripropylazuleno[*6,5-b*]furan (4d)

Following the general procedure II. 5-(Pent-1-yn-1-yl)benzofuran (18.4 mg, 0.1 mmol) and 4-octyene (44.0 μL, 0.3 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **4d** as a dark green solid (10.5 mg, 36% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.23 (s, 1H), 7.92 (d, *J* = 10.8 Hz, 1H), 7.55 (d, *J* = 2.0 Hz, 1H), 7.17 (d, *J* = 10.8 Hz, 1H), 6.92 (dd, *J* = 2.0, 0.8 Hz, 1H), 3.02 – 2.94 (m, 4H), 2.86 – 2.82 (m, 2H), 1.69 – 1.60 (m, 6H), 1.07 – 1.01 (m, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 158.1, 147.2, 142.1, 136.5, 131.9, 128.9, 127.7, 126.2, 124. 9, 120.9, 112.3, 107.0, 29.7, 28.2, 27.9, 26.2, 25.1, 24.8, 15.0, 14.8(overlapped). HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{21}H_{27}O^+$ 295.2056; found 295.2055.



8,9,10-Tripropylazuleno[*6,5-b*]benzo[*d*]thiophene (4e)

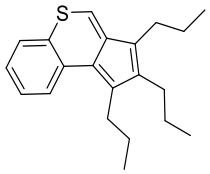
Following the general procedure II. 2-(Pent-1-yn-1-yl)dibenzo[*b,d*]thiophene (25.0 mg, 0.1 mmol) and 4-octyene (44.0 μL, 0.3 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **4e** as a deep blue oil (15.6 mg, 39% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.64 (s, 1H), 8.12 (d, *J* = 10.8 Hz, 1H), 8.05 – 8.03 (m, 1H), 7.54 (dd, *J* = 6.8, 2.0 Hz, 1H), 7.44 – 7.38 (m, 2H), 7.28 (s, 1H), 3.13 – 3.09 (m, 2H), 3.03 – 2.99 (m, 2H), 2.90 – 2.86 (m, 2H), 1.78 – 1.61 (m, 6H), 1.10 – 1.03 (m, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 160.1, 154.5, 148.0, 135.3, 132.9, 130.0, 129.4, 129.1, 128.0, 126.1, 123.2, 122.5, 119.0, 116.2, 111.1, 106.4, 29.7, 28.2, 28.0, 26.2, 25.3, 24.8, 15.1, 149, 14.9. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{25}H_{29}S^+$ 361.1984; found 361.1972.



1,2,3-Tripropylnaphtho[*2,3-f*]azulene (4f)

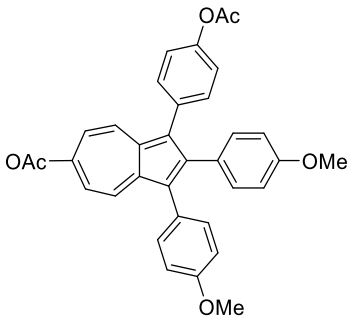
Following the general procedure II. 2-(Pent-1-yn-1-yl)anthracene (24.4 mg, 0.1 mmol) and 4-octyene (44.0 μL, 0.3 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether)

afforded **4f** as a dark green solid (15.1 mg, 43% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.34 – 8.33 (m, 1H), 8.07 (s, 1H), 7.96 – 7.90 (m, 3H), 7.53 – 7.45 (m, 2H), 7.28 (d, *J* = 12.0 Hz, 1H), 6.96 (d, *J* = 11.6 Hz, 1H), 2.84 (t, *J* = 8.0 Hz, 2H), 2.74 (t, *J* = 8.0 Hz, 2H), 2.63 (t, *J* = 8.0 Hz, 2H), 1.72 – 1.59 (m, 6H), 1.12 – 102 (m, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 145.5, 141.8, 140.1, 135.7, 134.8, 134.2, 133.3, 131.7, 131.6, 130.8, 130.58, 128.0, 127.5, 127.2, 126.1, 125.9, 124.8, 123.6, 29.2, 28.1, 27.4, 26.1, 24.4, 24.3, 14.9, 14.79, 14.76. HRMS (ESI$^+$) m/z: [M+H]$^+$ calcd for $C_{27}H_{31}^+$ 355.2420; found 355.2424.



1,2,3-Tripropylcyclopenta[*c*]thiochromene (4g)

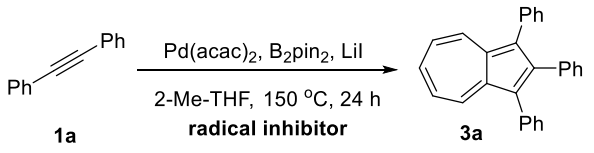
Following the general procedure II. 3-(Pent-1-yn-1-yl)benzo[*b*]thiophene (20.0 mg, 0.1 mmol) and 4-octyene (44.0 μL, 0.3 mmol) were used. Purification via flash column chromatography on silica gel (petroleum ether) afforded **4g** as a red oil (9.2 mg, 30% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.18 (d, *J* = 8.4 Hz, 1H), 7.74 (s, 1H), 7.60 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.46 – 7.42 (m, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 2.91 (t, *J* = 8.0 Hz, 2H), 2.68 (m, *J* = 8.0 Hz, 2H), 2.59 (m, *J* = 8.0 Hz, 2H), 1.75 – 1.50 (m, 6H), 1.11 (t, *J* = 7.2 Hz, 3H), 1.04 (t, *J* = 7.2 Hz, 3H), 0.98 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 144.2, 137.4, 135.2, 130.4, 127.4, 126.9, 126.4, 125.8, 123.5, 123.3, 117.6, 110.2, 30.3, 28.6, 27.3, 25.8, 24.6, 22.6, 14.9 (overlapped), 14.7. HRMS (ESI$^+$) m/z: [M+H]$^+$ calcd for $C_{21}H_{27}S^+$ 311.1828; found 311.1825.



4-(6-acetoxy-2,3-bis(4-methoxyphenyl)azulen-1-yl)phenyl acetate (3dc)

Following the procedure in Scheme S5. ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.34 (t, *J* = 11.2 Hz, 2H), 7.97 (d, *J* = 8.0 Hz, 2H), 7.76 (d, *J* = 10.4 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.94 (d, *J* = 8.4 Hz, 4H), 6.68 (d, *J* = 8.4 Hz, 2H), 3.86 (s, 3H), 3.76 (s, 3H), 2.73 (s, 3H), 2.65 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 200.5, 198.2, 159.1, 158.6, 151.1, 143.1, 141.4, 139.1, 138.5, 135.2, 134.1, 133.3, 132.8, 132.5, 131.7, 129.9, 128.4, 128.2, 127.9, 127.7, 123.4, 123.3, 114.0, 113.7, 55.4, 55.2, 27.7, 26.8. HRMS (ESI$^+$) m/z: [M+H]$^+$ calcd for $C_{43}H_{29}O_4^+$ 501.2060; found 501.2060.

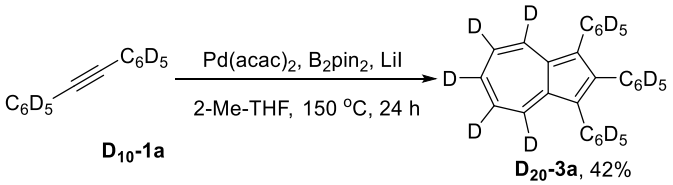
VI. Mechanistic study



1a 3a

BHT (1.0 equiv): 45%
BHT (3.0 equiv): 44%
pyrocatechol (1.0 equiv): 46%

A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with alkyne **1a** (0.2 mmol, 1.0 equiv), $Pd(acac)_2$ (10.0 mol%), B_2pin_2 (2.0 equiv), LiI (3.0 equiv), radical inhibitor and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether) to give the corresponding isolate yield of **3a**.



D_{10}-1a D_{20}-3a, 42%

A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with alkyne $\mathbf{D_{10}}$-**1a** (0.2 mmol, 1.0 equiv), $Pd(acac)_2$ (10.0 mol%), B_2pin_2 (2.0 equiv), LiI (3.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether) to provide $\mathbf{D_{20}}$-**3a** as the desired product (15.8 mg, 42%).

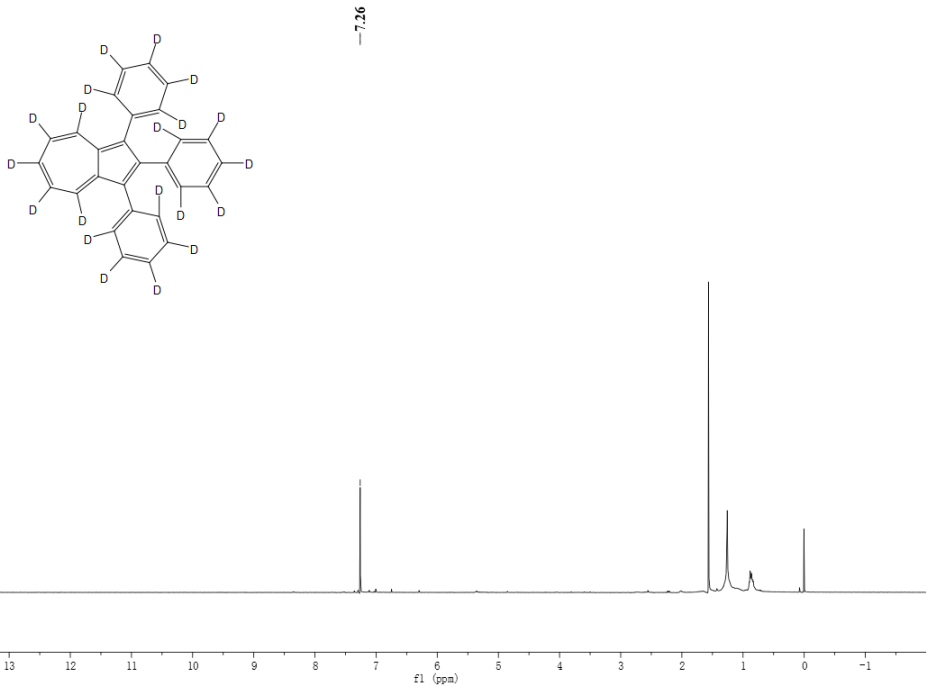
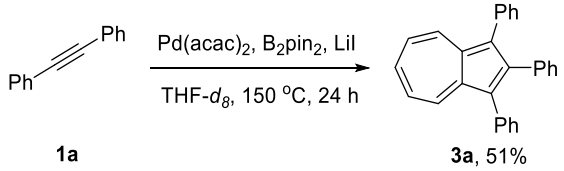


Figure S4. Copy of ^{1}H NMR spectrum of **D_{20}-3a**.



1a **3a**, 51%

A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with alkyne **1a** (0.2 mmol, 1.0 equiv), $Pd(acac)_2$ (10.0 mol%), B_2pin_2 (2.0 equiv), LiI (3.0 equiv) and THF-d_8 (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether) to provide **3a** as the desired product (18.2 mg, 51%).

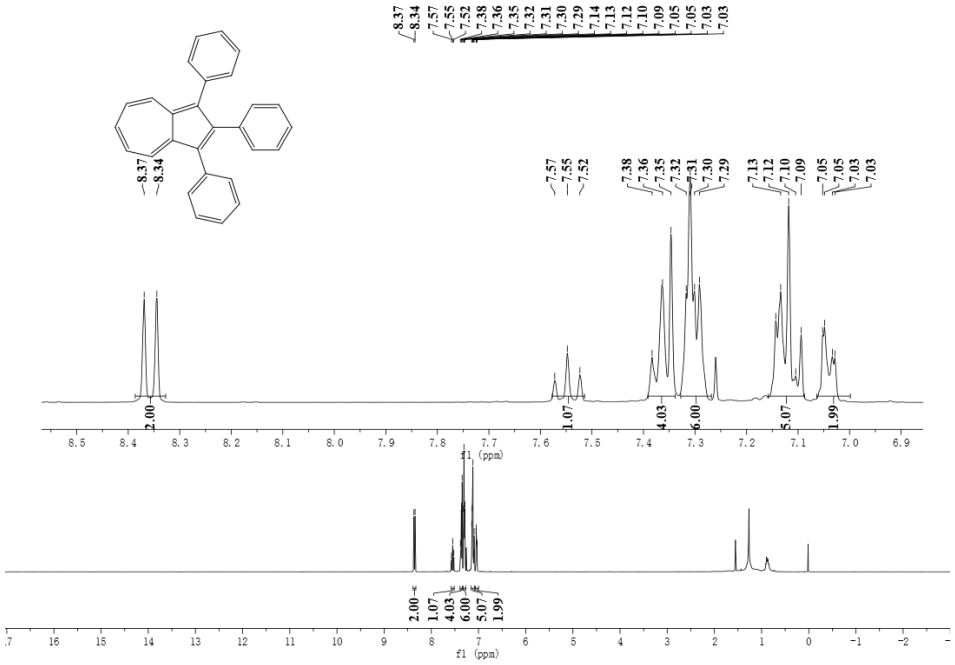
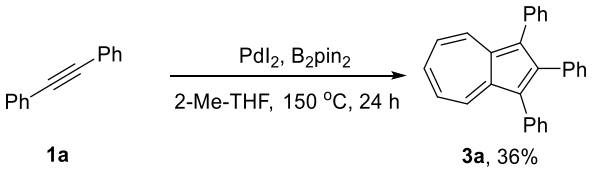
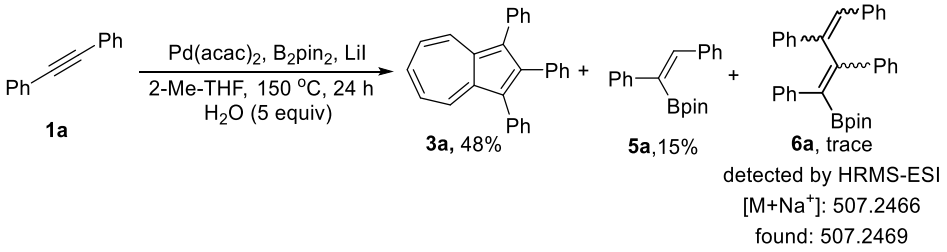


Figure S5. Copy of ^{1}H NMR spectrum of **3a**.



1a **3a**, 36%

A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with alkyne **1a** (0.2 mmol, 1.0 equiv), PdI_2 (10.0 mol%), B_2pin_2 (2.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether) to provide **3a** as the desired product (12.8 mg, 36%).



A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with alkyne **1a** (0.2 mmol, 1.0 equiv), $Pd(acac)_2$ (10.0 mol%), B_2pin_2 (2.0 equiv), LiI (3.0 equiv), H_2O (5.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether) to provide **3a** (15.8 mg, 48%). Then eluent was changed to petroleum ether/dichloromethane (5:1) to provide (*E*)-2-(1,2-diphenylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **5a** (9.2 mg, 15%). ^{1}H NMR ($CDCl_3$, 400 MHz): 7.46 – 7.43 (m, 4H), 7.35 – 7.22 (m, 7H), 1.29 (s, 12H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 142.7, 140.9, 138.9, 128.6, 128.4, 128.2, 127.7, 127.06, 127.02, 84.2, 25.0. The ^{1}H NMR and ^{13}C NMR data were in accordance with the reported data.[5] HRMS (ESI$^+$) m/z: $[M+Na]^+$ calcd for $C_{20}H_{23}BNaO_2^+$ 329.1683; found 329.1683.

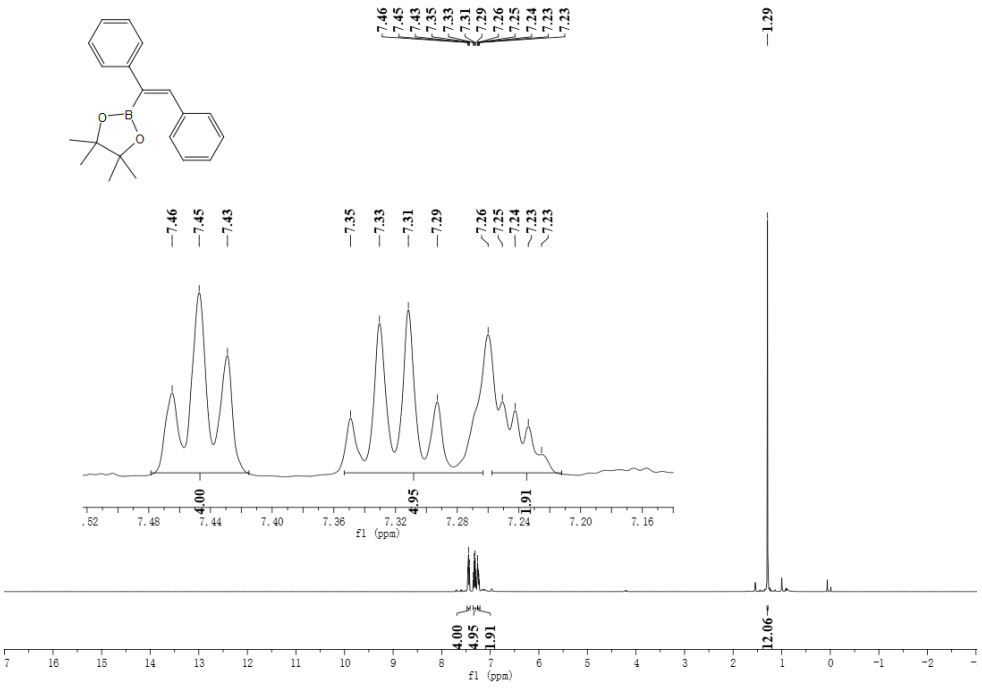


Figure S6. Copy of ^{1}H NMR spectrum of **5a**

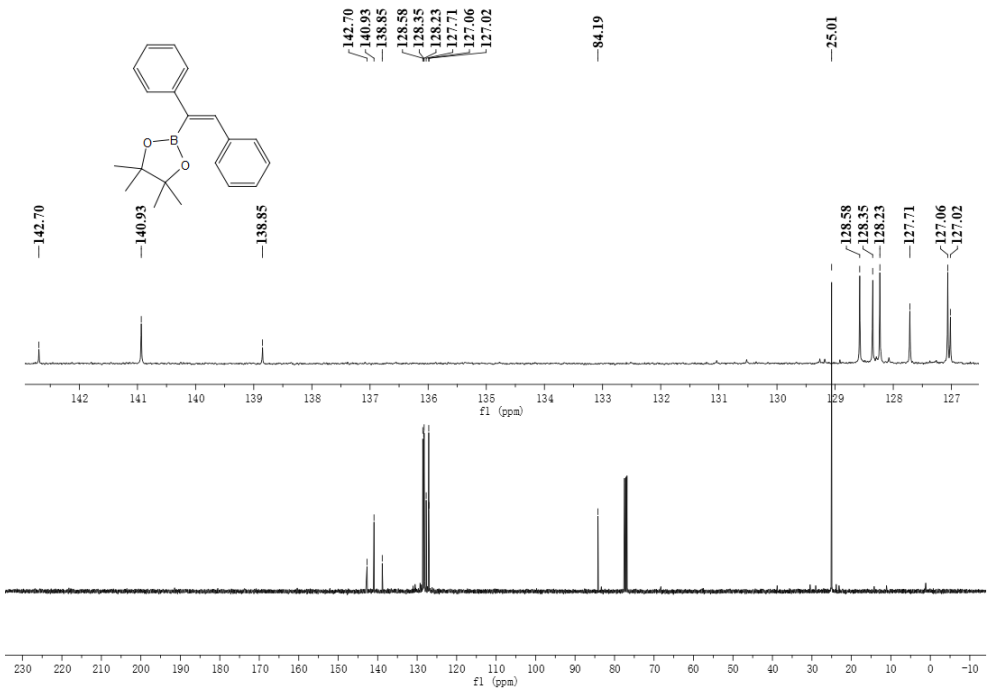


Figure S7. Copy of ^{13}C NMR spectrum of **5a**

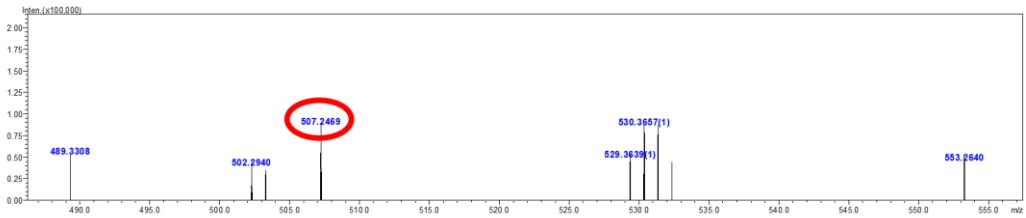
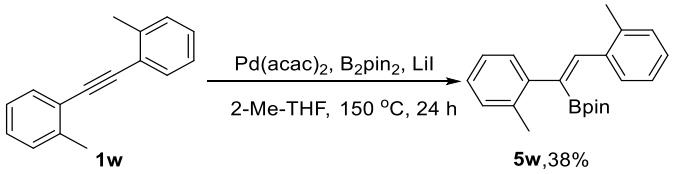


Figure S8. Copy of HRMS spectrum of **6a**.



A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with alkyne **1w** (0.2 mmol, 1.0 equiv), $Pd(acac)_2$ (10.0 mol%), B_2pin_2 (2.0 equiv), LiI (3.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/dichloromethane = 8:1) to give the (*E*)-2-(1,2-di-o-tolylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **5w** as the desired product (15.7 mg, 38%). ^1H NMR ($CDCl_3$, 400 MHz): 7.42 (d, *J* = 7.2 Hz, 1H), 7.26 – 7.18 (m, 5H), 7.16 – 7.14 (m, 2H), 7.08 (s, 1H), 2.38 (s, 3H), 2.32 (s, 3H), 1.16 (s, 12H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 143.5, 142.9, 138.2, 136.4, 135.5, 130.1, 129.8, 129.1, 128.7, 127.8, 126.8, 125.9, 125.3, 83.7, 24.9, 20.8, 20.3. HRMS (ESI^+) m/z: $[M+H]^+$ calcd for $C_{22}H_{28}BO_2^+$ 335.2177; found 335.2180. The ^1H NMR and ^{13}C

NMR of (*Z*)-2-(1,2-di-o-tolylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane is reported in the literature.[6]

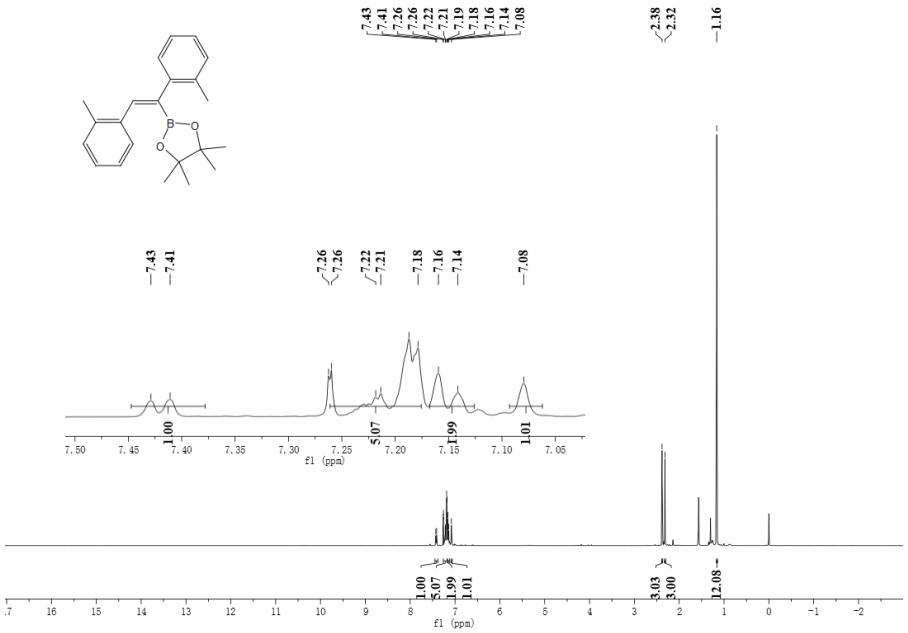


Figure S9. Copy of ^{1}H NMR spectrum of **5w**.

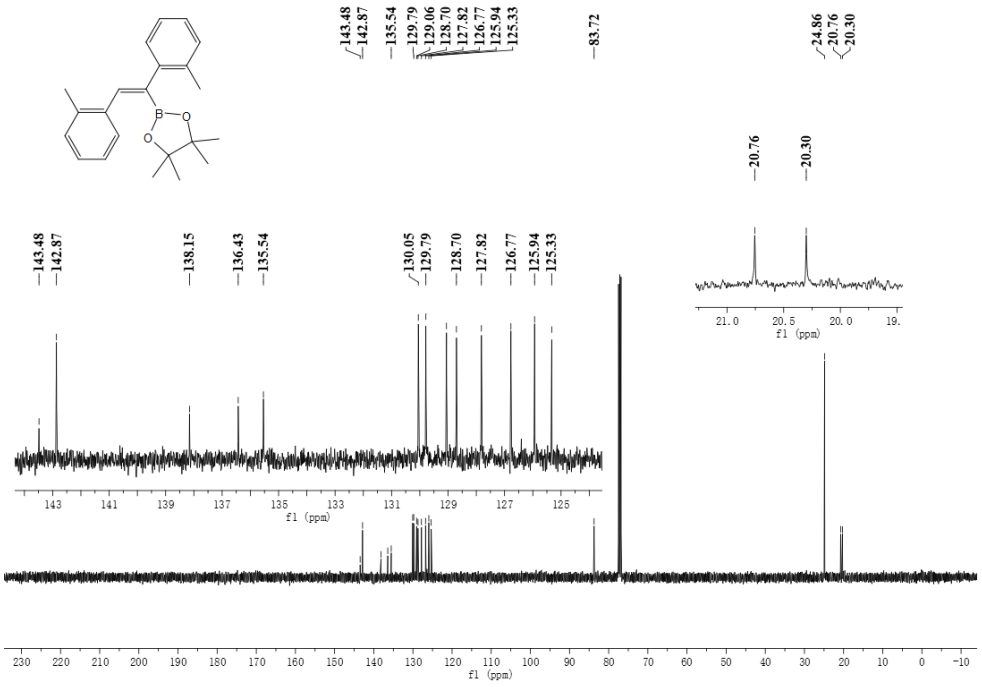
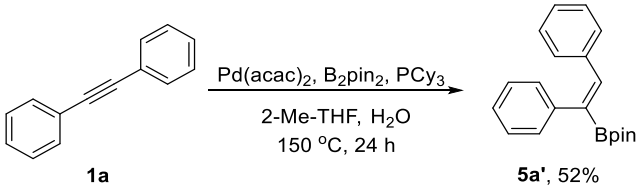


Figure S10. Copy of ^{13}C NMR spectrum of **5w**.



1a **5a'**, 52%

A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with alkyne **1a** (0.2 mmol, 1.0

equiv), $Pd(acac)_2$ (10.0 mol%), B_2pin_2 (2.0 equiv), PCy_3 (10 mol%), H_2O (5.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/dichloromethane = 8:1) to give the (*Z*)-2-(1,2-diphenylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **5a′** (31.8 mg, 52%). ^{1}H NMR ($CDCl_3$, 400 MHz): 7.36 (s, 1H), 7.28 – 7.15 (m, 5H), 7.12 – 7.04 (m, 5H),1.31 (s, 12H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 143.3, 140.6, 137.1, 130.1, 129.0, 128.4, 128.0, 127.7, 126.4, 83.9, 24.9. The ^{1}H NMR and ^{13}C NMR data were in accordance with the reported data.[5]

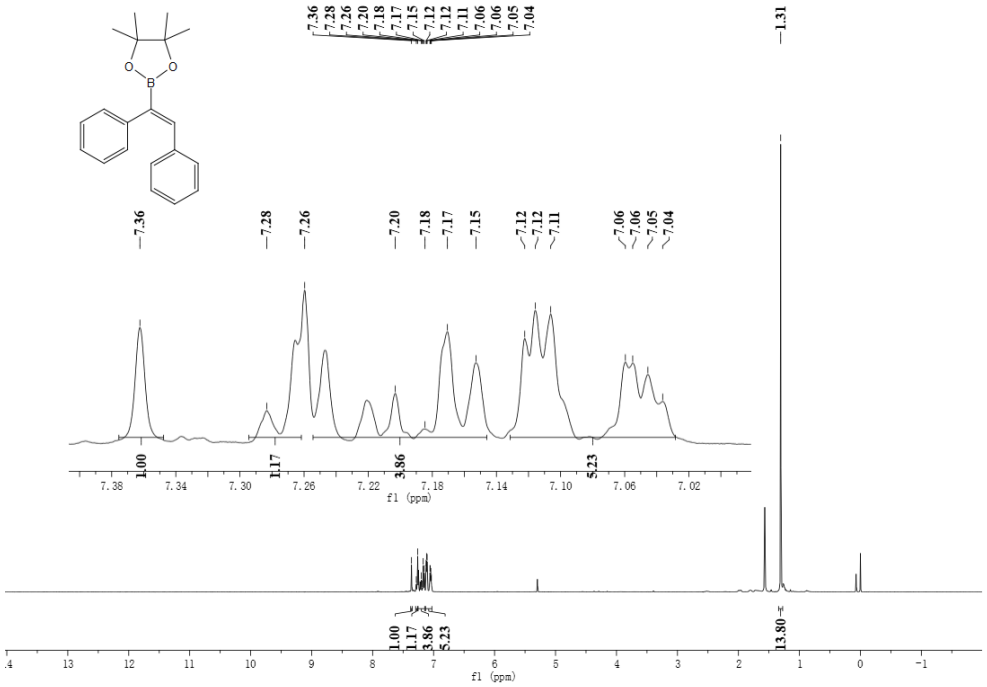


Figure S11. Copy of ^{1}H NMR spectrum of **5a′**.

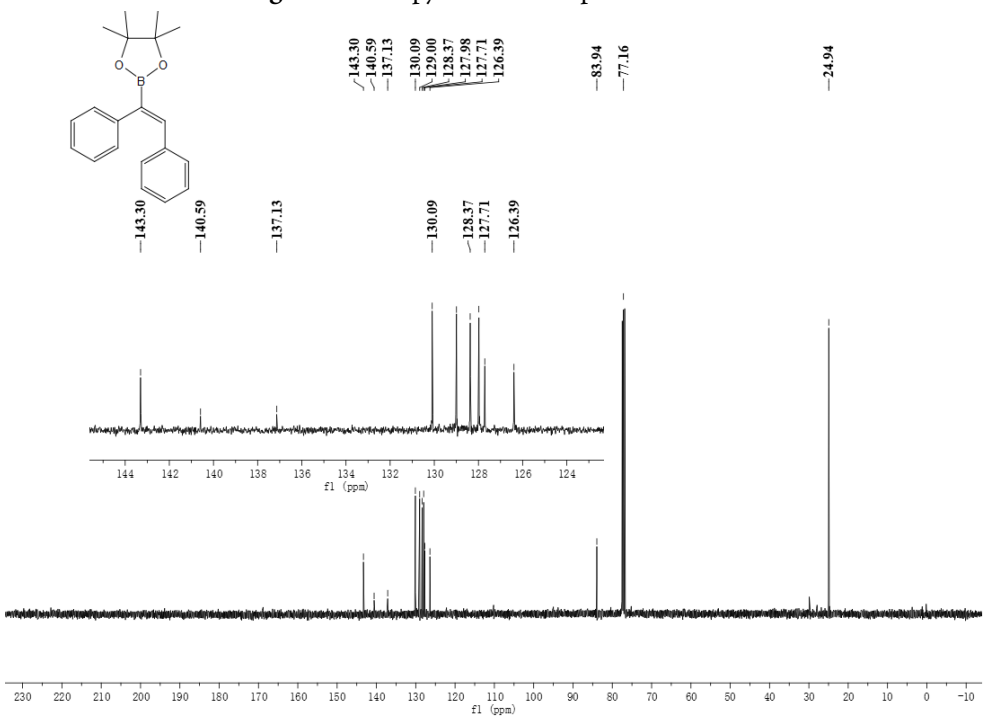
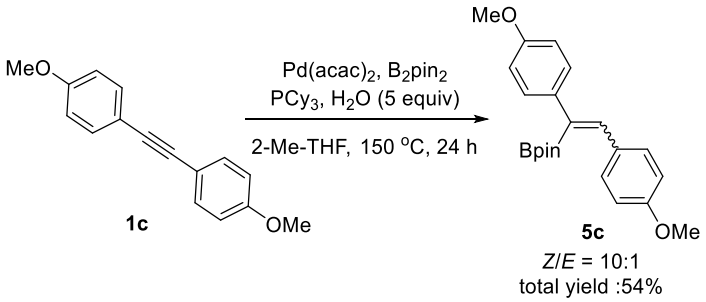


Figure S12. Copy of ^{13}C NMR spectrum of **5a′**.



A flame dried 25 mL Schlenk tube with a magnetic stir bar was charged with 1,2-bis(4-methoxyphenyl)ethyne **1c** (0.2 mmol, 1.0 equiv), $Pd(acac)_2$ (10.0 mol%), B_2pin_2 (2.0 equiv), PCy_3 (10 mol%), H_2O (5.0 equiv) and 2-Me-THF (1.0 mL) under N_2. The resulting solution was stirred at room temperature for 10 min and then 150 °C for 24 h. Subsequently, it was diluted with 20 mL of dichloromethane. The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/ ethyl acetate = 10:1) to give the unseparated mixture of (*E*)-2-(1,2-bis(4-methoxyphenyl)vinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(*E*)-5c** and (*Z*)-2-(1,2-bis(4-methoxyphenyl)vinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **(*Z*)-5c** (39.5 mg, *Z*/*E* = 10:1, total yield: 54%). The ^1H NMR data of **(*Z*)-5c** is reported in the literature.[6] HRMS (ESI$^+$) m/z: $[M+Na]^+$ calcd for $C_{22}H_{27}BO_4Na^+$ 389.1895; found 389.1894.

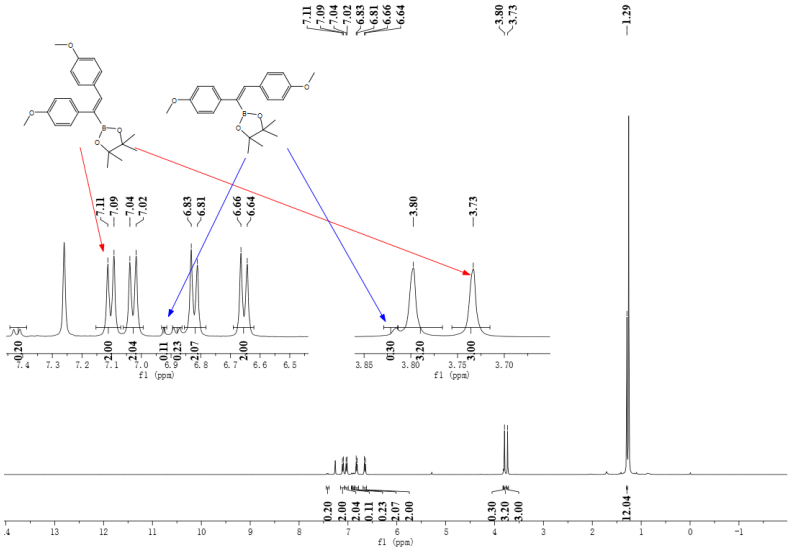


Figure S13. Copy of ^{13}C NMR spectrum of **5c**.

VII. Single-crystal X-ray diffraction analysis

The single crystals of compound **3a** was grown in chloroform by evaporating solvent from the saturated solution slowly. The detail structure information was uploaded to The Cambridge Crystallographic Data Centre (CCDC) and the data can be obtained free of charge via www.ccdc.cam.ac.uk/structures.

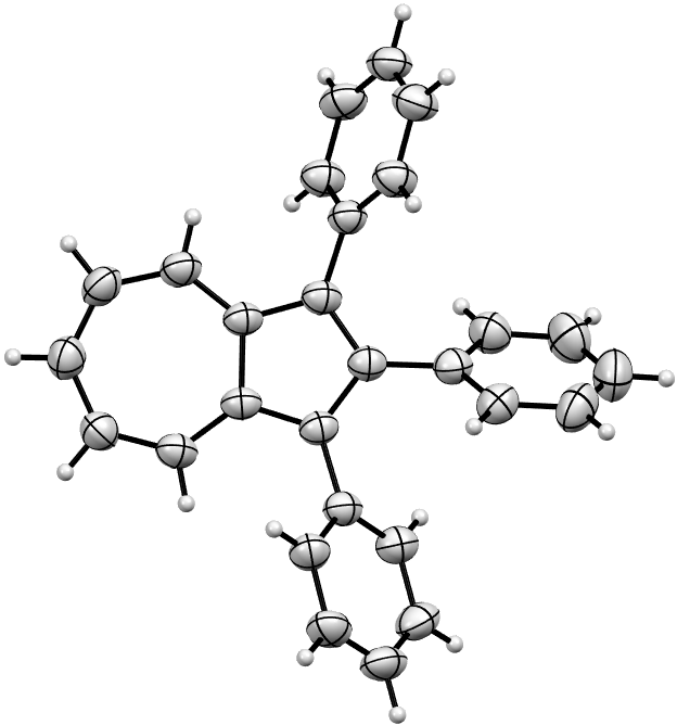


Figure S14. ORTEP drawing of **3a** with 50% probability thermal ellipsoids. (CCDC number: 2071102)

Table S3. Crystal data for 3a.

Identification code	**3a**
Empirical formula	$C_{28}H_{20}$
Formula weight	356.44
Temperature/K	291.4(7)
Crystal system	triclinic
Space group	P-1
a/Å	8.4176(5)
b/Å	10.9015(6)
c/Å	11.3672(7)
α/°	110.376(5)
β/°	95.240(5)
γ/°	92.506(5)
Volume/Å^3	970.55(10)
Z	2
ρ_{calc}g/cm^3	1.220
μ/mm^{-1}	0.521
F(000)	376.0
Crystal size/mm^3	0.7 × 0.5 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.352 to 143.318
Index ranges	-10 ≤ h ≤ 7, -13 ≤ k ≤ 13, -13 ≤ l ≤ 13
Reflections collected	8096

Independent reflections	3720 [R_{int} = 0.0353, R_{sigma} = 0.0396]
Data/restraints/parameters	3720/0/253
Goodness-of-fit on F^2	1.018
Final R indexes [I>=2σ (I)]	R_1 = 0.0627, wR_2 = 0.1746
Final R indexes [all data]	R_1 = 0.0706, wR_2 = 0.1885
Largest diff. peak/hole / e Å^{-3}	0.23/-0.31

VIII. Computational investigations

1. Computational method.

Geometry optimization was carried out with Gaussian 09 E.01[7] program package. PBE0-D3(BJ) level[8,9] and a slightly modified version of Ahlrichs' def2-SVP basis set[10] with corresponding pseudo-potential[11] were used. From the original def2-SVP basis set, all p polarization functions on H atoms were removed in order to save computational time and the corresponding basis set was named as def2-SVP(-p) in the main text. Such basis set is slightly larger and more precise than def2-SV(P) since the f polarization functions on Pd was kept. The default FINE integration grid was used. Solvation effect was modeled with IEFPCM solvation model[12] of THF, since reliable IEFPCM parameters of the 2-Me-THF was not accessible. Thermodynamic data based on Gaussian's frequency analysis at 423.15 K was obtained with Shermo 2.0.8 code[13] and Grimme's quasi-RRHO method[14] as implemented in Shermo. A ZPE scaling factor of 0.98055 was used for current optimization, which was obtained by fitting the ZPVE15/10 data set.[15] Gibbs free energies of all species were corrected to 1 M standard state in solution from standard state in gas phase by adding 2.98 kcal/mol to the calculated free energy. Single point energy calculations were carried out on ORCA 4.2.1 program package,[16] at *w*B97M-V/def2-QZVP level[17,10,11] with SMD solvation model[18] of THF. RI with def2/J auxiliary basis set[19] and RIJCOSX approximations[20] were used for accelerating calculation. GRID4 and GRIDX4 with TightSCF convergence criteria was applied. RDG analysis was performed with Multiwfn[21] 3.8 2021-May-8 dev version and visualized with VMD 1.9.3. package[22], based on the IEFPCM/PBE0/def2-SVP(-p) wavefunction.

2. Influence of diffuse functions on electronic energies

In order to evaluate the influence of diffuse functions in single point calculations, the absolute energy of I^- anion and the simplified **Cat.** [(acac)PdI(Bglycol)$^-$] were re-calculated using ma-def2-QZVP[23] and aug-def2-QZVP (def2-QZVP with aug-cc-pVQZ(-PP for Pd)[11b,24-26] diffuse functions) basis set and corresponding pseudo potential. All other computational settings were kept the same as main text except the auto-generated RI auxiliary basis set, namely AUTOAUX[27] in ORCA, was utilized instead of def2/J and threshold for basis set linear dependency was set to 10^{-6} (STHRESH 1E-6, does not change the def2-QZVP energy for current examples). For convenience of comparison, calculation using combination of def2-QZVP and AUTOAUX was also performed. The results listed below suggest that the error induced from not utilizing diffuse functions would be much lower than 1 kcal/mol.

Table S4. Influence of diffuse functions and aux basis set on single point energies.

Specie	Basis set	Aux basis set	E_{el} (Ha)	E_{rel} (kcal/mol)
I^-	def2-QZVP	def2/J	-297.862297372554	0.001
	def2-QZVP	AUTOAUX	-297.862298242401	0
	ma-def2-QZVP	AUTOAUX	-297.862465924638	-0.105
	aug-def2-QZVP	AUTOAUX	-297.862483827000	-0.116
Cat.	def2-QZVP	def2/J	-1025.038489032568	-0.402
	def2-QZVP	AUTOAUX	-1025.037848636010	0
	ma-def2-QZVP	AUTOAUX	-1025.038172648889	-0.203
	aug-def2-QZVP	AUTOAUX	-1025.038461104335	-0.384

3. Evaluation of ZPE scale factor

The ZPVE15/10 database[15] contains experimental ZPEs of totally 15 small main-group molecules. Since the utilized def2-SVP(-p) basis set is identical to def2-SV(P) for main-group elements, molecules in ZPVE15/10 database were optimized under PBE0-D3(BJ)/def2-SV(P) level and the calculated ZPE was lineally fitted to the experimental ZPE with the intercept of being 0. The result was listed below, showing that the scaling factor for ZPE correction is 0.98055 which is used in the present calculations.

Table S5. ZPE data for evaluating ZPE scale factor.

Molecule	Exp. ZPE (kcal/mol)	PBE0-D3(BJ)/def2-SV(P) Calc. ZPE	
		(Hartree)	(kcal/mol)
C_2H_2	16.49	0.027199	17.06762
CH_4	27.710	0.044675	28.03396
Cl_2	0.7983	0.001199	0.752383
CO_2	7.3	0.012002	7.531363
CO	3.0929144	0.005183	3.252379
F_2	1.3021	0.002453	1.539280
H_2CO	16.1	0.026887	16.87183
H_2O	13.26	0.020900	13.11494
H_2	6.2310	0.009960	6.249990
HCN	10.0	0.016466	10.33256
HF	5.68353	0.008925	5.600518
N_2O	6.770	0.011763	7.381388
N_2	3.3618	0.005764	3.616962
NH_3	21.200	0.034142	21.42441
·OH	5.2915	0.008256	5.180714

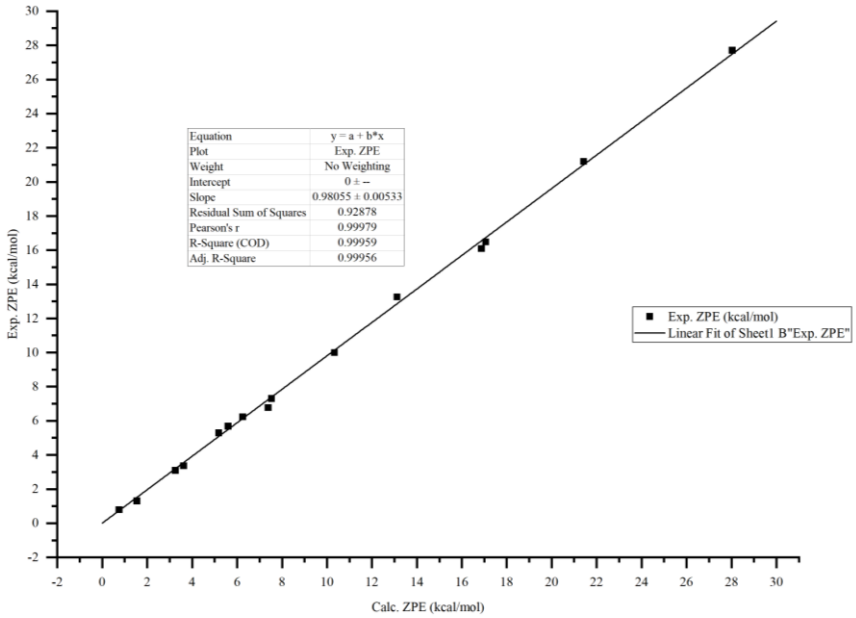


Figure S15. Linear fit graph of experimental to calculated ZPE.

4. Discussions of other possible pathways that are disfavored

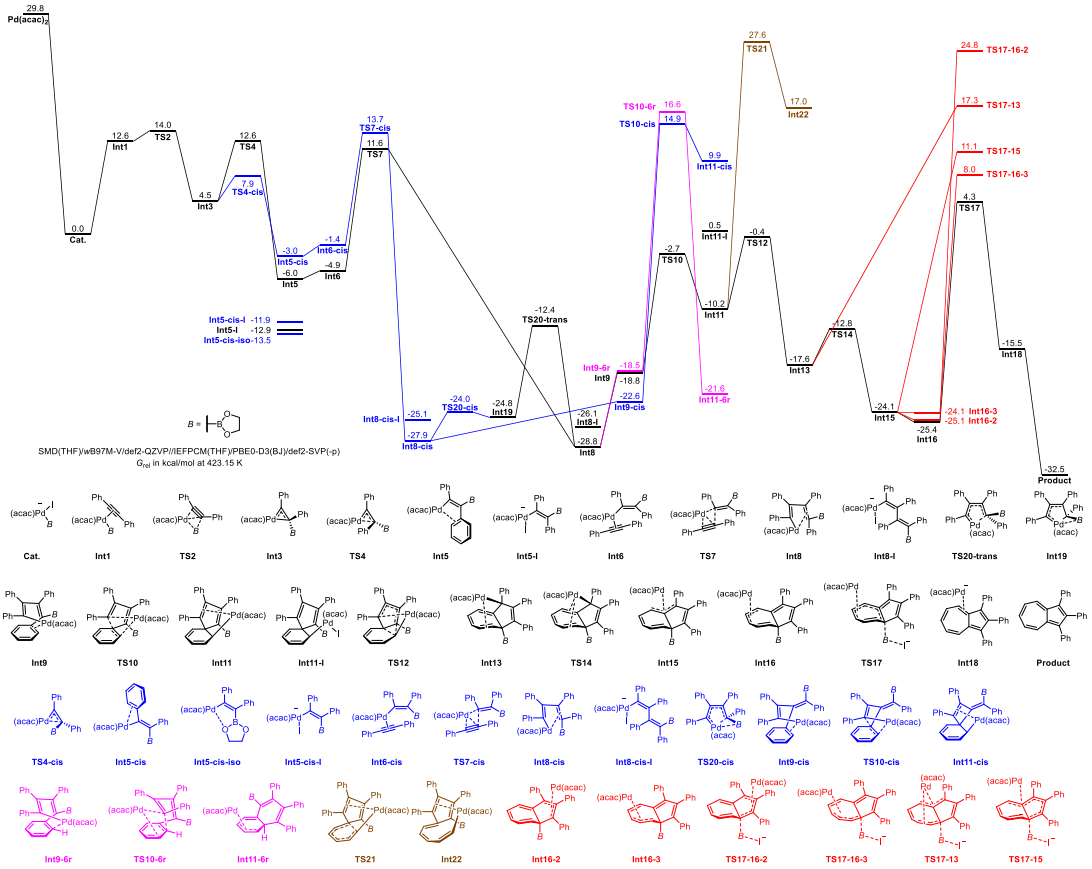


Figure S16. A general view of the whole considered.

4.1 Possible pathway after the *cis*-1st addition

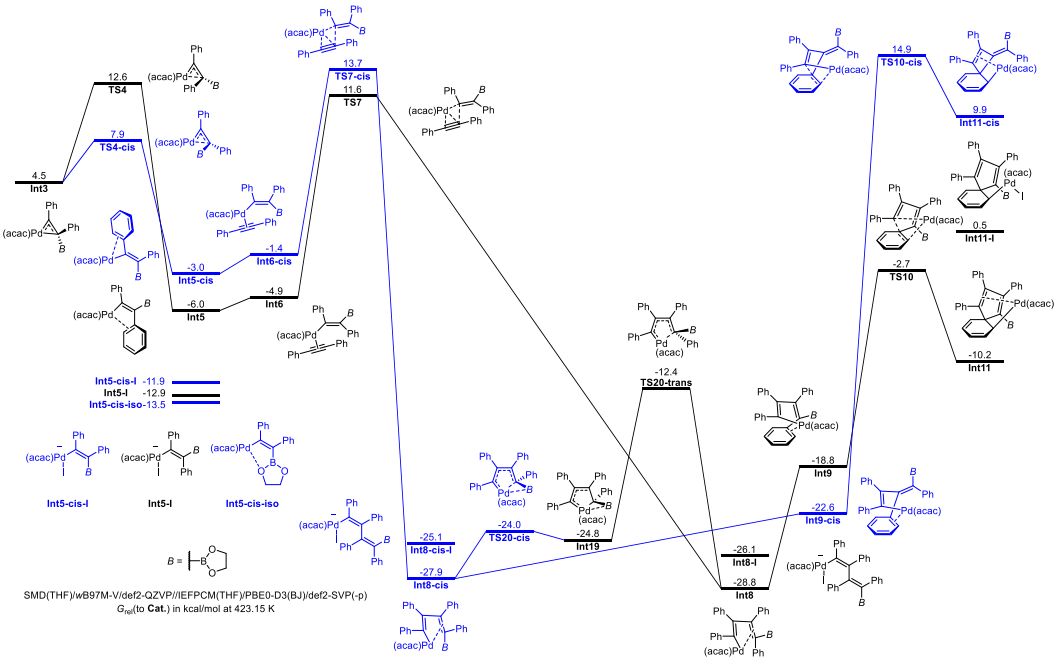


Figure S17. Possible reaction PES after the *cis*-1st addition.

As stated in the main text, the addition of Pd-B bond in **Int1** towards the diphenylacetylene gives **Int3**, in which the C=C double bond in the boryl vinyl is twisted to become a carbanion-carbene type ligand. The C–C bond in **Int3** may rotate to give either **Int5** or **Int5-cis** (via **TS4** and **TS4-cis**, respectively). The relative stability **Int5-cis-iso** with a borate group coordinating to Pd center was overestimated compared to the full model calculation in main text, (**Figure 2 (b)**) probably because of an overestimation of coordination ability of the borate group due to neglecting of the methyl groups. **Int5** and **Int5-cis** have similar reaction pathways to perform the second addition step to give corresponding **Int8** and **Int8-cis** and their iodo-complexes. Another isomerization pathway between **Int8** and **Int8-cis** occurs, via a direct rotation of the terminal C=C bond. Such pathway goes through **Int19**, **TS20-trans** and **TS20-cis**, with a $\Delta G^{\neq}$ of 15.5 kcal/mol (**Int8-cis** to **TS20-trans**). Since the δ-phenyl ring is not accessible for **Int8-cis** to perform the dearomatization, it may only go through **TS10-cis** to give a strained spiro-[5.3] skeleton **Int11-cis**, with highly disfavored $\Delta G^{\neq}$ and ΔG.

4.2 An insertion pathway towards 6/6 fused bicyclic rings

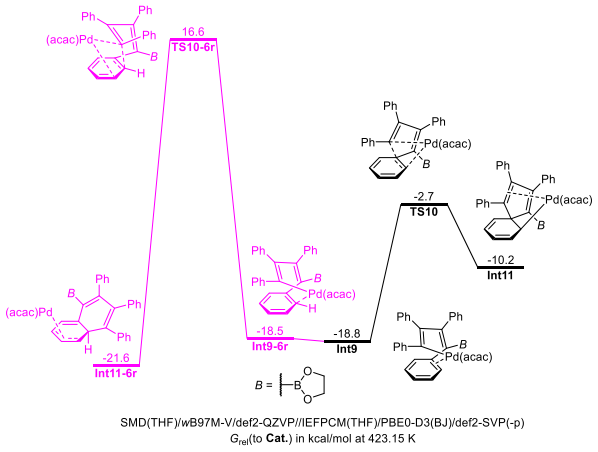


Figure S18. Possible farther insertion from **Int9**.

Another pathway forming a monohydronaphthene palladium(II) complex through insertion of the carbon-palladium bond to the π bond on C2-C3 instead of C1-C2 on the δ-Ph was found. Via **TS10-6r**, **Int11-6r** is generated with a high $\Delta G^{\neq}$ of 35.4 kcal/mol (**Int9** to **TS10-6r**), probably due to the strain in the transition state. This can be excluded for consideration.

4.3 A migration pathway via 6π-electrocyclic ring opening

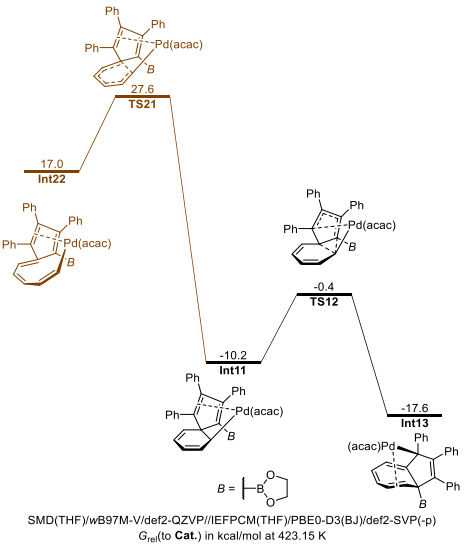


Figure S19. Possible 6π-electrocyclic ring opening from **Int11**.

Alternative pathway from **Int11** to **Int13** could occur through a 6π-electrocyclic ring opening to give **Int22**, which is followed by Suzuki coupling. Calculation shows the activation Gibbs free energy for the electrocyclic ring opening step is 37.8 kcal/mol (from **Int11** to **TS21**) and is endothermic by 27.2 kcal/mol. This pathway is disfavored compared to the vinyl [1,5] shift (via **TS12**) and can be ruled out.

4.4 Other possible TSs for E_1cb type dissociation

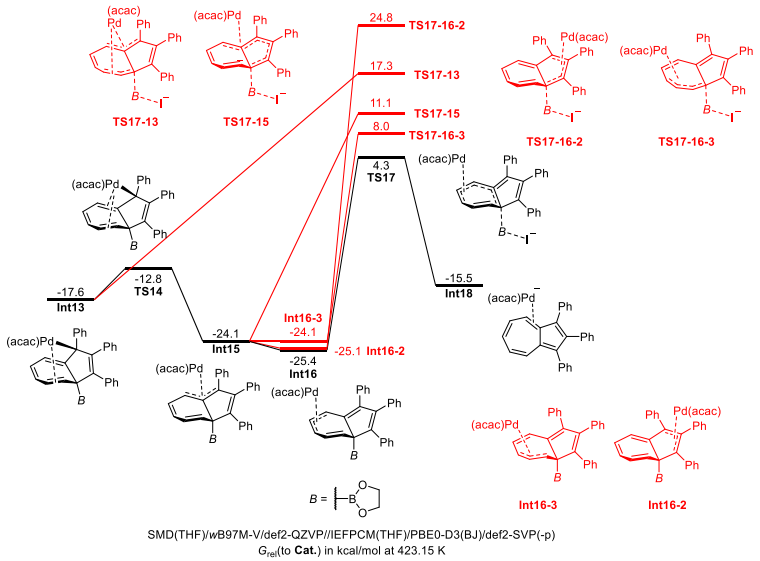


Figure S20. Several other unfavored TSs for boryl group dissociation.

Several isomers of **Int16** and **TS17** corresponding to the shifts of Pd(acac) group on the conjugative system were also located, but all of them are energetically disfavored and can be ruled out.

5. Optimized atomic coordinates and energies

acac-B

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -599.331378634803 a.u.

Thermal correction to G: 320.786 kJ/mol 76.670 kcal/mol 0.122181 a.u.

Optimized atomic Cartesian coordinates:

O	0.17682500	1.22164100	-0.12316800
C	1.45195800	1.20304400	0.01423100
O	0.18683200	-1.21875100	-0.16934700
C	1.46210500	-1.19404600	-0.02963400
C	2.16181300	0.00524100	0.10060800
H	3.24481600	0.00729400	0.21338000
C	2.11588400	2.53493000	0.05363700
H	1.71825100	3.11364000	0.90571900
H	3.20765600	2.44937800	0.14469200
H	1.86311700	3.09517600	-0.86333700
C	2.13642400	-2.52123900	-0.03289600
H	1.74414400	-3.12959300	0.80086900
H	1.88747300	-3.05455900	-0.96677200
H	3.22751700	-2.42963200	0.06050900
B	-0.71524200	-0.00463000	-0.08061900
O	-1.44781900	-0.00103900	1.13755000
O	-1.62412100	-0.01570100	-1.16891400
C	-2.79988300	-0.21958500	0.81873300
C	-2.91047600	0.21088700	-0.64769300
H	-3.45527100	0.36431700	1.48900300
H	-3.05888300	-1.29175200	0.93745700
H	-3.66342400	-0.36900800	-1.21016800
H	-3.17868000	1.28458800	-0.72566000

B2

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -508.076469489889 a.u.

Thermal correction to G: 224.725 kJ/mol 53.711 kcal/mol 0.085593 a.u.

Optimized atomic Cartesian coordinates:

B	0.00000300	0.85402800	0.00002800
O	-1.13057200	1.61081500	-0.12827200
O	1.13058000	1.61081000	0.12833100
C	0.75925900	2.98532000	0.13065300
H	1.32685300	3.51643400	-0.65068400
H	1.02091000	3.42538000	1.10773600
C	-0.75924500	2.98532400	-0.13059800
H	-1.32683700	3.51644200	0.65073800
H	-1.02089400	3.42538200	-1.10768300

B	-0.00000300	-0.85402800	0.00002800
O	1.13057200	-1.61081500	-0.12827200
O	-1.13058000	-1.61081000	0.12833100
C	0.75924500	-2.98532400	-0.13059800
C	-0.75925900	-2.98532000	0.13065300
H	1.32683700	-3.51644200	0.65073800
H	1.02089400	-3.42538200	-1.10768300
H	-1.32685300	-3.51643400	-0.65068400
H	-1.02091000	-3.42538000	1.10773600

Cat

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -1025.038489032568 a.u.

Thermal correction to G: 282.356 kJ/mol 67.485 kcal/mol 0.107544 a.u.

Optimized atomic Cartesian coordinates:

Pd	-0.22871400	-0.00719200	-0.00010600
O	-1.99021900	-1.34850900	0.00161200
C	-3.17674900	-0.94426900	-0.00212900
O	-1.53044300	1.60718600	-0.00391400
C	-2.79612000	1.55312900	-0.00809800
C	-3.60654800	0.40652100	-0.00739200
H	-4.68552200	0.57600800	-0.01111300
C	-4.24358300	-2.01853400	-0.00025500
H	-4.11391800	-2.65626500	0.89197100
H	-5.26783300	-1.61465700	-0.00805500
H	-4.10482300	-2.66872400	-0.88199300
C	-3.47303300	2.90499300	-0.01479800
H	-3.14726300	3.48046400	0.86957400
H	-3.14654500	3.47172600	-0.90459200
H	-4.57155900	2.83620900	-0.01508400
B	1.29436200	1.23625500	-0.00122000
O	1.86194200	1.77021100	1.13913400
O	1.83802800	1.79361200	-1.14183100
C	2.76114300	2.79946600	0.75830300
C	2.91173600	2.63967200	-0.76272700
H	3.71638300	2.68045300	1.29648600
H	2.33051300	3.77988800	1.03282300
H	2.84263300	3.59861600	-1.30299700
H	3.86814800	2.15734300	-1.03574600
I	1.66294900	-1.79329300	-0.00060000

I-

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -297.862297372554 a.u.

Thermal correction to G: -65.860 kJ/mol -15.741 kcal/mol -0.025085 a.u.
Optimized atomic Cartesian coordinates:

I	0.00000000	0.00000000	0.00000000

I-B
Charge = 0 Multiplicity = 1
wB97M-V single point energy: -551.761916518152 a.u.
Thermal correction to G: 57.472 kJ/mol 13.736 kcal/mol 0.021890 a.u.
Optimized atomic Cartesian coordinates:

B	0.00000000	0.00000000	-0.73259100
O	0.01595800	-1.14286400	-1.45384300
O	-0.01595800	1.14286400	-1.45384300
C	0.05330200	-0.76999600	-2.83447700
C	-0.05330200	0.76999600	-2.83447700
H	-0.78433400	-1.25623100	-3.35798500
H	0.99890800	-1.13033600	-3.27027800
H	0.78433400	1.25623100	-3.35798500
H	-0.99890800	1.13033600	-3.27027800
I	0.00000000	0.00000000	1.40020300

Pd(acac)2
Charge = 0 Multiplicity = 1
wB97M-V single point energy: -818.372342886382 a.u.
Thermal correction to G: 402.212 kJ/mol 96.131 kcal/mol 0.153194 a.u.
Optimized atomic Cartesian coordinates:

O	1.36455400	1.45026400	0.00000000
C	2.61824100	1.24969700	0.00000000
O	1.36455400	-1.45026400	0.00000000
C	2.61824100	-1.24969700	0.00000000
C	3.25844500	0.00000000	0.00000000
H	4.34924000	0.00000000	0.00000000
C	3.44862500	2.50263900	0.00000000
H	3.19464400	3.10759000	0.88764600
H	4.52777200	2.29210300	0.00000000
H	3.19464400	3.10759000	-0.88764600
C	3.44862500	-2.50263900	0.00000000
H	3.19464400	-3.10759000	0.88764600
H	3.19464400	-3.10759000	-0.88764600
H	4.52777200	-2.29210300	0.00000000
Pd	0.00000000	0.00000000	0.00000000
O	-1.36455400	-1.45026400	0.00000000
O	-1.36455400	1.45026400	0.00000000
C	-2.61824100	-1.24969700	0.00000000
C	-2.61824100	1.24969700	0.00000000

C	-3.25844500	0.00000000	0.00000000
C	-3.44862500	-2.50263900	0.00000000
C	-3.44862500	2.50263900	0.00000000
H	-4.34924000	0.00000000	0.00000000
H	-3.19464400	-3.10759000	0.88764600
H	-4.52777200	-2.29210300	0.00000000
H	-3.19464400	-3.10759000	-0.88764600
H	-3.19464400	3.10759000	0.88764600
H	-3.19464400	3.10759000	-0.88764600
H	-4.52777200	2.29210300	0.00000000

PhCCPh

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -539.480928707558 a.u.

Thermal correction to G: 347.976 kJ/mol 83.168 kcal/mol 0.132537 a.u.

Optimized atomic Cartesian coordinates:

C	0.00000000	0.00000000	0.60959600
C	0.00000000	0.00000000	-0.60959600
C	0.00000000	0.00000000	2.03488600
C	-0.00006100	1.21278800	2.75002900
C	0.00006100	-1.21278800	2.75002900
C	-0.00006000	1.20802200	4.14153800
H	-0.00010800	2.15769100	2.20040700
C	0.00006000	-1.20802200	4.14153800
H	0.00010800	-2.15769100	2.20040700
C	0.00000000	0.00000000	4.84189800
H	-0.00010700	2.15713000	4.68558700
H	0.00010700	-2.15713000	4.68558700
H	0.00000000	0.00000000	5.93580600
C	0.00000000	0.00000000	-2.03488600
C	0.00006100	1.21278800	-2.75002900
C	-0.00006100	-1.21278800	-2.75002900
C	0.00006000	1.20802200	-4.14153800
H	0.00010800	2.15769100	-2.20040700
C	-0.00006000	-1.20802200	-4.14153800
H	-0.00010800	-2.15769100	-2.20040700
C	0.00000000	0.00000000	-4.84189800
H	0.00010700	2.15713000	-4.68558700
H	-0.00010700	-2.15713000	-4.68558700
H	0.00000000	0.00000000	-5.93580600

Int1

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1266.656518202400 a.u.

Thermal correction to G: 734.139 kJ/mol 175.463 kcal/mol 0.279619 a.u.

Optimized atomic Cartesian coordinates:

Pd	-0.48850900	0.54935400	0.04897000
O	-1.89543800	0.07775000	-1.55558700
C	-2.94202600	0.73079300	-1.79500300
O	-1.65635200	2.15689000	0.55294200
C	-2.73761100	2.51270100	-0.02259600
C	-3.37339200	1.88940300	-1.10292800
H	-4.30418200	2.34558700	-1.44529400
C	-3.79997900	0.21460000	-2.92403400
H	-4.10328700	-0.82317200	-2.69956600
H	-4.69898700	0.82481500	-3.09757600
H	-3.19932200	0.18051100	-3.84972700
C	-3.36531800	3.74846000	0.56871800
H	-3.56022000	3.58002200	1.64232600
H	-2.64961400	4.58659400	0.49986200
H	-4.30358500	4.03222900	0.06949200
C	0.27410800	-1.37985000	-0.12684600
C	1.15778100	-0.59034000	-0.56006300
C	-0.39398200	-2.59265100	0.23963500
C	0.29803700	-3.81439700	0.13151700
C	-1.72111100	-2.59473000	0.70229100
C	-0.32839400	-5.00624300	0.47932300
H	1.33117400	-3.81791700	-0.22615600
C	-2.33923100	-3.79190600	1.04961200
H	-2.26051700	-1.64728000	0.78029800
C	-1.64722100	-4.99950300	0.93989000
H	0.21780500	-5.94994000	0.39191900
H	-3.37222900	-3.78238700	1.40895700
H	-2.13640600	-5.93872600	1.21404200
C	2.42054600	-0.17022300	-1.09777100
C	3.37553300	-1.14818200	-1.43771800
C	2.73029500	1.18648300	-1.29139000
C	4.60898500	-0.77138800	-1.95719600
H	3.13899400	-2.20534000	-1.28961200
C	3.96914200	1.55458900	-1.80861000
H	1.99312600	1.94612900	-1.02048000
C	4.91055600	0.58013900	-2.14386700
H	5.34330400	-1.53903000	-2.21809800
H	4.20096200	2.61378900	-1.95258500
H	5.88238800	0.87319300	-2.55164800
B	0.73794700	0.98748300	1.55013200
O	1.04493200	0.14482600	2.58162200
O	1.35704700	2.20277900	1.64694600

C	1.85836100	0.86365300	3.50617500
C	2.24282800	2.15373600	2.76229400
H	2.73110600	0.25032800	3.78049600
H	1.27046500	1.06458100	4.41830300
H	2.11319100	3.05854100	3.37676200
H	3.28153200	2.12851900	2.38931100

TS2

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1266.651549913502 a.u.

Thermal correction to G: 740.277 kJ/mol 176.930 kcal/mol 0.281957 a.u.

Optimized atomic Cartesian coordinates:

Pd	0.70762600	-0.41811600	-0.06216300
O	2.68581000	0.29468900	-0.50032400
C	3.73679500	-0.39833200	-0.60834900
O	1.53060800	-2.33673600	-0.05388600
C	2.74214700	-2.66376800	-0.22436400
C	3.81556900	-1.79898300	-0.49882200
H	4.80078400	-2.25336100	-0.61767700
C	-0.26887600	1.37036800	-0.05541400
C	-1.15347600	0.49128800	-0.34402700
C	0.13444300	2.73667000	0.14600400
C	-0.85062500	3.72277900	0.35125800
C	1.48920700	3.11199700	0.13800300
C	-0.48533100	5.05148900	0.53816200
H	-1.90536700	3.43660400	0.36324100
C	1.84472600	4.44494800	0.32560200
H	2.24548800	2.34032500	-0.03019900
C	0.86316600	5.41711500	0.52656200
H	-1.25873600	5.80885500	0.69634500
H	2.90131600	4.72889600	0.31507300
H	1.14800200	6.46285600	0.67589700
C	-2.49246600	0.13753200	-0.76589100
C	-2.71431300	-0.89348800	-1.69308100
C	-3.59216800	0.84202500	-0.24599200
C	-4.00728200	-1.19868100	-2.10460300
H	-1.85887100	-1.45083200	-2.08253000
C	-4.88436200	0.53007800	-0.66095000
H	-3.42651100	1.62615600	0.49741100
C	-5.09570500	-0.48913500	-1.59090400
H	-4.16892800	-1.99944300	-2.83199200
H	-5.73321000	1.08437700	-0.25008000
H	-6.11170300	-0.73456300	-1.91376300
B	-0.80434400	-1.27733700	0.93832800

O	-1.16860200	-0.87166800	2.19149900
O	-1.39025000	-2.44435700	0.55085100
C	-1.99664800	-1.89532100	2.74192900
C	-2.36383000	-2.77346200	1.53659300
H	-2.87355100	-1.43690900	3.22498100
H	-1.42114400	-2.44881800	3.50383400
H	-2.31905800	-3.85116200	1.75749400
H	-3.36502400	-2.53398300	1.13559200
C	5.00093600	0.38132500	-0.86660300
H	5.18309000	1.06528500	-0.01864300
H	5.88221300	-0.26303800	-1.00360000
H	4.86411200	1.00925200	-1.76402200
C	3.01530900	-4.14182700	-0.11008500
H	4.07393000	-4.39494200	-0.27027800
H	2.70549400	-4.49141700	0.89041600
H	2.39645000	-4.68407000	-0.84619400

Int3

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1266.667144596439 a.u.

Thermal correction to G: 741.402 kJ/mol 177.199 kcal/mol 0.282385 a.u.

Optimized atomic Cartesian coordinates:

Pd	0.88497800	0.00657500	-0.14004900
O	2.26478900	1.56551600	-0.05339500
C	3.48053200	1.50006600	-0.40841100
O	2.38645700	-1.23523300	-0.93395900
C	3.58485300	-0.89960900	-1.14882900
C	4.14476300	0.37566000	-0.92569100
H	5.20085900	0.49998300	-1.17186000
C	4.25264600	2.78381100	-0.23853400
H	3.77556900	3.57651000	-0.84139600
H	4.19907900	3.10417100	0.81654200
H	5.30747500	2.69033700	-0.53651300
C	4.47164500	-1.98824300	-1.69794900
H	4.46436100	-2.84678500	-1.00385400
H	4.05517900	-2.34602700	-2.65601000
H	5.50929000	-1.65867500	-1.85597100
C	-0.79842100	0.69646200	0.34924400
C	-1.18635400	-0.62693900	0.31795600
C	-1.41163300	1.98146700	0.46780600
C	-2.76497400	2.10701500	0.85110800
C	-0.64717900	3.14084100	0.22000400
C	-3.34080200	3.36467900	0.96220000
H	-3.34900300	1.20512000	1.05347100

C	-1.22985100	4.39644400	0.34109800
H	0.40631300	3.02185700	-0.05150700
C	-2.57471800	4.50768500	0.70549900
H	-4.39017400	3.46319200	1.25353400
H	-0.63824400	5.29624300	0.15122000
H	-3.03258500	5.49735300	0.79602400
C	-2.32979500	-1.10686100	-0.49817700
C	-3.10570100	-2.20185800	-0.08870300
C	-2.68343900	-0.44590500	-1.68674800
C	-4.20834100	-2.61258600	-0.83596000
H	-2.84145000	-2.73625900	0.82716700
C	-3.78648800	-0.85388900	-2.43113000
H	-2.07071700	0.39141900	-2.03531700
C	-4.55586500	-1.93963500	-2.00776600
H	-4.80196300	-3.46736300	-0.49773100
H	-4.04189600	-0.32629600	-3.35509200
H	-5.41999400	-2.26512300	-2.59456800
B	-0.36629700	-1.59891100	1.23608600
O	0.16902400	-1.24292900	2.45900900
O	-0.25516700	-2.94662000	0.98918400
C	0.33769300	-3.54896800	2.13035500
H	1.12389900	-4.25223100	1.81309900
H	-0.43511300	-4.11293400	2.68300900
C	0.88697100	-2.36882400	2.94424800
H	0.72180100	-2.47573300	4.02796100
H	1.96622000	-2.21314300	2.76575700

TS4

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1266.656061791030 a.u.

Thermal correction to G: 746.087 kJ/mol 178.319 kcal/mol 0.284170 a.u.

Optimized atomic Cartesian coordinates:

Pd	-0.87612900	0.06969400	-0.19727900
O	-2.17959200	1.60566100	0.28920100
C	-3.40243800	1.67013900	-0.04666500
O	-2.45123900	-0.92008000	-1.20747900
C	-3.63136300	-0.48913200	-1.31647000
C	-4.12406500	0.72715000	-0.79460800
H	-5.17551900	0.95250700	-0.98187100
C	0.84607200	0.59683000	0.30597400
C	1.24997100	-0.72695200	0.14790300
C	1.50973500	1.85318800	0.47404400
C	2.86452900	1.90655600	0.86796600
C	0.79570100	3.05659100	0.29109100

C	3.49272600	3.13152100	1.04601800
H	3.40750700	0.97257900	1.03439300
C	1.42858500	4.27860000	0.47856200
H	-0.26160200	2.99928200	0.01725500
C	2.77628900	4.31680500	0.84914300
H	4.54355600	3.16995800	1.34631900
H	0.87386900	5.21028000	0.33687200
H	3.27296000	5.28093200	0.99423700
C	0.66322800	-1.78246300	1.02449900
C	0.48543300	-3.10514300	0.57793900
C	0.31434400	-1.48155900	2.35757200
C	-0.03725300	-4.07867500	1.42425500
H	0.75477600	-3.36138800	-0.44898300
C	-0.21705100	-2.45708500	3.19720300
H	0.47969100	-0.46786300	2.73621300
C	-0.39757200	-3.76207600	2.73626600
H	-0.17079300	-5.09892100	1.05127000
H	-0.48099000	-2.19606300	4.22673100
H	-0.80986000	-4.53015100	3.39719500
B	2.37911500	-1.04471000	-0.87398700
O	2.89864900	-0.10074500	-1.71863100
O	2.95014300	-2.27690300	-1.03660400
C	3.84879600	-2.19937200	-2.13644200
H	3.41805000	-2.75275000	-2.98892100
H	4.80681600	-2.66966700	-1.86382900
C	3.97933600	-0.69385600	-2.42424500
H	4.92867100	-0.27670600	-2.04449900
H	3.89840700	-0.45360900	-3.49622300
C	-4.11197300	2.91069500	0.43433900
H	-3.60386300	3.80175200	0.02545400
H	-5.17259400	2.93501500	0.14344800
H	-4.03473900	2.97101300	1.53393800
C	-4.58097500	-1.38067300	-2.07650300
H	-5.58986000	-0.95248000	-2.17203000
H	-4.17039700	-1.57445400	-3.08276700
H	-4.64923700	-2.35608500	-1.56342800

TS4-cis

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1266.664068286217 a.u.

Thermal correction to G: 747.472 kJ/mol 178.650 kcal/mol 0.284697 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.07052700	-0.13589200	0.13482900
O	-2.19726500	1.55374600	-0.17919200

C	-3.45289000	1.61346100	0.00151200
O	-2.76786600	-1.21019600	0.76433900
C	-3.93506500	-0.73160000	0.79480000
C	-4.30057400	0.58914500	0.45380900
H	-5.35922500	0.84014900	0.54058300
C	0.67414900	0.52376800	-0.24767400
C	1.33344400	-0.67365400	-0.20178900
C	1.16377200	1.88138200	-0.37328800
C	2.30792900	2.14387900	-1.15421500
C	0.50778600	2.95654800	0.25424300
C	2.78515200	3.44145600	-1.29310300
H	2.81422400	1.31224600	-1.65175800
C	0.99530700	4.25301300	0.11990100
H	-0.38913800	2.75667500	0.84331400
C	2.13236700	4.49878200	-0.65250300
H	3.67234600	3.63355600	-1.90356100
H	0.48300700	5.08095400	0.61866100
H	2.51089600	5.51979700	-0.75970100
C	2.71789400	-0.80355000	0.32254500
C	3.62057900	-1.71688200	-0.24474000
C	3.16338400	-0.00398800	1.38825200
C	4.93039600	-1.81106800	0.22198600
H	3.29463800	-2.35545100	-1.07050800
C	4.47104200	-0.09928000	1.85660300
H	2.46620800	0.69488000	1.85950800
C	5.36255300	-1.00166000	1.27330500
H	5.61947100	-2.52425100	-0.24068800
H	4.79484200	0.53166900	2.68999200
H	6.38963300	-1.07884700	1.64235400
B	0.57908600	-1.97776200	-0.64231100
O	-0.43008800	-2.00105800	-1.58713700
O	0.88162800	-3.22697300	-0.17467500
C	0.09078400	-4.16840900	-0.89137600
H	-0.33685400	-4.90074300	-0.18922500
H	0.73548200	-4.70393000	-1.61012300
C	-0.97832500	-3.31783700	-1.58974900
H	-1.17573900	-3.62943300	-2.62665900
H	-1.92936500	-3.29986800	-1.03057100
C	-4.05320400	2.95752100	-0.32452800
H	-3.84756400	3.20005500	-1.38174300
H	-5.13852800	2.99266700	-0.14944500
H	-3.56031300	3.73392500	0.28616400
C	-5.01543400	-1.68383000	1.23992500
H	-6.01592300	-1.22673100	1.24654100

H	-5.02205500	-2.56163300	0.57011900
H	-4.77871900	-2.05340800	2.25306100

Int5

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1266.685043835749 a.u.

Thermal correction to G: 744.401 kJ/mol 177.916 kcal/mol 0.283527 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.01515900	-0.10759700	0.20257100
O	-2.98742300	-0.83932900	0.06445500
C	-3.99265500	-0.13932900	-0.22951900
O	-1.67633100	1.77825300	-0.16074600
C	-2.87843200	2.10151100	-0.42204900
C	-3.99186600	1.25245100	-0.47102900
H	-4.95101300	1.71355800	-0.71286000
C	-5.29911800	-0.88595100	-0.32056100
H	-5.49708100	-1.38775100	0.64263400
H	-6.14944000	-0.23468000	-0.57148600
H	-5.21040600	-1.67836000	-1.08429100
C	-3.06614800	3.56996400	-0.70096200
H	-2.70375900	4.15357400	0.16290800
H	-2.44388800	3.85711300	-1.56675000
H	-4.11448800	3.83294900	-0.90503800
C	0.88514600	0.38204800	0.19118500
C	1.51753700	-0.80626500	0.06133800
C	1.43375500	1.73398900	0.24568600
C	2.32758000	2.08055100	1.27293600
C	1.08868600	2.70795200	-0.70594800
C	2.86428000	3.36372500	1.34469200
H	2.59876500	1.32678700	2.01739000
C	1.63865500	3.98552300	-0.63968800
H	0.38723600	2.44989000	-1.50146000
C	2.52342400	4.32076000	0.38751900
H	3.55827300	3.61727800	2.15201900
H	1.36977800	4.73014400	-1.39534700
H	2.94660400	5.32841300	0.44186900
C	0.47283000	-1.87755000	0.15416200
C	-0.29238100	-1.98242300	1.34672600
C	0.22646200	-2.80745600	-0.88910300
C	-1.27161400	-2.99239800	1.47705800
H	0.00685300	-1.40453900	2.22704300
C	-0.73762700	-3.78569500	-0.74287400
H	0.81942900	-2.74090000	-1.80507300
C	-1.49551600	-3.87789000	0.44203500

H	-1.84089500	-3.06850900	2.40737500
H	-0.91598500	-4.49693400	-1.55491100
H	-2.25360000	-4.65997100	0.54167400
B	3.00434700	-1.10854600	-0.23981300
O	3.45560500	-2.38858000	-0.42645900
O	3.99042800	-0.17055000	-0.36692100
C	5.18627000	-0.83571900	-0.74796600
H	6.01046500	-0.51961200	-0.08820000
H	5.44258100	-0.54932000	-1.78277100
C	4.86216500	-2.33712900	-0.61975300
H	5.13238400	-2.91083600	-1.52102000
H	5.36097900	-2.80148800	0.24859100

Int5-cis

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1266.680787697671 a.u.

Thermal correction to G: 745.812 kJ/mol 178.253 kcal/mol 0.284065 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.18412500	-0.49741700	-0.22310600
O	1.50814800	1.46161100	0.31762500
C	2.65165400	1.95547900	0.56704300
O	3.24979900	-0.84511100	-0.33322500
C	4.13032000	0.00203800	-0.01751800
C	3.89542500	1.31917100	0.43236300
H	4.77528100	1.91355800	0.68523200
C	2.62661700	3.38550900	1.04304800
H	1.89607200	3.48358300	1.86369200
H	3.61188100	3.73466500	1.38541000
H	2.28819300	4.04079000	0.22095400
C	5.55640900	-0.46930900	-0.14654600
H	5.69070900	-1.38952200	0.44806600
H	5.75543100	-0.73428800	-1.20003600
H	6.28879800	0.28439300	0.17857200
C	-0.77344900	-0.51492200	-0.14345500
C	-1.76257900	0.38343200	-0.12291600
C	-0.48258600	-1.91009300	0.01083700
C	0.36877500	-2.45287900	-1.00540800
C	-0.65994900	-2.63856300	1.22422700
C	1.02013900	-3.69145100	-0.78194600
H	0.33610700	-2.04024100	-2.02062800
C	-0.03267500	-3.85125600	1.39545600
H	-1.30107100	-2.21589100	2.00224300
C	0.82575700	-4.37445200	0.39907800
H	1.65448400	-4.10995400	-1.56808900

H	-0.18812100	-4.41530600	2.31995400
H	1.32296200	-5.33407800	0.56633700
C	-3.19302300	0.00238500	-0.05645800
C	-3.64599400	-1.26809400	-0.45284000
C	-4.14428600	0.92633200	0.40968700
C	-4.99288000	-1.60770900	-0.36589800
H	-2.93171200	-1.99526900	-0.84879800
C	-5.49304700	0.58533500	0.49802100
H	-3.81329200	1.91942600	0.72686000
C	-5.92482400	-0.68374000	0.11306800
H	-5.32065300	-2.60236200	-0.68361100
H	-6.21249900	1.31998900	0.87264500
H	-6.98366400	-0.95116400	0.17876900
B	-1.35726100	1.89685400	-0.21915400
O	-0.91173900	2.45583400	-1.38122400
O	-1.48942100	2.79771400	0.79870100
C	-1.08791800	4.07298500	0.31516800
H	-0.29167600	4.47309200	0.96275800
H	-1.94948300	4.76034500	0.35769800
C	-0.60593300	3.81844300	-1.12785600
H	-1.12214300	4.45248800	-1.86690100
H	0.48092800	3.96667400	-1.24025700

Int5-cis-I

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -1564.572012783140 a.u.

Thermal correction to G: 731.191 kJ/mol 174.759 kcal/mol 0.278496 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.15476700	0.11800200	-0.00742700
O	1.23872700	1.19373500	-1.78889700
C	2.29760800	1.55933900	-2.37542300
O	3.28846200	0.02345400	0.01003200
C	4.03476500	0.55612200	-0.85216300
C	3.62165200	1.29163600	-1.98530100
H	4.41036300	1.69083000	-2.62632900
C	2.06685900	2.37050900	-3.62834700
H	1.48178700	3.27121700	-3.37238800
H	3.00250500	2.67473500	-4.12160400
H	1.45814200	1.78161800	-4.33674600
C	5.51808300	0.37672700	-0.62422500
H	5.79020700	0.81204100	0.35356500
H	5.74930800	-0.70155300	-0.57080500
H	6.13484900	0.84053100	-1.40904600
C	-0.78915700	0.31044500	-0.09908400

C	-1.64772400	-0.65974200	-0.50965800
C	-1.17639000	1.70752300	0.17998400
C	-1.72030700	2.50131500	-0.84443400
C	-0.97573800	2.29288200	1.44185600
C	-2.06569000	3.83063200	-0.61149000
H	-1.86529500	2.05749700	-1.83288600
C	-1.33669900	3.61780100	1.67792000
H	-0.53711200	1.68607400	2.24007900
C	-1.88162400	4.39447800	0.65260900
H	-2.48512800	4.43237500	-1.42434500
H	-1.18490900	4.05140900	2.67159800
H	-2.15621000	5.43778800	0.83695000
C	-3.11687400	-0.45122200	-0.59562000
C	-3.84231500	0.19329900	0.42030400
C	-3.83425600	-0.92634600	-1.70642400
C	-5.21979200	0.37756200	0.31833400
H	-3.31073500	0.54780900	1.30712200
C	-5.21184400	-0.74184300	-1.81421000
H	-3.29455400	-1.44142600	-2.50810100
C	-5.91306800	-0.08421700	-0.80228900
H	-5.75890900	0.88257600	1.12643800
H	-5.74194000	-1.11475200	-2.69665500
H	-6.99489300	0.06085900	-0.88273200
B	-1.10331300	-2.07882000	-0.82777900
O	-1.81543500	-3.22770600	-0.57290100
O	0.11695100	-2.34844000	-1.40038900
C	0.33550200	-3.74609600	-1.32135000
H	1.04761600	-3.95160400	-0.50173500
H	0.77211700	-4.11159600	-2.26487300
C	-1.05523300	-4.33200600	-1.03382400
H	-1.53058400	-4.74520000	-1.94237200
H	-1.03617900	-5.12003000	-0.26336300
I	0.92961200	-1.22543600	2.24624600

Int5-cis-iso

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1266.692651568076 a.u.

Thermal correction to G: 752.602 kJ/mol 179.876 kcal/mol 0.286651 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.27102700	-0.41105200	-0.09867600
O	-3.20236500	-1.19786500	-0.09133600
C	-4.24816100	-0.49974900	0.02226800
O	-1.95348100	1.44709500	0.13295300
C	-3.18288200	1.76532800	0.21129400

C	-4.28773200	0.90330600	0.16372500
H	-5.27279000	1.36501500	0.24981300
C	-5.54603700	-1.26351600	-0.00020400
H	-5.54107000	-2.01179400	0.81150800
H	-6.42648900	-0.61381800	0.11155400
H	-5.62393900	-1.81919700	-0.95113600
C	-3.41035600	3.24407100	0.37516000
H	-2.91377100	3.58682300	1.29956000
H	-2.93083400	3.77904600	-0.46286000
H	-4.47733800	3.50756200	0.41590600
C	0.61911100	0.18489100	-0.09547400
C	1.57589800	-0.79609300	-0.08318600
C	0.91438200	1.62356000	-0.01050700
C	0.51350800	2.50658400	-1.02467300
C	1.59837500	2.14202800	1.09999500
C	0.81745500	3.86322100	-0.94695700
H	-0.03700300	2.11424300	-1.88442000
C	1.88445400	3.50288200	1.18757300
H	1.91065300	1.46192800	1.89790200
C	1.50167800	4.36788300	0.16113000
H	0.51026100	4.53550700	-1.75411700
H	2.41707100	3.89026100	2.06165100
H	1.73261500	5.43551500	0.22600800
C	3.04048000	-0.56789300	-0.08807000
C	3.63752400	0.42822400	-0.87919500
C	3.88039000	-1.37845800	0.69382900
C	5.01691400	0.62011700	-0.87112700
H	3.00796400	1.05665000	-1.51420200
C	5.26098400	-1.18416200	0.70635900
H	3.43986900	-2.17005500	1.30652200
C	5.83674600	-0.18127300	-0.07397700
H	5.45710300	1.40192600	-1.49802300
H	5.89192500	-1.82371700	1.33162900
H	6.92027500	-0.02871700	-0.06702400
B	0.97002000	-2.20755400	-0.06132600
O	-0.40815600	-2.29303900	-0.31549600
O	1.48468500	-3.43542000	0.19547100
C	0.44979200	-4.40551800	0.03598300
H	0.49885600	-5.13169400	0.86100800
H	0.60822500	-4.93763000	-0.91691200
C	-0.85832000	-3.60469400	0.03513100
H	-1.59032300	-3.95213100	-0.70707900
H	-1.33510700	-3.56206300	1.02776500

Int5-I

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -1564.572976625466 a.u.

Thermal correction to G: 729.354 kJ/mol 174.320 kcal/mol 0.277796 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.22437900	-0.05651700	-1.11724700
O	1.79738300	-0.76921800	0.76613100
C	2.89669400	-0.51889600	1.34298800
O	3.13687300	0.90694800	-1.29703500
C	4.02752200	0.89741800	-0.40922800
C	3.95997400	0.25432000	0.84858400
H	4.83252800	0.35442300	1.49734100
C	3.03845300	-1.14749300	2.70888200
H	2.95539700	-2.24459600	2.61334100
H	3.99210700	-0.89976000	3.19922200
H	2.20272900	-0.81654400	3.35006000
C	5.29087500	1.65409600	-0.74935500
H	5.74459900	1.21239100	-1.65406100
H	5.03241700	2.69831100	-0.99657500
H	6.03163500	1.64669800	0.06466700
C	-0.47697600	-0.98772600	-0.86476100
C	-1.62865500	-0.42644100	-0.40726700
C	-0.31889400	-2.44197100	-1.05680100
C	-0.50299300	-3.31006400	0.03373500
C	0.05174900	-2.99753100	-2.29306900
C	-0.34439800	-4.68719800	-0.11064700
H	-0.76679200	-2.88413700	1.00661100
C	0.19705600	-4.37478100	-2.44007100
H	0.21347800	-2.32799700	-3.14304400
C	0.00103700	-5.22729400	-1.35048100
H	-0.49000800	-5.34437100	0.75292900
H	0.47081700	-4.78855900	-3.41596700
H	0.12583600	-6.30846800	-1.46645500
C	-1.71656600	1.00803700	-0.04154600
C	-0.73495300	1.62957700	0.74912700
C	-2.80256700	1.78921800	-0.46812400
C	-0.82465700	2.98165800	1.07817600
H	0.09875900	1.02783500	1.12194800
C	-2.89318000	3.14216700	-0.14602700
H	-3.58370900	1.32811300	-1.08128900
C	-1.90131400	3.74738700	0.62792000
H	-0.04569600	3.43982200	1.69632100
H	-3.74400900	3.73004100	-0.50535000
H	-1.97056400	4.80946800	0.88325200

B	-2.92408000	-1.27449300	-0.26888000
O	-3.87587700	-1.03892200	0.69841500
O	-3.27993300	-2.31386300	-1.09327800
C	-4.43261900	-2.93129300	-0.55074400
H	-4.13853200	-3.88091500	-0.06676200
H	-5.15036200	-3.15937200	-1.35536300
C	-4.97009600	-1.91031300	0.46351500
H	-5.81694400	-1.32715300	0.05815200
H	-5.29055400	-2.37318800	1.41108400
I	0.41089400	0.76742500	-3.47748600

Int6

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.195994560189 a.u.

Thermal correction to G: 1188.154 kJ/mol 283.976 kcal/mol 0.452544 a.u.

Optimized atomic Cartesian coordinates:

Pd	0.00415100	-1.13292600	-0.32704800
O	-0.37854600	-3.17245100	0.12280300
C	-0.51629200	-4.07959900	-0.74180500
O	0.02553000	-1.57068500	-2.34057900
C	-0.16542000	-2.72750700	-2.83860900
C	-0.42491100	-3.91608900	-2.14305500
H	-0.56670100	-4.81257900	-2.74909000
C	-0.79615500	-5.45695000	-0.19740700
H	-1.68265000	-5.41362500	0.45864500
H	-0.96161000	-6.20565900	-0.98622000
H	0.05396600	-5.77621400	0.43101000
C	-0.09841100	-2.76701400	-4.34234000
H	-0.85253200	-2.07519200	-4.75671200
H	0.88934100	-2.39968700	-4.67166200
H	-0.26594800	-3.77418700	-4.75148500
C	-0.46735500	-0.60180200	1.67648600
C	0.77051000	-0.79425900	1.61591700
C	-1.77116700	-0.28466100	2.17960400
C	-1.89545100	0.70645000	3.16965500
C	-2.91668400	-0.95485800	1.72294500
C	-3.14619800	1.01122000	3.69675600
H	-1.00279100	1.23560900	3.51365700
C	-4.16197200	-0.64439600	2.25722200
H	-2.81395800	-1.71570900	0.94561200
C	-4.28108700	0.33599400	3.24372800
H	-3.23668100	1.78448800	4.46528000
H	-5.05107200	-1.16615000	1.89287600
H	-5.26422900	0.58008400	3.65691500

C	2.15140900	-0.86793800	1.99458200
C	2.54988500	-0.28130300	3.21016600
C	3.11366800	-1.48781400	1.18205800
C	3.88471200	-0.31764300	3.59868300
H	1.80250800	0.20856900	3.84007300
C	4.44768500	-1.51445200	1.57553900
H	2.80639100	-1.93450700	0.23327000
C	4.83782900	-0.93059500	2.78184900
H	4.18597500	0.14203700	4.54455100
H	5.19117000	-1.99127700	0.93067000
H	5.88840700	-0.95045100	3.08618700
C	0.35947800	0.76766000	-0.73453000
C	-0.60371500	1.70662000	-0.85760400
C	1.80358100	1.05974500	-0.76504800
C	-2.05411000	1.40203000	-0.79854100
B	-0.15769700	3.18808000	-1.08761600
C	2.64383200	0.44888700	-1.71052000
C	2.37683200	1.91558800	0.18902800
C	-2.59050600	0.33598800	-1.53987400
C	-2.93521900	2.19363900	-0.04390000
O	0.64791100	3.58868500	-2.11755000
O	-0.53123500	4.23019000	-0.27669000
C	4.01260400	0.70263100	-1.71051300
H	2.20123300	-0.22673000	-2.44826300
C	3.74889700	2.16098600	0.19356500
H	1.73447400	2.37160400	0.94884400
C	-3.95603700	0.05599400	-1.50889800
H	-1.92237400	-0.25892300	-2.16894000
C	-4.29845500	1.90946300	-0.00938300
H	-2.53806300	3.03523900	0.52908700
C	0.98340300	4.95183700	-1.90454200
C	-0.01501800	5.43041700	-0.83921400
C	4.57193900	1.55615400	-0.75633600
H	4.65222300	0.22635100	-2.46013600
H	4.17932500	2.82235700	0.95188800
C	-4.81655900	0.83960900	-0.74089000
H	-4.35013900	-0.77818900	-2.09820300
H	-4.96328500	2.52796000	0.60141600
H	0.90377600	5.50862200	-2.85159000
H	2.02808000	5.00923900	-1.54984000
H	0.45656600	6.03646900	-0.04938600
H	-0.84789800	6.01002700	-1.27481900
H	5.64974400	1.74460300	-0.75077300
H	-5.88825300	0.61989500	-0.71309700

Int6-cis

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.190664805456 a.u.

Thermal correction to G: 1188.812 kJ/mol 284.133 kcal/mol 0.452794 a.u.

Optimized atomic Cartesian coordinates:

Pd	0.82987600	-0.95051400	-0.01687800
O	2.68012600	-1.80699700	-0.59547800
C	3.18405800	-2.85108100	-0.09491000
O	0.56915300	-2.47158900	1.33873000
C	1.36865300	-3.43774800	1.53804400
C	2.60308500	-3.65573400	0.90653300
H	3.16451300	-4.53794700	1.21887600
C	4.53146300	-3.24181800	-0.64490000
H	5.24074600	-2.41207500	-0.47848200
H	4.93251300	-4.15892100	-0.18852100
H	4.45220800	-3.38308600	-1.73692000
C	0.89565200	-4.42382500	2.57329800
H	0.75352800	-3.90048800	3.53499900
H	-0.09187100	-4.81436000	2.27132300
H	1.59332900	-5.26227600	2.71554600
C	1.63564800	0.79389100	-0.87069700
C	0.69512900	0.46905800	-1.63119800
C	2.81205800	1.49533500	-0.43257000
C	3.15933200	2.68479300	-1.09721300
C	3.61260200	1.03796200	0.62521900
C	4.28339100	3.40444800	-0.70287800
H	2.53613300	3.03997500	-1.92223600
C	4.73917000	1.75973300	1.00866600
H	3.33950200	0.11679500	1.14373500
C	5.07613400	2.94465400	0.35073700
H	4.54321200	4.33086800	-1.22319500
H	5.35698500	1.39691800	1.83496700
H	5.95917000	3.51142000	0.65989300
C	-0.33962400	0.48280800	-2.62557500
C	-1.30194500	1.50639900	-2.59893600
C	-0.41693900	-0.52199800	-3.60404700
C	-2.33040100	1.51406900	-3.53706100
H	-1.23885200	2.27852200	-1.82795600
C	-1.44580000	-0.50183000	-4.54088200
H	0.33146300	-1.31900000	-3.61415100
C	-2.40630700	0.51171800	-4.50599600
H	-3.08297000	2.30720300	-3.50674500
H	-1.50238800	-1.28589500	-5.30128400

H	-3.21873500	0.51948700	-5.23849000
C	-0.97059800	-0.28354900	0.47843700
C	-1.28825100	0.96809400	0.87382500
C	-1.93695200	-1.39755300	0.38713200
C	-2.69820800	1.38755600	1.10927000
B	-0.24615900	2.11189600	1.08600100
C	-2.60859300	-1.83119300	1.54190100
C	-2.18181400	-2.07107700	-0.81955800
C	-3.71812300	1.10487100	0.18702000
C	-3.03043800	2.12771200	2.25503700
O	-0.36074200	3.32299700	0.45573900
O	0.78337900	2.07911400	1.98515000
C	-3.50536300	-2.89480700	1.48872900
H	-2.41567300	-1.31983400	2.48887100
C	-3.08501600	-3.13118300	-0.87464400
H	-1.67046400	-1.74636000	-1.72937600
C	-5.02631200	1.52636400	0.41453900
H	-3.47350600	0.55346000	-0.72460900
C	-4.33971300	2.54624400	2.48788900
H	-2.24907400	2.36527900	2.98546000
C	0.66123100	4.18323900	0.93731400
C	1.40486300	3.35817500	2.00757300
C	-3.74965400	-3.54920900	0.27919400
H	-4.01860000	-3.21752700	2.39997400
H	-3.27085600	-3.63408400	-1.82869900
C	-5.34540500	2.24440100	1.56881000
H	-5.80429500	1.29479000	-0.31978600
H	-4.57568100	3.11229000	3.39442800
H	0.20159000	5.09746400	1.34853200
H	1.31888400	4.46889600	0.10042200
H	2.47736700	3.24554000	1.78440000
H	1.29982400	3.78624000	3.01869700
H	-4.45541000	-4.38440500	0.23718700
H	-6.37350400	2.57357400	1.74778800

TS7

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.169795853846 a.u.

Thermal correction to G: 1191.891 kJ/mol 284.869 kcal/mol 0.453967 a.u.

Optimized atomic Cartesian coordinates:

Pd	0.73761700	1.16496500	0.07657600
O	2.55559300	2.21253100	0.20897200
C	2.72951900	3.44881400	-0.00495000
O	-0.15455400	2.94856600	-0.57380300

C	0.39679400	4.08028300	-0.66699700
C	1.74736700	4.37451400	-0.39442700
H	2.06672500	5.40960000	-0.52864600
C	1.45442200	-0.60160500	0.70135500
C	0.23962800	-0.72301600	1.11564100
C	2.72261600	-1.27726800	0.58906200
C	2.74502100	-2.68157700	0.68896700
C	3.92505200	-0.58811200	0.35930100
C	3.94437800	-3.37553600	0.56996500
H	1.80670100	-3.22031600	0.84512100
C	5.12082500	-1.29172800	0.23989100
H	3.89615000	0.50127800	0.27766000
C	5.13710400	-2.68415700	0.34406000
H	3.94802800	-4.46721100	0.64500200
H	6.05279600	-0.74654200	0.06145700
H	6.07896400	-3.23229100	0.24559200
C	-0.54017300	-1.35299800	2.17190500
C	-1.82335200	-1.88711700	1.98608500
C	0.07560900	-1.47750800	3.43139100
C	-2.46920800	-2.53555100	3.03552200
H	-2.32215900	-1.79816700	1.01917900
C	-0.57452300	-2.12900700	4.47526500
H	1.07222200	-1.05226400	3.57873400
C	-1.85168700	-2.65849900	4.28111500
H	-3.46957800	-2.94847600	2.87576300
H	-0.08269800	-2.21828100	5.44839200
H	-2.36692800	-3.16474400	5.10286500
C	-1.00682500	0.17312700	-0.21561600
C	-1.17518500	-0.75670600	-1.20815700
C	-2.12676100	0.95867600	0.34458200
C	-0.05123000	-1.46646600	-1.84161600
B	-2.60232800	-1.20823900	-1.67779400
C	-3.17309200	1.37967400	-0.49389000
C	-2.15404000	1.37627400	1.68541900
C	1.07282300	-0.79777600	-2.35217400
C	-0.08249100	-2.87070300	-1.92187300
O	-3.00416900	-1.16605000	-2.98282500
O	-3.54570100	-1.74848700	-0.84747800
C	-4.23509200	2.13421200	-0.00105400
H	-3.13405500	1.14844000	-1.56283000
C	-3.21383100	2.13037900	2.18053500
H	-1.33191800	1.10605100	2.35178400
C	2.15420100	-1.50917600	-2.87133100
H	1.08154100	0.29567300	-2.36444300

C	0.99984300	-3.58143600	-2.42956700
H	-0.95429400	-3.41086700	-1.53690300
C	-4.28600300	-1.78019400	-3.06615300
C	-4.73615700	-1.93281400	-1.60377500
C	-4.26587200	2.50578700	1.34302300
H	-5.03389500	2.44994300	-0.67891700
H	-3.21424300	2.43301800	3.23188100
C	2.12789300	-2.90161200	-2.89803700
H	3.02445100	-0.96743600	-3.25292500
H	0.96904900	-4.67484800	-2.45363300
H	-4.18118400	-2.75301000	-3.57690600
H	-4.96235700	-1.14458400	-3.65881100
H	-5.46541200	-1.15838400	-1.30755900
H	-5.16466900	-2.92288900	-1.38388600
H	-5.09575200	3.10293500	1.73244800
H	2.98120300	-3.46078800	-3.29294600
C	4.14704900	3.92871800	0.17754400
H	4.80138100	3.40685300	-0.54321300
H	4.25308100	5.01469100	0.03640600
H	4.49726000	3.65547700	1.18802400
C	-0.50833600	5.19177900	-1.13335800
H	-0.02055700	6.17785200	-1.11697700
H	-0.84562400	4.97479700	-2.16254600
H	-1.41001800	5.21478400	-0.49754300

TS7-cis

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.167893770431 a.u.

Thermal correction to G: 1192.350 kJ/mol 284.978 kcal/mol 0.454142 a.u.

Optimized atomic Cartesian coordinates:

Pd	0.86475400	1.09561500	0.13366200
O	2.73678400	2.01919500	0.06376300
C	2.97449000	3.24426300	-0.16001100
O	0.02599300	2.95181300	-0.36607100
C	0.63355000	4.04599000	-0.51988800
C	2.02481700	4.24475200	-0.41634100
H	2.39853600	5.25697300	-0.58075900
C	1.54256000	-0.71685100	0.62452700
C	0.35196700	-0.84886700	1.09519900
C	2.77551300	-1.44577300	0.43301700
C	2.74869400	-2.84756300	0.56976300
C	3.97876700	-0.81457500	0.07931400
C	3.90036600	-3.59687100	0.35384300
H	1.80791100	-3.34051200	0.83043700

C	5.12789100	-1.57334100	-0.13294700
H	3.98565300	0.27290500	-0.02682500
C	5.09437000	-2.96268700	-0.00029300
H	3.86622600	-4.68549200	0.45845900
H	6.06125200	-1.07375100	-0.40967900
H	5.99865100	-3.55372700	-0.17331400
C	-0.45100400	-1.57873900	2.06481600
C	-1.49299900	-2.42966100	1.67055500
C	-0.12249900	-1.47662800	3.42693000
C	-2.20045200	-3.15675000	2.62442300
H	-1.73217300	-2.52932800	0.61008700
C	-0.83786800	-2.20071600	4.37676900
H	0.69462400	-0.81606700	3.73004900
C	-1.88175200	-3.03785400	3.97832100
H	-3.00833300	-3.82208500	2.30651800
H	-0.57889700	-2.11038500	5.43567300
H	-2.44631500	-3.60303100	4.72569900
C	-0.98422600	0.25218600	-0.04050500
C	-1.22746600	-0.59602000	-1.07844000
C	-1.97681400	1.11624200	0.63310500
C	-2.57403600	-0.89208000	-1.62098400
B	-0.06040100	-1.41981700	-1.73619200
C	-2.83837500	1.89730200	-0.15768100
C	-2.04205300	1.26300300	2.02577700
C	-3.70220100	-1.06133600	-0.79959500
C	-2.72917700	-1.07349500	-3.00577700
O	-0.01743500	-2.78432000	-1.67533400
O	0.94204500	-0.88469000	-2.49299800
C	-3.75870000	2.76079000	0.42583400
H	-2.76901600	1.82957300	-1.24576700
C	-2.96930200	2.12392800	2.61132500
H	-1.36189500	0.69754600	2.66424300
C	-4.94023500	-1.38354200	-1.34781300
H	-3.60403800	-0.94581400	0.28252800
C	-3.97142700	-1.38288500	-3.55609600
H	-1.86204200	-0.95062300	-3.66365000
C	1.05298500	-3.23007000	-2.50088600
C	1.80172500	-1.94549200	-2.90021600
C	-3.83596100	2.87259900	1.81604300
H	-4.41669400	3.35969200	-0.21121800
H	-3.00750800	2.21252000	3.70118800
C	-5.08354900	-1.53885600	-2.72853500
H	-5.80348600	-1.51670000	-0.68872900
H	-4.06923400	-1.50639000	-4.63883400

H	0.63062200	-3.76071100	-3.37156700
H	1.68719800	-3.92994800	-1.93497900
H	2.76441000	-1.84230200	-2.37251600
H	1.98152400	-1.87311900	-3.98449700
H	-4.56031400	3.55150800	2.27601400
H	-6.05900000	-1.78786100	-3.15679000
C	4.43577000	3.61375700	-0.14831100
H	4.95835200	3.05004400	-0.94136700
H	4.60485600	4.68987400	-0.30242200
H	4.88215200	3.30787100	0.81378200
C	-0.24679000	5.22157700	-0.85934300
H	0.30642500	6.17140500	-0.90764100
H	-0.73327700	5.03818200	-1.83379600
H	-1.05143700	5.30016700	-0.10810400

Int8

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.238481364024 a.u.

Thermal correction to G: 1199.997 kJ/mol 286.806 kcal/mol 0.457055 a.u.

Optimized atomic Cartesian coordinates:

Pd	-0.76559100	-0.70405900	-0.39152400
O	-0.89030400	-2.52292900	-1.31439100
C	-1.95730500	-3.15958700	-1.57764700
O	-2.88503800	-0.60363200	-0.34511300
C	-3.65976000	-1.52932700	-0.71614300
C	-3.27112700	-2.74866000	-1.30677800
H	-4.06888300	-3.43836700	-1.58731100
C	-1.73086600	-4.48780500	-2.25000800
H	-1.04696500	-5.09532500	-1.63260600
H	-2.66421300	-5.04422800	-2.42075500
H	-1.22708200	-4.32040700	-3.21833400
C	-5.12851700	-1.26850900	-0.50352500
H	-5.43084900	-0.38802800	-1.09741600
H	-5.76055300	-2.12338800	-0.78581500
H	-5.30289700	-1.02235500	0.55831800
C	1.20227900	-0.71650700	-0.37957600
C	1.51713600	0.58596200	-0.24834600
C	2.00404800	-1.93258400	-0.43005800
C	2.12868400	-2.70613600	-1.59443000
C	2.65765200	-2.35276000	0.74208200
C	2.90800400	-3.86084500	-1.59070100
H	1.61185000	-2.39067400	-2.50358400
C	3.43008900	-3.51171300	0.74151500
H	2.54953800	-1.75527700	1.65286400

C	3.56033000	-4.26818800	-0.42500600
H	3.00556800	-4.45126800	-2.50695400
H	3.93536800	-3.82676400	1.65968300
H	4.16878600	-5.17760700	-0.42534800
C	2.80505600	1.28424600	-0.29973000
C	3.97080200	0.64166300	-0.75424600
C	2.90418600	2.62588600	0.10622800
C	5.18864200	1.31380200	-0.78535100
H	3.91662400	-0.39567400	-1.09206300
C	4.12359700	3.29910900	0.07159200
H	2.01153100	3.15435200	0.45213900
C	5.27325200	2.64569500	-0.37179300
H	6.08274200	0.79337200	-1.14200000
H	4.17383700	4.34347000	0.39399200
H	6.23170200	3.17247700	-0.39984300
C	0.18753500	1.26926400	-0.08165400
C	-0.60759900	0.92609100	1.03943800
C	-0.14366200	2.32501300	-1.07256900
C	-0.50574700	3.61175600	-0.65591900
C	0.02127600	2.07826200	-2.44246600
C	-0.71510800	4.62494600	-1.58832700
H	-0.61105400	3.82178200	0.41138700
C	-0.20401800	3.08578400	-3.37676800
H	0.31882300	1.07754600	-2.77056700
C	-0.57198900	4.36376000	-2.95153700
H	-0.99164100	5.62697500	-1.24706700
H	-0.08626900	2.87388200	-4.44348900
H	-0.74096500	5.15897800	-3.68379700
C	0.01806400	0.31414100	2.25517300
C	1.18193200	0.86539900	2.80792700
C	-0.55428800	-0.79896800	2.88959000
C	1.77877800	0.30097500	3.93455400
H	1.63414300	1.74649600	2.34566700
C	0.04167200	-1.36648100	4.01306700
H	-1.47202500	-1.23299100	2.48449800
C	1.21567200	-0.82322100	4.53837100
H	2.69183700	0.74617400	4.34140300
H	-0.41410500	-2.24461900	4.48035600
H	1.68572500	-1.27111000	5.41903900
B	-2.09910400	1.41408600	1.21328500
O	-2.78326300	2.22167100	0.35552600
O	-2.82463000	1.06543700	2.31671300
C	-4.12712500	2.29650400	0.80072800
C	-4.11812000	1.63640900	2.19296300

H	-4.77000600	1.75469500	0.08737000
H	-4.44557900	3.35122000	0.82831800
H	-4.26852100	2.36375800	3.00906400
H	-4.87863400	0.84457300	2.29077700

Int8-cis

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.236134482141 a.u.

Thermal correction to G: 1197.316 kJ/mol 286.165 kcal/mol 0.456034 a.u.

Optimized atomic Cartesian coordinates:

Pd	-0.37182900	-1.06673600	-0.35842500
O	0.26177300	-2.88418800	-1.03810600
C	-0.47046500	-3.87192900	-1.36285300
O	-2.35882200	-1.72007200	-0.59135800
C	-2.72480900	-2.86389000	-0.97141600
C	-1.86970700	-3.92149200	-1.34723600
H	-2.33778700	-4.85830800	-1.65414900
C	0.30118800	-5.08746400	-1.80469700
H	1.00336300	-5.38199400	-1.00573900
H	-0.35091600	-5.93851800	-2.05043700
H	0.90962200	-4.82968900	-2.68947700
C	-4.21526500	-3.07974900	-1.02186800
H	-4.65771200	-2.37388000	-1.74688300
H	-4.49083200	-4.10662800	-1.30432300
H	-4.64791800	-2.83914700	-0.03559400
C	1.45353200	-0.35586600	-0.18554500
C	1.24539400	0.97500900	-0.15517000
C	2.70106300	-1.11029200	-0.11481200
C	3.10839100	-1.99661700	-1.12452200
C	3.53243900	-0.93252800	1.00569500
C	4.32134800	-2.67423800	-1.01978400
H	2.46464600	-2.14670600	-1.99266900
C	4.74020200	-1.61765000	1.10958200
H	3.21553800	-0.23934900	1.78990700
C	5.14032800	-2.49106000	0.09615000
H	4.63043000	-3.35552600	-1.81864400
H	5.37614100	-1.46622400	1.98730700
H	6.08990700	-3.02882500	0.17588600
C	2.19417300	2.09563800	-0.18021300
C	3.43005700	1.99803800	-0.83962200
C	1.87094300	3.29891800	0.46600700
C	4.31862900	3.06975100	-0.84208800
H	3.68679200	1.07331100	-1.36282100
C	2.75981400	4.37158000	0.46218100

H	0.91586600	3.38622200	0.99221900
C	3.98811900	4.26060200	-0.19101900
H	5.27641300	2.97802300	-1.36331700
H	2.49247300	5.30026900	0.97534000
H	4.68674800	5.10266500	-0.19638800
C	-0.23454100	1.19164200	-0.12526700
C	-0.98099100	0.63240900	0.92783800
C	-0.77667200	2.12235100	-1.14959900
C	-1.48413700	3.27169500	-0.77417800
C	-0.50935800	1.89904700	-2.50553900
C	-1.92624200	4.17281300	-1.73954500
H	-1.68502500	3.46077600	0.28377800
C	-0.96674000	2.79172900	-3.47285700
H	0.05351300	1.00682400	-2.79748400
C	-1.67601700	3.93161200	-3.09167700
H	-2.47195100	5.07024100	-1.43360400
H	-0.76347100	2.59862800	-4.53022100
H	-2.03049300	4.63671400	-3.84940500
C	-2.44391300	0.86339000	1.07289100
C	-3.33585900	0.88497600	-0.01219600
C	-2.95898000	1.11531400	2.35388900
C	-4.68520700	1.16185800	0.17927700
H	-2.96992400	0.66792600	-1.01556500
C	-4.31015600	1.39896900	2.54810800
H	-2.28972900	1.10221100	3.21954800
C	-5.17975400	1.42340100	1.45912800
H	-5.36085500	1.16827700	-0.68137000
H	-4.68243400	1.59937200	3.55712800
H	-6.24204200	1.64076300	1.60607500
B	-0.22880500	0.03612600	2.17998700
O	0.84048800	0.62538700	2.79912600
O	-0.67701100	-1.07609500	2.84212100
C	1.11610000	-0.10245200	3.98945300
C	0.24710600	-1.36635900	3.88214400
H	0.84540800	0.52208900	4.85839100
H	2.19297300	-0.32840700	4.04526500
H	0.83762100	-2.25371200	3.59573200
H	-0.29970400	-1.59335900	4.81103600

Int8-cis-I

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -2104.110052938832 a.u.

Thermal correction to G: 1186.453 kJ/mol 283.569 kcal/mol 0.451896 a.u.

Optimized atomic Cartesian coordinates:

Pd	0.09619400	1.63078600	-0.42180800
O	-0.16454100	2.35082100	1.50900400
C	-1.04304800	3.18514500	1.87033700
O	-1.32990400	3.05980700	-1.11362400
C	-2.03123800	3.78879900	-0.36320900
C	-1.94644200	3.87556300	1.04314300
H	-2.63631300	4.56261300	1.53727200
C	-1.08658800	3.43595600	3.35747600
H	-0.09209100	3.76909800	3.70236000
H	-1.83984600	4.18581100	3.64363400
H	-1.30995100	2.48327100	3.86906900
C	-3.05691900	4.64585500	-1.06842600
H	-3.74503700	3.99408000	-1.63518900
H	-3.64107200	5.27398000	-0.37868900
H	-2.54750900	5.29225600	-1.80446400
C	1.33434500	0.31642600	0.35599900
C	0.86378100	-0.81990800	0.91898000
C	2.75547400	0.70093800	0.33759000
C	3.18517700	1.96581300	0.77542700
C	3.71700600	-0.19084900	-0.16955500
C	4.53312800	2.31643300	0.73091400
H	2.44108800	2.66738500	1.16442100
C	5.06278700	0.16477500	-0.22238800
H	3.38111500	-1.17043900	-0.52134200
C	5.47944200	1.41837800	0.23133500
H	4.84881500	3.30263800	1.08655300
H	5.79574500	-0.54322800	-0.62318700
H	6.53703200	1.69737100	0.18977100
C	1.64928100	-1.70175300	1.81957800
C	2.53351200	-1.16365400	2.77157200
C	1.48146500	-3.09677300	1.79974700
C	3.24572500	-1.98574000	3.64097900
H	2.64629600	-0.07872000	2.83424300
C	2.19282100	-3.92139500	2.66979200
H	0.78658200	-3.53669900	1.08108900
C	3.08365400	-3.37222700	3.59325100
H	3.92571700	-1.53767600	4.37269600
H	2.04863000	-5.00581600	2.62515600
H	3.63959500	-4.01901000	4.27911100
C	-0.57095800	-1.20127900	0.71152400
C	-0.98306800	-1.93242000	-0.35730200
C	-1.51549700	-0.67703300	1.73622300
C	-1.31220700	-0.91375200	3.10347600
C	-2.60695900	0.11401300	1.34974000

C	-2.19506700	-0.40071800	4.05329700
H	-0.45778400	-1.51584300	3.42416300
C	-3.47914200	0.64063100	2.29848500
H	-2.75442600	0.33393800	0.28913000
C	-3.28304400	0.37778900	3.65540900
H	-2.02743900	-0.60790000	5.11499300
H	-4.31464800	1.26843000	1.97428200
H	-3.97046900	0.78733600	4.40212500
C	-2.41118600	-2.32046600	-0.51291600
C	-3.05948500	-3.07546600	0.47602700
C	-3.14447900	-1.94764800	-1.64949500
C	-4.40108400	-3.43003900	0.34664800
H	-2.49684800	-3.37973000	1.36372800
C	-4.48897300	-2.29364500	-1.77707900
H	-2.65326100	-1.36484100	-2.43261900
C	-5.12452600	-3.03574500	-0.77993500
H	-4.88579700	-4.01708000	1.13329500
H	-5.04637100	-1.97860900	-2.66503300
H	-6.17959300	-3.30830500	-0.88215500
B	-0.00245200	-2.39658400	-1.48326400
O	1.34882200	-2.56882200	-1.34926100
O	-0.45981800	-2.79828100	-2.71242300
C	1.88231000	-2.93472900	-2.60808600
C	0.65438000	-3.12364000	-3.52255500
H	2.48163100	-3.85445800	-2.49787600
H	2.53994900	-2.12410200	-2.96535900
H	0.67887300	-2.44484800	-4.39188700
H	0.54819100	-4.15935000	-3.88900000
I	0.62724100	0.77738200	-2.84804500

Int8-I

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -2104.111940875383 a.u.

Thermal correction to G: 1187.165 kJ/mol 283.739 kcal/mol 0.452167 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.69490500	-0.33470400	-0.66871600
O	-0.17228800	-0.83361100	-1.99153700
C	-0.02917500	-1.97131900	-2.52945200
O	-2.75394200	-2.07343800	-1.28254000
C	-2.23785400	-3.01768800	-1.93447400
C	-0.95162300	-3.03118800	-2.51727300
H	-0.65947200	-3.94046600	-3.04630400
C	1.29271500	-2.18195300	-3.22607800
H	2.09474600	-2.21822900	-2.46608700

H	1.31613600	-3.11259900	-3.81351200
H	1.51093100	-1.32589800	-3.88594200
C	-3.10166900	-4.24714800	-2.08822900
H	-4.07757000	-3.95784900	-2.51463300
H	-2.64229900	-5.02054800	-2.72250900
H	-3.30028000	-4.67233700	-1.08821900
C	-0.62368600	1.21021000	-0.08417100
C	0.61362900	1.03741900	0.45515400
C	-1.19401500	2.54315700	-0.35530300
C	-1.58065000	2.89512800	-1.65854500
C	-1.37396900	3.48944700	0.66710900
C	-2.10280200	4.15731600	-1.93598000
H	-1.46085900	2.15948000	-2.46025500
C	-1.90764700	4.74607700	0.39378900
H	-1.09065700	3.22324800	1.68911700
C	-2.26927700	5.09034100	-0.91058800
H	-2.38770700	4.41294400	-2.96164300
H	-2.04288700	5.46576400	1.20772700
H	-2.68663200	6.07901700	-1.12554000
C	1.50423000	2.16950400	0.84172800
C	1.76604900	3.25409700	-0.00790500
C	2.13140200	2.15203200	2.09702300
C	2.62136500	4.28167200	0.38230500
H	1.30765100	3.27617500	-0.99875800
C	2.97718300	3.18508200	2.49744900
H	1.95296400	1.30654100	2.76900600
C	3.22948600	4.25591200	1.63881400
H	2.82117800	5.10874500	-0.30644800
H	3.44733400	3.14950000	3.48551800
H	3.90153100	5.06376900	1.94484900
C	1.17328100	-0.32228300	0.68915600
C	2.43193800	-0.67145400	0.29647100
C	0.33030100	-1.31254700	1.39919600
C	0.23105500	-2.63560900	0.94138200
C	-0.35730600	-0.95813000	2.56845600
C	-0.51693700	-3.58042800	1.64059700
H	0.71454800	-2.91447000	0.00088400
C	-1.08948500	-1.90429900	3.27893500
H	-0.31740600	0.07909000	2.91277700
C	-1.17414900	-3.21978000	2.81731000
H	-0.60048200	-4.60065800	1.25290800
H	-1.61698600	-1.60909200	4.19087600
H	-1.76726400	-3.95803600	3.36572100
C	3.26762700	0.20162200	-0.55958400

C	4.59224400	0.49566900	-0.20183200
C	2.76899900	0.72364200	-1.76310800
C	5.38680100	1.31332500	-1.00382100
H	4.99534800	0.09470900	0.73466400
C	3.56804400	1.52641100	-2.57405800
H	1.73947400	0.48263100	-2.04385900
C	4.87695600	1.83224200	-2.19551600
H	6.41118800	1.54696200	-0.69668500
H	3.16255400	1.92442300	-3.51007500
H	5.50033600	2.47149800	-2.82860400
B	3.05873300	-2.04258700	0.68766400
O	3.58070200	-2.91035100	-0.24255500
O	3.21265700	-2.50252900	1.97055400
C	4.17756400	-3.99440400	0.45422100
C	3.67097500	-3.84292500	1.89663800
H	5.27666800	-3.90607600	0.38498300
H	3.87528600	-4.94745500	-0.00872900
H	2.82410100	-4.52050700	2.10993100
H	4.45527600	-4.01382400	2.65127100
I	-3.65153700	0.35900700	0.96245200

Int9

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.221198311828 a.u.

Thermal correction to G: 1196.404 kJ/mol 285.948 kcal/mol 0.455686 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.50759800	-0.84290900	0.04958500
O	-1.98010900	-0.30153100	1.98591500
C	-2.57069200	-1.05744200	2.81783000
O	-2.40954100	-2.72198800	0.32617600
C	-2.93697200	-3.10976800	1.40557100
C	-3.03691600	-2.36370300	2.59825700
H	-3.52286800	-2.85466800	3.44317900
C	-2.77237100	-0.43697900	4.17654100
H	-3.36630500	0.48767500	4.06935600
H	-3.27781600	-1.11183500	4.88302300
H	-1.79194300	-0.14431700	4.59101000
C	-3.49852000	-4.50832000	1.38229600
H	-4.24983600	-4.58435700	0.57694300
H	-2.68956000	-5.21865300	1.13689700
H	-3.95945100	-4.80186700	2.33698800
C	-0.70286700	0.95081600	-0.12707500
C	0.63014000	1.18585000	0.01210700
C	-1.70310300	1.97848200	-0.44559300

C	-2.94639700	2.05986500	0.21136300
C	-1.45443000	2.87406300	-1.50467700
C	-3.89329200	3.00638600	-0.16983100
H	-3.14706100	1.37969400	1.04195100
C	-2.40805600	3.81134400	-1.89198200
H	-0.49240700	2.82870000	-2.01934500
C	-3.63240700	3.88269100	-1.22589800
H	-4.84765900	3.06077200	0.36300700
H	-2.19208800	4.49392500	-2.71971500
H	-4.38179800	4.62088500	-1.52731600
C	1.16583000	2.55896800	0.20690200
C	0.56491500	3.45577400	1.10288700
C	2.29747800	2.98776800	-0.50405400
C	1.06472900	4.74523500	1.26705600
H	-0.30348800	3.12660000	1.68028400
C	2.79857800	4.27816200	-0.34253600
H	2.78507800	2.29973700	-1.20195700
C	2.18277500	5.16397900	0.54272100
H	0.58161300	5.42789700	1.97295600
H	3.67759700	4.59409000	-0.91285100
H	2.57733500	6.17613600	0.67361000
C	1.63484400	0.10109700	-0.10627500
C	1.50401900	-0.86299700	-1.06146800
C	2.78789100	0.12207900	0.82076600
C	4.09303700	-0.12885100	0.37538900
C	2.58297500	0.39773300	2.18059700
C	5.16307000	-0.13095300	1.26754700
H	4.27314900	-0.29593200	-0.69181900
C	3.65005200	0.38987600	3.07535700
H	1.56841800	0.60760200	2.53365300
C	4.94393500	0.12423500	2.62205900
H	6.17636800	-0.32146100	0.90113400
H	3.47181900	0.59517400	4.13516100
H	5.78354100	0.12687400	3.32365300
C	0.33927800	-0.78848500	-1.97432100
C	0.20848600	0.21132400	-2.94598300
C	-0.71719100	-1.72562600	-1.81827400
C	-0.95980800	0.32546300	-3.69550800
H	1.02532700	0.92517300	-3.08272200
C	-1.91408500	-1.57073700	-2.55696500
H	-0.53180100	-2.65953100	-1.27632600
C	-2.03801900	-0.53956800	-3.48210500
H	-1.04362400	1.12072300	-4.44209700
H	-2.71844100	-2.29746400	-2.41636400

H	-2.96422900	-0.41681900	-4.04936800
B	2.40804100	-2.12868000	-1.16616200
O	2.74926300	-2.92310300	-0.10843400
O	2.87627400	-2.60132300	-2.36241200
C	3.64164200	-3.92097200	-0.58502100
C	3.52513900	-3.84379900	-2.11701100
H	3.35002700	-4.90267300	-0.17982300
H	4.66108300	-3.68521300	-0.23122400
H	4.50335400	-3.85646300	-2.62318800
H	2.90574400	-4.65755600	-2.53273800

Int9-6r

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.221039339821 a.u.

Thermal correction to G: 1197.269 kJ/mol 286.154 kcal/mol 0.456016 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.53880800	-0.77749400	0.06316800
O	-1.98535800	-0.20224900	1.99646800
C	-2.60997100	-0.92425700	2.83359700
O	-2.52376600	-2.61317800	0.35448300
C	-3.07100800	-2.96733200	1.43559900
C	-3.13678000	-2.20885200	2.62280500
H	-3.64594500	-2.67032300	3.47069300
C	-2.78072200	-0.28650700	4.18850400
H	-3.32221300	0.66905700	4.07524800
H	-3.32399900	-0.92888600	4.89716500
H	-1.78654400	-0.04628400	4.60409800
C	-3.70000100	-4.33701400	1.42090100
H	-4.45734400	-4.37947200	0.61866800
H	-2.92796300	-5.08727800	1.17559000
H	-4.17137500	-4.60321900	2.37849400
C	-0.65590000	0.97726100	-0.12970000
C	0.68735600	1.15459000	0.00217300
C	-1.61042500	2.04581200	-0.45398900
C	-2.85182300	2.18042400	0.19767000
C	-1.32106900	2.92702700	-1.51492200
C	-3.75788600	3.16346300	-0.19050900
H	-3.08312300	1.51166800	1.02945600
C	-2.23404800	3.90105800	-1.90920300
H	-0.36010000	2.84078900	-2.02635900
C	-3.45712600	4.02462400	-1.24843000
H	-4.71136500	3.25846000	0.33816900
H	-1.98726200	4.57128200	-2.73840800
H	-4.17459100	4.79163200	-1.55554100

C	1.28072600	2.50491700	0.18901200
C	0.72807500	3.42431900	1.09277700
C	2.41903100	2.88829200	-0.53691100
C	1.28148500	4.69249000	1.25102000
H	-0.14549300	3.12965400	1.68097900
C	2.97364500	4.15732700	-0.38164100
H	2.86963500	2.18193600	-1.24138400
C	2.40587400	5.06637400	0.51223500
H	0.83544600	5.39346800	1.96333300
H	3.85701200	4.43818600	-0.96347400
H	2.84271900	6.06164700	0.63825000
C	1.64346400	0.02703600	-0.11076900
C	1.45989700	-0.94569900	-1.04982500
C	2.80713600	0.01925300	0.80314200
C	4.10159000	-0.25405600	0.34124600
C	2.62349700	0.29903800	2.16499100
C	5.18255700	-0.27228700	1.21966100
H	4.26358200	-0.42770000	-0.72764700
C	3.70122800	0.27325000	3.04661800
H	1.61708700	0.52721900	2.53000500
C	4.98464200	-0.01332000	2.57682000
H	6.18795200	-0.47981200	0.84090500
H	3.53982100	0.48167300	4.10850300
H	5.83307300	-0.02418300	3.26767200
C	0.29701000	-0.82250000	-1.96012500
C	0.21462000	0.17747900	-2.93793400
C	-0.80215100	-1.70818200	-1.80227100
C	-0.94440700	0.34144400	-3.69147900
H	1.06439400	0.85137200	-3.07656200
C	-1.98852100	-1.50277400	-2.54633200
H	-0.66127000	-2.64777300	-1.25692000
C	-2.06212700	-0.47247700	-3.47702500
H	-0.98924400	1.13518100	-4.44301700
H	-2.82609800	-2.19060700	-2.40399300
H	-2.97980200	-0.31065000	-4.04839300
B	2.29045800	-2.25992800	-1.14614100
O	2.71942500	-2.99530100	-0.07748700
O	2.59294500	-2.84080200	-2.34876100
C	3.50497200	-4.06890000	-0.57580000
C	3.20928700	-4.09558200	-2.08521600
H	3.22243600	-5.00292100	-0.06519200
H	4.56869000	-3.86145800	-0.36235900
H	4.11793400	-4.19811000	-2.69935700
H	2.50808400	-4.90241000	-2.36138900

Int9-cis

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.228803449580 a.u.

Thermal correction to G: 1200.261 kJ/mol 286.869 kcal/mol 0.457155 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.85461800	-0.50952200	0.05486500
O	3.27440300	0.58015800	-0.95161100
C	4.40900500	0.17064600	-1.34922000
O	3.11142300	-2.19155700	-0.11624800
C	4.26317500	-2.21596000	-0.62445500
C	4.92999400	-1.12297100	-1.21700200
H	5.93073400	-1.30135600	-1.61410300
C	5.23712100	1.22840100	-2.03117400
H	4.69950700	1.58783900	-2.92620500
H	5.34891700	2.09270000	-1.35388800
H	6.23119700	0.86397100	-2.32949300
C	4.95923900	-3.55259800	-0.58070500
H	5.02373600	-3.89298600	0.46742100
H	4.34894200	-4.29521100	-1.12403300
H	5.96867400	-3.52522900	-1.01721000
C	0.72706800	1.09196500	0.21077600
C	-0.62306500	0.93116000	0.17892200
C	1.40564000	2.36793200	0.48223100
C	1.99599300	3.13215500	-0.53674000
C	1.46781200	2.84631500	1.80131700
C	2.61599600	4.34470100	-0.24471700
H	1.95672500	2.76771400	-1.56496800
C	2.09228500	4.05768600	2.09297600
H	1.00876700	2.25960700	2.60305300
C	2.66873300	4.81203800	1.07015300
H	3.06203800	4.93295600	-1.05279900
H	2.12442300	4.41690600	3.12623200
H	3.15696700	5.76475600	1.29671800
C	-1.55269100	2.07757800	0.35988600
C	-1.48134400	3.21393600	-0.45874800
C	-2.50400100	2.05724200	1.39058200
C	-2.32948400	4.29870100	-0.25073900
H	-0.75881500	3.23410200	-1.27794400
C	-3.35453900	3.14206500	1.60082700
H	-2.57690700	1.17636200	2.03500100
C	-3.27071000	4.26735300	0.78095600
H	-2.25948000	5.17445200	-0.90324100
H	-4.08802300	3.10605400	2.41194100

H	-3.93893500	5.11849700	0.94326200
C	-1.13509200	-0.44106400	0.08969000
C	-2.41313200	-0.76233200	-0.26341600
C	-0.13499900	-1.48879300	0.47054300
C	-0.07667900	-2.72544000	-0.23677700
C	0.56023600	-1.39730400	1.71139900
C	0.58339200	-3.81088800	0.29507100
H	-0.59077900	-2.80088600	-1.19742700
C	1.19653000	-2.53744000	2.25750600
H	0.40006800	-0.52228500	2.34757100
C	1.20292600	-3.72688000	1.55907500
H	0.61870100	-4.75037200	-0.26346300
H	1.67171500	-2.46319800	3.23929600
H	1.69750400	-4.60711100	1.97947500
C	-2.99271100	-2.11333200	-0.09035100
C	-2.84613500	-2.82454300	1.11288200
C	-3.75860700	-2.69773000	-1.11274200
C	-3.41638700	-4.08433400	1.27521000
H	-2.27991000	-2.37508400	1.93407100
C	-4.32398500	-3.96154300	-0.95527200
H	-3.89419200	-2.15830700	-2.05633100
C	-4.15215400	-4.66277800	0.23919900
H	-3.28808200	-4.61861000	2.22162400
H	-4.90459700	-4.40160000	-1.77180200
H	-4.59841900	-5.65367800	0.36594800
B	-3.38978600	0.29388600	-0.88123500
O	-4.65190800	0.51449900	-0.40624500
O	-3.11663900	0.99405300	-2.02283100
C	-5.25297100	1.53004300	-1.19571100
C	-4.22976900	1.82700800	-2.31275900
H	-5.44127200	2.41146300	-0.55997100
H	-6.21745300	1.16484300	-1.58600200
H	-4.61239000	1.57972500	-3.31720800
H	-3.90123800	2.87937600	-2.30970400

TS10

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.196391388048 a.u.

Thermal correction to G: 1198.479 kJ/mol 286.443 kcal/mol 0.456477 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.35038700	-0.95282400	-0.46019100
O	2.28181700	0.59993900	-1.55053600
C	3.04647600	0.42501600	-2.53999800
O	2.22723200	-2.36190800	-1.72010700

C	3.00053500	-2.09191800	-2.68537900
C	3.41440600	-0.81320800	-3.10452900
H	4.08891700	-0.77681000	-3.96210900
C	3.59971500	1.68908400	-3.14981300
H	4.15733500	2.24826700	-2.37806000
H	4.26129300	1.49972200	-4.00835600
H	2.76234600	2.33264800	-3.47226300
C	3.51170800	-3.29349800	-3.44108400
H	4.05091000	-3.95920100	-2.74439000
H	2.65453200	-3.86660100	-3.83600400
H	4.17983900	-3.02430800	-4.27261800
C	0.47136300	0.41245500	0.78456000
C	-0.63108200	1.08348300	0.26689000
C	1.44729100	1.07194300	1.68847000
C	2.81462900	0.75764800	1.68681000
C	0.98871100	2.00079600	2.64058500
C	3.69348400	1.36250500	2.58438000
H	3.19789400	0.03178500	0.96439000
C	1.86194400	2.60557200	3.53810600
H	-0.07608900	2.24577100	2.67724600
C	3.22254900	2.29072400	3.51194100
H	4.75608200	1.10368800	2.55639600
H	1.47749500	3.32445500	4.26798200
H	3.91162100	2.76438100	4.21773200
C	-0.64022700	2.54371400	0.05984100
C	0.47620500	3.16220200	-0.52798400
C	-1.73233700	3.34076800	0.44031700
C	0.49855300	4.54071800	-0.72403600
H	1.31464200	2.53499600	-0.84770800
C	-1.70326900	4.71996100	0.25044100
H	-2.60661000	2.87750000	0.90472700
C	-0.58859000	5.32494000	-0.33361800
H	1.37189500	5.00726300	-1.19009300
H	-2.55805600	5.32791800	0.56173400
H	-0.56973400	6.40816700	-0.48744200
C	-1.81438000	0.25548400	0.07578600
C	-1.71216200	-0.97025000	0.67406800
C	-2.99328200	0.73573300	-0.67141600
C	-4.28092600	0.65457500	-0.12634800
C	-2.83092000	1.30108800	-1.94424000
C	-5.38306800	1.12050800	-0.83966800
H	-4.41314500	0.23646800	0.87567300
C	-3.93332400	1.75666300	-2.66305000
H	-1.82693100	1.37668800	-2.37260100

C	-5.21271000	1.67038400	-2.11117100
H	-6.38236800	1.05723500	-0.39856500
H	-3.79237500	2.18674900	-3.65905600
H	-6.07825600	2.03702900	-2.67118200
C	-0.39260300	-1.21695100	1.31235800
C	-0.21774300	-1.03684200	2.74828700
C	0.37554700	-2.31445900	0.68757700
C	0.77086800	-1.68582700	3.42232800
H	-0.86493600	-0.31197400	3.24891000
C	1.38520800	-2.98353000	1.46463700
H	-0.13063200	-2.89757400	-0.09557000
C	1.61242500	-2.64164600	2.77027700
H	0.90968400	-1.49329400	4.49028300
H	1.95274600	-3.79061600	0.99183900
H	2.40268900	-3.13684700	3.34144600
B	-2.69896900	-2.16453500	0.58449800
O	-3.65663600	-2.34301900	-0.37354100
O	-2.65730200	-3.18836000	1.49356300
C	-4.40147600	-3.50558800	-0.03785000
C	-3.58643200	-4.18074800	1.07959800
H	-4.51479700	-4.14116400	-0.93031700
H	-5.40663800	-3.20061000	0.30255900
H	-4.20588800	-4.48865500	1.93692600
H	-3.02981100	-5.06268000	0.71734900

TS10-6r

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.165104883417 a.u.

Thermal correction to G: 1197.050 kJ/mol 286.102 kcal/mol 0.455932 a.u.

Optimized atomic Cartesian coordinates:

Pd	0.63135900	-1.42266100	-0.21210600
O	2.11479300	-0.82743900	-1.59401400
C	2.25789400	-1.24615400	-2.78065300
O	-0.00312100	-2.88181900	-1.67664600
C	0.46197600	-3.00814100	-2.84100700
C	1.52073100	-2.26503800	-3.40719000
H	1.79182700	-2.50254700	-4.43764800
C	3.33412200	-0.54225800	-3.56990900
H	4.27622400	-0.55628900	-2.99539800
H	3.50202200	-0.98810700	-4.56180900
H	3.05044000	0.51807600	-3.69808700
C	-0.20073300	-4.06545700	-3.69166300
H	-0.13446100	-5.03984700	-3.17668100
H	-1.27420300	-3.82732600	-3.79376900

H	0.24491100	-4.15517100	-4.69376700
C	0.94933400	0.19596400	1.00317500
C	0.07022100	1.10687300	0.38101900
C	2.32771400	0.55333200	1.42545400
C	3.40707700	-0.30773900	1.19340500
C	2.55208700	1.72656200	2.16294100
C	4.68334100	0.01084400	1.65513800
H	3.23964400	-1.22840400	0.62970500
C	3.82488600	2.04419600	2.62815600
H	1.71461100	2.39861000	2.36977200
C	4.89833500	1.18832000	2.37141000
H	5.51668800	-0.66903600	1.45375500
H	3.98051300	2.96647800	3.19607700
H	5.89992600	1.43740600	2.73490000
C	0.59452300	2.39356500	-0.13583500
C	1.68224900	2.38446000	-1.02394200
C	0.05863500	3.63072600	0.25579000
C	2.21415100	3.57730700	-1.50850400
H	2.09830000	1.42018900	-1.33215200
C	0.59748000	4.82270100	-0.22254200
H	-0.78108100	3.66095200	0.95445700
C	1.67527700	4.80137900	-1.10968200
H	3.05803400	3.54944400	-2.20492200
H	0.17145400	5.77715400	0.10145400
H	2.09406800	5.73854100	-1.48891200
C	-1.37074600	0.81381300	0.34449200
C	-1.84524800	-0.34542700	0.91660500
C	-2.28945600	1.79566700	-0.27757900
C	-3.30196500	2.40742400	0.47090400
C	-2.14404300	2.13739600	-1.62856000
C	-4.15039500	3.34364800	-0.11639700
H	-3.41278100	2.15285200	1.52891300
C	-2.99985300	3.06310600	-2.22029800
H	-1.35022000	1.66825200	-2.21717100
C	-4.00252900	3.67313300	-1.46431300
H	-4.93184200	3.82046900	0.48300800
H	-2.87971400	3.31448100	-3.27828700
H	-4.66824900	4.40834400	-1.92647000
C	-0.77527400	-1.22147400	1.44762400
C	0.10293600	-0.56627600	2.43213700
C	-0.55432700	-2.58786700	1.16348400
C	0.95938400	-1.37307100	3.23592600
H	-0.31259600	0.32262600	2.92171100
C	0.44729400	-3.30421800	1.87278400

H	-1.24453000	-3.12582400	0.50922300
C	1.16446700	-2.70396800	2.91486400
H	1.46334300	-0.92031900	4.09330000
H	0.59373600	-4.36245700	1.64209900
H	1.87047700	-3.30576200	3.49448500
B	-3.30167800	-0.85254800	0.97668500
O	-4.34334300	-0.42170300	0.20211500
O	-3.65527000	-1.88007500	1.81656600
C	-5.51360300	-1.11038900	0.61587000
C	-5.00237900	-2.23240900	1.53719200
H	-6.04910800	-1.49252800	-0.26787100
H	-6.17756900	-0.40459800	1.14569200
H	-5.56996500	-2.30568300	2.47872900
H	-5.01983500	-3.21972400	1.04315300

TS10-cis

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.167767553980 a.u.

Thermal correction to G: 1196.821 kJ/mol 286.047 kcal/mol 0.455845 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.39913700	-0.93835600	-0.55157700
O	-2.72437200	0.58271000	-1.19899900
C	-3.46735400	0.48523600	-2.21394600
O	-2.01005200	-2.16782500	-2.10589900
C	-2.87552100	-1.84891100	-2.97470300
C	-3.57715000	-0.63283400	-3.06831000
H	-4.28206700	-0.54347400	-3.89717100
C	-4.30065900	1.70572900	-2.51892100
H	-3.62853300	2.55448500	-2.73873000
H	-4.98315300	1.56058300	-3.36966800
H	-4.88415700	1.98035400	-1.62319900
C	-3.15224500	-2.91610300	-4.00465700
H	-2.21513700	-3.16171700	-4.53456500
H	-3.48477600	-3.83689500	-3.49418300
H	-3.91377200	-2.61486700	-4.73923700
C	-0.72751000	0.24663700	1.02231300
C	0.36801000	0.98350100	0.57116700
C	-1.83903100	0.61233400	1.90381600
C	-2.81171000	-0.34796200	2.23852200
C	-1.93952800	1.88984400	2.48416200
C	-3.86028100	-0.03570300	3.09911000
H	-2.73622400	-1.35492600	1.81617000
C	-2.99256000	2.20205300	3.33902800
H	-1.18452200	2.64657400	2.26223000

C	-3.96009600	1.24344000	3.64806000
H	-4.60556400	-0.79861300	3.34287300
H	-3.05596100	3.20479300	3.77236600
H	-4.78602400	1.49176600	4.32129000
C	0.53622600	2.42725800	0.40151800
C	1.62963600	3.10326200	0.96442700
C	-0.41220300	3.15183300	-0.33901500
C	1.77666400	4.47759300	0.78253200
H	2.35656100	2.55107000	1.56586100
C	-0.25706900	4.52276400	-0.52330500
H	-1.26696900	2.61767300	-0.76718700
C	0.83760100	5.18916800	0.03435300
H	2.62816200	4.99621500	1.23311100
H	-0.99612300	5.07853400	-1.10800200
H	0.95597400	6.26697000	-0.11142500
C	1.34182000	-0.09222500	0.54382700
C	2.61951600	-0.16303200	0.08096000
C	0.40837900	-1.12795700	1.15187000
C	0.41763900	-1.43061400	2.58060500
C	-0.01674600	-2.19941400	0.22335100
C	-0.20973300	-2.54380400	3.04466500
H	0.85039900	-0.69148500	3.26198300
C	-0.67918900	-3.34999500	0.79204200
H	0.62617700	-2.37002600	-0.65340800
C	-0.80583100	-3.49413600	2.14528600
H	-0.26286200	-2.72791300	4.12190700
H	-1.05459100	-4.12229400	0.11332100
H	-1.32544800	-4.36273900	2.55998300
C	3.48572300	-1.34807700	0.16945600
C	3.30539700	-2.37789800	1.11350300
C	4.55991100	-1.47655800	-0.73324600
C	4.14697400	-3.48537000	1.13852200
H	2.50427800	-2.30826500	1.85231300
C	5.39718000	-2.58847800	-0.71462600
H	4.73823000	-0.69161100	-1.47516300
C	5.19445700	-3.60211200	0.22210100
H	3.98335100	-4.26684000	1.88677700
H	6.21599700	-2.66137800	-1.43660000
H	5.85251300	-4.47582000	0.24274200
B	3.15261200	1.08889000	-0.70357000
O	2.52377200	1.55829900	-1.81878700
O	4.26929700	1.79917600	-0.37233900
C	3.15873100	2.77207600	-2.20185400
C	4.42709900	2.84201100	-1.32866800

H	2.46693500	3.60771400	-2.00128100
H	3.38044600	2.74578600	-3.28050600
H	5.35033200	2.66079600	-1.90502500
H	4.52533800	3.80527600	-0.80266000

Int11

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.208982827046 a.u.

Thermal correction to G: 1200.413 kJ/mol 286.906 kcal/mol 0.457213 a.u.

Optimized atomic Cartesian coordinates:

Pd	-0.88210000	-0.37088000	0.98391000
O	-2.41963300	1.10087900	0.94833700
C	-3.20004500	1.37003800	1.89961200
O	-1.39108300	-0.78945300	2.93892300
C	-2.32442500	-0.24620600	3.60958400
C	-3.19442200	0.76432200	3.17552700
H	-3.93846000	1.11497500	3.89299800
C	-4.22135100	2.44117600	1.61100600
H	-4.85818200	2.11389800	0.77032800
H	-4.85817000	2.67524000	2.47716500
H	-3.70062700	3.35603700	1.27827600
C	-2.46946400	-0.77473100	5.01329000
H	-2.64652700	-1.86382200	4.97426700
H	-1.52240700	-0.62144200	5.55987300
H	-3.28888800	-0.29386000	5.56776600
C	-0.23911500	-0.85773300	-1.00513900
C	0.10928100	0.49574200	-0.84318400
C	-1.34050500	-1.40058000	-1.83386200
C	-2.69386500	-1.19265300	-1.52911800
C	-1.02022300	-2.08113000	-3.01966100
C	-3.69520500	-1.66495900	-2.37476500
H	-2.96044000	-0.63648100	-0.62650600
C	-2.02237700	-2.54677100	-3.86874700
H	0.02565300	-2.22457600	-3.29581200
C	-3.36457700	-2.34716600	-3.54592900
H	-4.74413900	-1.49291100	-2.11598500
H	-1.74975500	-3.06796000	-4.79133500
H	-4.15165000	-2.71717500	-4.20981200
C	-0.60987500	1.67290500	-1.38281000
C	-0.70730800	2.85146300	-0.62937800
C	-1.14530100	1.65313400	-2.67680300
C	-1.33527400	3.97736600	-1.15122600
H	-0.29761500	2.87499600	0.38285200
C	-1.77064200	2.78377700	-3.20264700

H	-1.06280400	0.74891000	-3.28409000
C	-1.87060600	3.94734200	-2.44094600
H	-1.40881800	4.88627900	-0.54664600
H	-2.17994100	2.75270400	-4.21681400
H	-2.36353800	4.83341200	-2.85239200
C	1.55206400	0.57200400	-0.47885900
C	2.08410700	-0.67520400	-0.39037000
C	2.25648500	1.84075700	-0.21113400
C	2.40370700	2.81833900	-1.20431800
C	2.78105700	2.08629900	1.06457200
C	3.06885600	4.01102100	-0.92814900
H	1.99669400	2.63811900	-2.20302900
C	3.43924400	3.28262500	1.34369200
H	2.65675700	1.32904700	1.84474400
C	3.58524700	4.24813100	0.34685400
H	3.18289200	4.76275500	-1.71489500
H	3.83925400	3.46244800	2.34611900
H	4.10173000	5.18803600	0.56388100
C	0.97284200	-1.69117600	-0.48999400
C	1.26961000	-2.97401200	-1.20677100
C	0.46056700	-1.87943800	0.95804900
C	0.69115600	-4.12469300	-0.82255000
H	1.93723800	-2.94010000	-2.07367300
C	-0.20881900	-3.15796800	1.23131800
H	1.17247500	-1.58066700	1.74737800
C	-0.14712700	-4.19686900	0.36858800
H	0.87789200	-5.04580400	-1.38428900
H	-0.73020700	-3.25474100	2.19012000
H	-0.65452000	-5.13860300	0.59905700
B	3.53862600	-1.05107100	-0.02320800
O	4.62505600	-0.25626700	-0.26393500
O	3.86794700	-2.24448200	0.56044500
C	5.76324600	-0.88839600	0.30445700
C	5.28478600	-2.30760900	0.66022900
H	6.08093500	-0.31848100	1.19521400
H	6.59053200	-0.88478900	-0.42300900
H	5.65978500	-3.06690800	-0.04793200
H	5.56964300	-2.61302200	1.67968800

Int11-6r

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.229560259224 a.u.

Thermal correction to G: 1206.435 kJ/mol 288.345 kcal/mol 0.459507 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.71034800	-1.55426200	-0.10838700
O	-3.34310900	-1.92314100	1.15382600
C	-3.37186000	-1.68976900	2.39741300
O	-0.63084700	-0.82312600	1.52890900
C	-1.04581100	-0.78814000	2.72333300
C	-2.32391900	-1.16649000	3.17750500
H	-2.51875200	-1.04832500	4.24497000
C	-4.67752700	-2.02153100	3.07625900
H	-4.91336200	-3.08735400	2.91077800
H	-4.66271500	-1.81796100	4.15734800
H	-5.48861600	-1.43573900	2.60903900
C	-0.04012900	-0.30287200	3.73769100
H	0.76933400	-1.05008000	3.82329000
H	0.42135300	0.63521200	3.38662400
H	-0.48101700	-0.14754300	4.73395900
C	-0.39135100	1.37203200	-1.39266900
C	0.79075100	1.30159000	-0.72823800
C	-1.27650900	2.55458000	-1.29175600
C	-2.54662600	2.43909400	-0.70637600
C	-0.85816400	3.80950200	-1.75260800
C	-3.37084700	3.55464700	-0.57586200
H	-2.87700900	1.46463800	-0.33344900
C	-1.68585900	4.92468000	-1.62868000
H	0.13167400	3.90864600	-2.20693300
C	-2.94375500	4.80114100	-1.03813800
H	-4.35295000	3.45070000	-0.10477500
H	-1.34329300	5.89779000	-1.99343100
H	-3.59183100	5.67680400	-0.93593600
C	1.21303600	2.39407500	0.19159700
C	0.47123800	2.64288900	1.35326200
C	2.33747100	3.18571200	-0.07070700
C	0.84462200	3.65679900	2.23405200
H	-0.41045200	2.02922700	1.55514100
C	2.71231800	4.20110200	0.80794600
H	2.92227400	3.00996300	-0.97745300
C	1.96892500	4.43841200	1.96479100
H	0.25335200	3.83603300	3.13732000
H	3.59215000	4.81267100	0.58589000
H	2.26487100	5.23382000	2.65552300
C	1.60923400	0.08320800	-0.80325600
C	1.07701000	-1.09547400	-1.24739000
C	2.96037100	0.09698900	-0.17531700
C	4.10540300	0.43814200	-0.90167600
C	3.08779900	-0.24786200	1.17551800

C	5.35739900	0.43464500	-0.28911600
H	4.01284200	0.69854600	-1.96030600
C	4.33988400	-0.24890300	1.79014600
H	2.18675100	-0.50873700	1.73847800
C	5.47785100	0.09325900	1.05922200
H	6.24710100	0.69769200	-0.86944300
H	4.42614000	-0.51871000	2.84724000
H	6.46096300	0.09256000	1.53971900
C	-0.31495900	-1.09122800	-1.70299900
C	-0.77637000	0.21962000	-2.30658800
C	-1.05309300	-2.28079200	-1.93793800
C	-2.20260100	0.21136800	-2.76913900
H	-0.14877600	0.36724400	-3.22093600
C	-2.46003200	-2.10494100	-2.01931200
H	-0.59261500	-3.26815000	-1.84452200
C	-2.98864300	-0.86438700	-2.60254100
H	-2.58260800	1.11390900	-3.25548200
H	-3.09918500	-2.99284100	-2.04677600
H	-4.03481700	-0.84533700	-2.92276700
B	1.87177400	-2.42540300	-1.05625600
O	3.14395600	-2.62754700	-1.50901300
O	1.35754100	-3.52165800	-0.41385100
C	3.59648100	-3.87522200	-1.00022600
C	2.32357100	-4.56485600	-0.48345700
H	4.32535100	-3.68484800	-0.19322600
H	4.09873700	-4.44152200	-1.80023600
H	1.95747600	-5.34426600	-1.17391300
H	2.45259900	-5.01329400	0.51389800

Int11-cis

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.176371751444 a.u.

Thermal correction to G: 1198.731 kJ/mol 286.504 kcal/mol 0.456572 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.37744200	-0.57228300	-0.76347200
O	-2.73315600	1.05587400	-0.58246500
C	-3.71601600	1.25912500	-1.34298500
O	-2.44693800	-1.27792900	-2.37574300
C	-3.48774300	-0.73381000	-2.86477900
C	-4.10936400	0.44612000	-2.42994100
H	-4.99305600	0.76575500	-2.98510000
C	-4.52899200	2.48915400	-1.02881000
H	-3.85485600	3.36159100	-0.97836400
H	-5.32539000	2.67966700	-1.76357100

H	-4.98246300	2.37470800	-0.02806500
C	-4.07801900	-1.47061900	-4.03933700
H	-3.31888800	-1.55203800	-4.83693300
H	-4.33302800	-2.49959500	-3.73067000
H	-4.97636000	-0.98071200	-4.44310500
C	-0.38289200	-0.67568600	1.10425100
C	0.15535400	0.48267500	0.49180200
C	-1.34075400	-0.89415000	2.18967100
C	-1.26543500	-2.03289600	3.00685000
C	-2.36184000	0.04619000	2.43365400
C	-2.17437500	-2.21910500	4.04768200
H	-0.48252900	-2.77043000	2.82700100
C	-3.26517100	-0.14563600	3.47215700
H	-2.46138100	0.91290700	1.77565400
C	-3.17418300	-1.27769900	4.28723700
H	-2.09805100	-3.11125600	4.67639900
H	-4.05473700	0.59210600	3.64376900
H	-3.88678400	-1.42652200	5.10402600
C	-0.05831400	1.93314400	0.62951400
C	-0.17910500	2.52359100	1.89302300
C	-0.08705400	2.74559800	-0.51159900
C	-0.34243700	3.90250500	2.01195600
H	-0.13936900	1.89706400	2.78806300
C	-0.25566700	4.12308300	-0.39217100
H	0.00309000	2.28393900	-1.49838600
C	-0.38693000	4.70463700	0.87051300
H	-0.43510200	4.35407500	3.00406600
H	-0.29064300	4.74612600	-1.29079100
H	-0.52099100	5.78635500	0.96527700
C	1.37657500	-0.22784800	0.07745600
C	2.62429000	0.19361900	-0.21560900
C	0.73551600	-1.57479200	0.42215000
C	1.46261000	-2.61659500	1.19883500
C	-0.02868400	-2.06943400	-0.80034400
C	1.03636800	-3.89350200	1.12763100
H	2.29314800	-2.32185500	1.84729300
C	-0.57404800	-3.42784200	-0.66098900
H	0.47039300	-1.90628700	-1.77301800
C	-0.07951500	-4.27859700	0.26920400
H	1.52428800	-4.67042400	1.72549000
H	-1.33364800	-3.76243000	-1.37665600
H	-0.46478500	-5.30051400	0.34171000
C	3.75494600	-0.72434100	-0.44894100
C	3.59837300	-1.98494400	-1.05295300

C	5.05321800	-0.33439400	-0.07038200
C	4.69040200	-2.82771500	-1.24627400
H	2.61130100	-2.29954000	-1.39637800
C	6.14516700	-1.17676200	-0.26287600
H	5.20167700	0.64096400	0.40488700
C	5.96838600	-2.43091600	-0.84977400
H	4.54082600	-3.80249800	-1.72045400
H	7.14228200	-0.85140000	0.04905300
H	6.82513700	-3.09327900	-1.00544500
B	2.92738300	1.73321500	-0.23826800
O	2.98760400	2.47241400	-1.38448700
O	3.20453200	2.45807700	0.88461700
C	3.33178800	3.80723600	-1.03430400
C	3.33133100	3.82436000	0.50647400
H	2.58852800	4.49863300	-1.46349300
H	4.32072200	4.04467600	-1.46205300
H	4.26026500	4.23777900	0.93077400
H	2.47278900	4.38136500	0.91675100

TS12

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.193543773525 a.u.

Thermal correction to G: 1200.587 kJ/mol 286.947 kcal/mol 0.457280 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.27751900	-0.90407600	-0.55701200
O	3.09169100	0.12592500	-0.62622100
C	4.06448900	-0.16236700	-1.38178000
O	1.96577800	-2.21705500	-2.03528600
C	3.10901900	-2.16494400	-2.57224500
C	4.12300900	-1.22345200	-2.30410500
H	5.05066900	-1.32901800	-2.86973600
C	5.25745500	0.75018100	-1.24880500
H	5.57865300	0.77498400	-0.19305000
H	6.10423900	0.44568900	-1.88182500
H	4.95742200	1.77878700	-1.51790300
C	3.37759700	-3.23436000	-3.60214500
H	3.24776800	-4.22730200	-3.13723600
H	2.62898200	-3.15639300	-4.41015400
H	4.38572800	-3.16774800	-4.03770600
C	0.36868900	0.19750900	0.96684800
C	-0.43849400	1.21962500	0.31134900
C	1.32185200	0.52008500	2.06703900
C	2.34780900	-0.36836800	2.42826800
C	1.17222600	1.69372900	2.82126000

C	3.20103000	-0.08712700	3.49275300
H	2.48234700	-1.29099700	1.85612400
C	2.03021800	1.98147400	3.88167000
H	0.36735400	2.39135300	2.57781500
C	3.05108000	1.09384700	4.22136100
H	3.99455200	-0.79518900	3.75022100
H	1.89371500	2.90631200	4.45051300
H	3.72518000	1.31895300	5.05334300
C	0.03866600	2.58101000	0.01464500
C	1.37396000	2.80850000	-0.35593500
C	-0.81886700	3.68651500	0.14667000
C	1.82845500	4.10122900	-0.60764400
H	2.06053900	1.96103200	-0.44301800
C	-0.35986400	4.97771300	-0.10016600
H	-1.85317600	3.53293500	0.46399300
C	0.96526700	5.19091100	-0.48471000
H	2.87144400	4.25723400	-0.90055000
H	-1.04227500	5.82538600	0.01399900
H	1.32503100	6.20554700	-0.68083000
C	-1.72272100	0.73512400	0.05456100
C	-1.86157000	-0.59468600	0.56226500
C	-2.78190300	1.38964100	-0.73517600
C	-4.09224900	1.46835100	-0.24164500
C	-2.50955900	1.91732600	-2.00617500
C	-5.10432000	2.05986900	-0.99551200
H	-4.31546600	1.07976100	0.75754100
C	-3.52059300	2.50841400	-2.76040700
H	-1.49201800	1.85653700	-2.40346200
C	-4.82107000	2.58301800	-2.25773900
H	-6.11947100	2.11799900	-0.59138200
H	-3.29197000	2.91179500	-3.75146300
H	-5.61379400	3.04934700	-2.85030500
C	-0.55745800	-0.99341700	1.10571800
C	-0.41318800	-1.93258600	2.24163700
C	-0.61425600	-1.72848200	-0.31621100
C	-0.56696300	-3.26419400	2.11789700
H	-0.19251300	-1.47869900	3.21172500
C	-0.80726100	-3.16868900	-0.31085800
H	-0.87221200	-1.20902800	-1.24784600
C	-0.80430000	-3.89353400	0.83309000
H	-0.48666700	-3.89957900	3.00470500
H	-0.91923500	-3.65747100	-1.28274200
H	-0.93086500	-4.97909100	0.79267600
B	-3.17024600	-1.45011300	0.59719700

O	-3.86679400	-1.79535000	-0.52135600
O	-3.73822200	-1.89425000	1.75261700
C	-5.06403400	-2.44068100	-0.10486700
C	-4.86899600	-2.68690700	1.40265300
H	-5.19847000	-3.37166900	-0.67752700
H	-5.91708500	-1.77253300	-0.31483800
H	-5.73627700	-2.37399300	2.00484200
H	-4.64532700	-3.74272100	1.63124300

Int13

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.222520513084 a.u.

Thermal correction to G: 1204.639 kJ/mol 287.916 kcal/mol 0.458823 a.u.

Optimized atomic Cartesian coordinates:

Pd	0.94870700	-1.06946300	-0.50497100
O	2.91904600	-0.31833700	-0.48245800
C	3.82746300	-0.64989400	-1.29491200
O	1.40110900	-2.18985200	-2.18431900
C	2.54354400	-2.26859600	-2.72742400
C	3.70959300	-1.58224200	-2.34432300
H	4.60455600	-1.76449300	-2.94198100
C	5.14421800	0.05648600	-1.09543500
H	5.44525600	-0.02894100	-0.03733900
H	5.94426000	-0.33485800	-1.74148700
H	5.00880700	1.13286500	-1.30539900
C	2.61100800	-3.19704700	-3.91344400
H	2.29288500	-4.20739200	-3.60242400
H	1.89644400	-2.85612800	-4.68302500
H	3.61703000	-3.25359500	-4.35493800
C	0.41185800	0.27269400	1.16348000
C	-0.36551500	1.26615900	0.37517200
C	1.50073800	0.61835900	2.10348300
C	2.51657000	-0.29524500	2.42439200
C	1.48651400	1.85847700	2.76095800
C	3.48920900	0.02301500	3.36922100
H	2.55608700	-1.25734300	1.90927300
C	2.45982600	2.17642000	3.70579900
H	0.69536400	2.57880100	2.54020500
C	3.46800500	1.26180100	4.01124900
H	4.27549300	-0.70211600	3.59949200
H	2.42675100	3.14748300	4.20877800
H	4.23551000	1.51359800	4.74929000
C	0.14789400	2.59195700	-0.00538200
C	1.49198100	2.74249100	-0.38351000

C	-0.68718800	3.71879400	-0.00790900
C	1.97932200	3.98868700	-0.77167800
H	2.15232800	1.86916800	-0.37565200
C	-0.19497100	4.96438700	-0.39121200
H	-1.73042000	3.61435400	0.30220200
C	1.13933700	5.10366700	-0.77760700
H	3.02722900	4.08934100	-1.07064600
H	-0.85825100	5.83462500	-0.38459800
H	1.52524900	6.08243400	-1.07820000
C	-1.53346400	0.70062000	-0.03631400
C	-1.60474100	-0.74930900	0.41152000
C	-2.48994400	1.24731800	-1.01132100
C	-3.85802000	1.34646600	-0.71648700
C	-2.04435100	1.65238900	-2.27980300
C	-4.75522800	1.84245200	-1.66042000
H	-4.21872000	1.06557400	0.27734200
C	-2.94215600	2.14262200	-3.22525200
H	-0.97973600	1.57317300	-2.51901400
C	-4.30044100	2.23999400	-2.91839200
H	-5.81714900	1.92247000	-1.40960400
H	-2.57853000	2.44886200	-4.21067700
H	-5.00546900	2.62626300	-3.66048500
C	-0.38326000	-0.89041400	1.29806600
C	-0.23044400	-1.98751200	2.20095200
C	-1.09191600	-1.64295700	-0.70756800
C	-0.70924900	-3.24638600	1.94461200
H	0.31386200	-1.80179300	3.13338200
C	-1.16874700	-3.06645000	-0.51745200
H	-1.30119500	-1.29650600	-1.72958300
C	-1.12909600	-3.74983900	0.67493300
H	-0.61205000	-3.98753800	2.74552300
H	-1.24720500	-3.66873900	-1.42951100
H	-1.29431200	-4.83159800	0.62693600
B	-2.99191200	-1.13154800	1.06553900
O	-3.96848000	-1.83677400	0.43104200
O	-3.35006400	-0.70904500	2.31259800
C	-5.12009600	-1.83537000	1.26590900
C	-4.62851900	-1.26114100	2.60764000
H	-5.51138200	-2.86092700	1.35603500
H	-5.89689500	-1.20512900	0.79854000
H	-5.28772700	-0.47316000	3.00490200
H	-4.51030700	-2.04078200	3.37947300

TS14

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.214680629169 a.u.

Thermal correction to G: 1204.303 kJ/mol 287.835 kcal/mol 0.458695 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.30863400	-1.02625100	-0.23924800
O	2.90615300	0.24271800	-0.78560200
C	3.88573700	-0.08346800	-1.51558100
O	2.16164600	-2.54103800	-1.40618600
C	3.24855800	-2.45809600	-2.04536700
C	4.09392700	-1.33351700	-2.12651200
H	4.99839700	-1.44210200	-2.72779800
C	4.90741000	1.00655800	-1.72532200
H	5.29261300	1.33364000	-0.74365200
H	5.74931400	0.68951500	-2.35875000
H	4.41513800	1.88108100	-2.18619400
C	3.64701600	-3.70911800	-2.78910500
H	3.70822200	-4.55146400	-2.07815200
H	2.86007400	-3.96172300	-3.52142900
H	4.60839400	-3.60725100	-3.31436700
C	0.34606000	0.32129100	1.02441700
C	-0.51205400	1.19018900	0.17180600
C	1.17645700	0.88845900	2.12189500
C	2.41008400	0.33553800	2.49218600
C	0.69725600	1.99224900	2.84456800
C	3.14387200	0.87065400	3.55062800
H	2.80922400	-0.51417800	1.93036200
C	1.42883100	2.52746300	3.90186300
H	-0.26581000	2.43322300	2.57363900
C	2.65772700	1.96946600	4.25850400
H	4.10711400	0.42634700	3.81871900
H	1.03536600	3.38792300	4.45148000
H	3.23553600	2.39182500	5.08610900
C	-0.16592700	2.58268000	-0.15815300
C	1.16871600	2.93555000	-0.41383900
C	-1.15169700	3.58006400	-0.21029600
C	1.50051900	4.25074200	-0.73385700
H	1.94351300	2.16273400	-0.38236300
C	-0.81521100	4.89479300	-0.52382800
H	-2.19090100	3.32023900	0.00851600
C	0.51240200	5.23494200	-0.79044300
H	2.54401900	4.50879100	-0.94007100
H	-1.59566400	5.66112900	-0.55593100
H	0.77649800	6.26796700	-1.03663200
C	-1.58662900	0.49195700	-0.28392300

C	-1.55459100	-0.94212200	0.22252800
C	-2.55641300	0.92645800	-1.30299800
C	-3.93844600	0.89857600	-1.06216800
C	-2.10378200	1.36191500	-2.55879100
C	-4.84149500	1.29846000	-2.04527900
H	-4.31158800	0.59539400	-0.07981600
C	-3.00632500	1.75757200	-3.54328200
H	-1.02800000	1.38339200	-2.75648000
C	-4.37864800	1.72714900	-3.29002400
H	-5.91502500	1.27955800	-1.83501100
H	-2.63500900	2.09013300	-4.51729400
H	-5.08791900	2.03828400	-4.06272500
C	-0.35844800	-0.93675600	1.14556300
C	-0.01701600	-2.02465300	1.95467700
C	-1.07419700	-1.88759500	-0.85278800
C	-0.51914800	-3.33152300	1.79663400
H	0.67002300	-1.83687100	2.78783000
C	-0.99773000	-3.24832700	-0.64723000
H	-1.01045200	-1.50230600	-1.87709600
C	-0.97507800	-3.89143100	0.60919900
H	-0.36391100	-4.01840000	2.63555100
H	-0.90015600	-3.88726300	-1.53215700
H	-1.14992700	-4.97289500	0.61479900
B	-2.90542300	-1.36634600	0.93654700
O	-3.85579500	-2.16491700	0.37896400
O	-3.24600500	-0.89217800	2.16882800
C	-4.97847800	-2.18016900	1.25320500
C	-4.48039800	-1.49678200	2.54019500
H	-5.30319900	-3.21960200	1.41724500
H	-5.80666100	-1.62671000	0.77722900
H	-5.17201900	-0.72419000	2.91152800
H	-4.29240300	-2.21864900	3.35305500

Int15

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.232807668772 a.u.

Thermal correction to G: 1204.769 kJ/mol 287.947 kcal/mol 0.458872 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.76592100	-0.67173300	-0.03982600
O	2.51858300	0.96975500	-1.09777100
C	3.53847200	0.95180300	-1.84905200
O	3.34497000	-1.83166400	-0.74023400
C	4.23742600	-1.44386000	-1.54780300
C	4.36713300	-0.15484200	-2.10206900

H	5.20533700	0.00399100	-2.78291700
C	3.85906600	2.26749300	-2.51149300
H	4.03455100	3.03190500	-1.73411500
H	4.73996000	2.21324700	-3.16838200
H	2.98641000	2.60006500	-3.10030000
C	5.25080300	-2.49462600	-1.92550400
H	5.77074800	-2.84142600	-1.01515400
H	4.72599700	-3.36827600	-2.34953400
H	5.99533600	-2.13133300	-2.64936700
C	0.13354700	0.28028400	0.93613300
C	-0.83747800	0.97752500	0.06089000
C	0.63900600	0.89906100	2.19234400
C	1.67690300	1.84064200	2.19706700
C	0.02941600	0.55350800	3.40676000
C	2.09869800	2.41972100	3.39244200
H	2.16608500	2.09981500	1.25519300
C	0.45618900	1.13044300	4.60274800
H	-0.79627600	-0.16473700	3.39881700
C	1.49129800	2.06584100	4.59873800
H	2.91345400	3.14996500	3.38214800
H	-0.02783500	0.85087800	5.54356600
H	1.82599900	2.51976700	5.53642400
C	-0.92024800	2.44872800	-0.00334300
C	0.16539800	3.20252700	-0.47170900
C	-2.08251000	3.11096200	0.41344200
C	0.07995700	4.59285000	-0.53305800
H	1.06815900	2.68036700	-0.80674100
C	-2.16291500	4.50110600	0.35608200
H	-1.69317400	2.10941800	-2.39155800
C	-1.08242000	5.24600200	-0.11971300
H	0.92949000	5.17172500	-0.90866600
H	-3.07527400	5.00692500	0.68643300
H	-1.14614500	6.33742000	-0.16620900
C	-1.63101900	0.07359200	-0.58002400
C	-1.27529300	-1.34751500	-0.15782800
C	-2.65803900	0.34335200	-1.59378900
C	-3.75850700	-0.51826600	-1.75257200
C	-2.55746600	1.44605800	-2.46306900
C	-4.73588400	-0.26995200	-2.71387100
H	-3.85742600	-1.40358500	-1.11876100
C	-3.53244300	1.69158200	-3.42504200
H	-2.92708300	2.52365700	0.78562500
C	-4.63199900	0.83994500	-3.55154500
H	-5.58437200	-0.95409600	-2.80910100

H	-3.42755100	2.55451700	-4.08952300
H	-5.39763200	1.03496100	-4.30829000
C	-0.11191100	-1.11763300	0.77610500
C	0.79488900	-2.06758100	1.29426800
C	-0.95155800	-2.24084200	-1.32648800
C	0.74858400	-3.49331000	0.99993900
H	1.30531500	-1.79728100	2.22704000
C	-0.32308300	-3.43086100	-1.27486100
H	-1.29655500	-1.88502600	-2.30349100
C	0.25604700	-4.08516000	-0.11559000
H	1.22761700	-4.14069100	1.74214700
H	-0.23768600	-3.98377700	-2.21822100
H	0.37876800	-5.17161600	-0.19600600
B	-2.41972300	-1.92629700	0.79393300
O	-3.17722200	-3.02223700	0.52191100
O	-2.71599900	-1.34057600	1.98895500
C	-4.02320800	-3.26074500	1.64376100
C	-3.82129100	-2.03593900	2.55687100
H	-3.71214500	-4.20246100	2.12550700
H	-5.06319100	-3.37001300	1.29874300
H	-4.69666100	-1.36514600	2.56279700
H	-3.58398500	-2.31151100	3.59631600

Int16

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.235533486297 a.u.

Thermal correction to G: 1206.270 kJ/mol 288.305 kcal/mol 0.459444 a.u.

Optimized atomic Cartesian coordinates:

Pd	2.89326000	-0.65523500	0.29474000
O	3.37748300	1.27602000	-0.30875700
C	4.27497800	1.59326400	-1.14477600
O	4.41578300	-1.39096600	-0.93834800
C	5.16628500	-0.69228000	-1.67746800
C	5.14521000	0.71081900	-1.80655100
H	5.86557500	1.15391900	-2.49649800
C	4.37758900	3.06987200	-1.42912300
H	4.54257300	3.61274500	-0.48200300
H	5.18601300	3.31447300	-2.13407200
H	3.41730900	3.42662700	-1.84166500
C	6.16762400	-1.47441500	-2.48991500
H	6.79794700	-2.07474700	-1.81087100
H	5.62958400	-2.18419300	-3.14259100
H	6.81180900	-0.83219900	-3.10865000
C	-0.72493200	1.00235900	0.48502100

C	-1.92011300	0.64867100	-0.27475200
C	-0.41869800	2.35527100	0.97867300
C	-1.41023600	3.10944600	1.62958600
C	0.86035800	2.91333400	0.82724100
C	-1.13023200	4.38318900	2.11672700
H	-2.40817900	2.68369500	1.76341800
C	1.13581200	4.19158200	1.31413700
H	1.64677100	2.35019500	0.31422900
C	0.14455400	4.93164700	1.95826000
H	-1.91377900	4.95279200	2.62570500
H	2.13782000	4.61216800	1.18144100
H	0.36248700	5.93511200	2.33651100
C	-2.94933300	1.62126700	-0.68877300
C	-2.60724500	2.76108100	-1.42977100
C	-4.29015500	1.42767600	-0.32704400
C	-3.58549800	3.67663300	-1.81367400
H	-1.56303400	2.92537600	-1.71092500
C	-5.26747100	2.34447600	-0.70746200
H	-3.23679700	0.03039500	-2.75790400
C	-4.91846000	3.47113500	-1.45462600
H	-3.30417400	4.55849900	-2.39716300
H	-6.30925000	2.18079200	-0.41546500
H	-5.68549100	4.19180700	-1.75375500
C	-1.94483800	-0.70625500	-0.48535400
C	-0.77794100	-1.32640900	0.23374800
C	-2.91288200	-1.49100000	-1.25373200
C	-3.25256900	-2.80162000	-0.87003100
C	-3.51003600	-0.97095800	-2.41749300
C	-4.17202200	-3.55028800	-1.60159100
H	-2.79436500	-3.24756500	0.01807900
C	-4.42740700	-1.71988500	-3.14762600
H	-4.55861800	0.54826100	0.26554800
C	-4.76941500	-3.01163100	-2.74105500
H	-4.42286000	-4.56410700	-1.27547100
H	-4.87523200	-1.29254500	-4.04994000
H	-5.49139700	-3.59887100	-3.31608600
C	-0.00215800	-0.13937800	0.74375700
C	1.19956300	-0.25063100	1.54941300
C	-0.02287400	-2.37226300	-0.52346300
C	1.83649300	-1.47462600	1.90175100
H	1.38564300	0.59838700	2.21860400
C	1.18530600	-2.86530100	-0.19700900
H	-0.52053000	-2.77769500	-1.41058800
C	2.04075300	-2.49123100	0.93013400

H	2.42966600	-1.51381000	2.82130100
H	1.60700500	-3.63996500	-0.84637200
H	2.77995300	-3.25300800	1.20543300
B	-1.39577100	-1.91406500	1.59722400
O	-1.15350900	-3.17753900	2.04200100
O	-2.21653800	-1.19749800	2.41536300
C	-1.77500800	-3.31714000	3.31640600
C	-2.64946700	-2.05825800	3.46173500
H	-0.98900900	-3.37557200	4.08806800
H	-2.35824400	-4.25088900	3.33868500
H	-3.72268100	-2.27418600	3.32324700
H	-2.51659400	-1.55377200	4.43174600

Int16-1

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.234096174249 a.u.

Thermal correction to G: 1203.726 kJ/mol 287.697 kcal/mol 0.458475 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.13153700	-0.67299300	-0.29200800
O	-3.13263400	-0.45888500	-0.88276000
C	-3.96272800	-1.40421300	-1.02400400
O	-1.38905000	-2.74025400	-0.26584900
C	-2.47110700	-3.35497700	-0.49397700
C	-3.70709700	-2.77489400	-0.83688500
H	-4.54286600	-3.45805000	-0.99849200
C	-5.34654800	-0.97665900	-1.44222900
H	-5.28655100	-0.46132800	-2.41709900
H	-6.04907300	-1.81934300	-1.52361900
H	-5.73687100	-0.24484400	-0.71368800
C	-2.38134700	-4.85578200	-0.38553200
H	-1.98838000	-5.12444600	0.61031300
H	-3.34846200	-5.35559300	-0.54434300
H	-1.65518000	-5.22916900	-1.12902300
C	-0.34652600	1.30837200	-0.29499700
C	0.22149500	0.52200900	0.76758500
C	-1.15332700	2.53421000	-0.08943600
C	-2.45056800	2.65745300	-0.59923200
C	-0.58074400	3.61221900	0.59977500
C	-3.16493600	3.84205200	-0.41577700
H	-2.90450100	1.80369800	-1.10985500
C	-1.29667200	4.79318900	0.78258000
H	0.43620300	3.51635600	0.99208900
C	-2.59165800	4.91084200	0.27396700
H	-4.18171400	3.92777800	-0.81118600

H	-0.84094500	5.62721100	1.32478400
H	-3.15537200	5.83764700	0.41784100
C	0.06814100	0.77125800	2.21102200
C	1.21873500	0.84115600	3.00760500
C	-1.18635300	0.98826400	2.79499400
C	1.11435000	1.11799800	4.36910700
H	2.19688000	0.68452200	2.54445000
C	-1.28829200	1.26066600	4.15710800
H	-2.08490300	0.93017300	2.17377700
C	-0.13897000	1.32519100	4.94747800
H	2.01822000	1.17193500	4.98308700
H	-2.27294500	1.42163500	4.60559300
H	-0.22078500	1.53778500	6.01759700
C	0.96286200	-0.51958000	0.12243000
C	1.45973700	-0.00849200	-1.23420500
C	1.60085600	-1.65841800	0.80725700
C	2.82689200	-2.17568400	0.36071900
C	0.98634600	-2.26979100	1.91460200
C	3.43362900	-3.24738500	1.01577800
H	3.32396500	-1.74130300	-0.51084700
C	1.59173000	-3.33706400	2.56758300
H	0.01263200	-1.90945300	2.25438600
C	2.82190900	-3.82993500	2.12395500
H	4.39159800	-3.62932800	0.65067700
H	1.09425800	-3.79632500	3.42696900
H	3.29506700	-4.67282700	2.63641800
C	0.48139100	1.13014200	-1.49607800
C	0.48010600	1.91324200	-2.60459100
C	1.37122500	-1.03330500	-2.33143200
C	1.29879100	1.71322700	-3.77283800
H	-0.19109000	2.77978200	-2.60834300
C	1.60429700	-0.77113700	-3.63460400
H	1.12100800	-2.05843700	-2.03368100
C	1.81290800	0.53266800	-4.22395900
H	1.43970700	2.59284700	-4.41227100
H	1.61133400	-1.62029100	-4.32937300
H	2.33153000	0.55227100	-5.18975100
B	2.89826100	0.64160300	-1.02563700
O	4.03227200	0.30980800	-1.70108500
O	3.09492900	1.60220000	-0.07422000
C	5.11312700	1.03701100	-1.12594400
C	4.44479300	2.04140000	-0.16831000
H	5.69162200	1.52624400	-1.92511700
H	5.77422900	0.32924000	-0.59741700

H	4.90008700	2.04551600	0.83451600
H	4.45784200	3.07128200	-0.56361400

Int16-2

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.233759716539 a.u.

Thermal correction to G: 1207.035 kJ/mol 288.488 kcal/mol 0.459735 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.95780700	-1.59016400	-0.71208000
O	1.32058900	-0.29720000	-2.20587800
C	1.96971300	0.70792000	-2.61529500
O	3.86452400	-0.74651500	-0.80348700
C	4.15068800	0.31425200	-1.43147000
C	3.29426800	1.04411400	-2.27745000
H	3.70399800	1.94723900	-2.73323800
C	1.20687200	1.61829200	-3.54415500
H	0.72325100	1.01735400	-4.33238000
H	0.40129000	2.11565500	-2.97397500
H	1.84229900	2.38957400	-4.00478000
C	5.55793900	0.81547700	-1.22454400
H	6.27273300	0.02736000	-1.51921400
H	5.77465100	1.73142200	-1.79418000
H	5.71873000	1.01056800	-0.14956800
C	-0.19329900	0.87952600	1.29401000
C	-1.22845200	0.91180200	0.26643500
C	0.36083800	2.06356900	1.96866900
C	1.74800500	2.27557100	1.99896200
C	-0.48057100	3.01089300	2.57291600
C	2.28089100	3.40018500	2.62769100
H	2.40761900	1.55837900	1.50113800
C	0.05330100	4.13059000	3.20553100
H	-1.56342700	2.85968700	2.54918500
C	1.43548300	4.32927600	3.23475400
H	3.36411100	3.55421900	2.63707000
H	-0.61489500	4.85637200	3.67875000
H	1.85278700	5.21259700	3.72749700
C	-1.86514700	2.14312000	-0.23553900
C	-1.08293200	3.22428000	-0.66902600
C	-3.26130300	2.25391400	-0.29832900
C	-1.68225700	4.37964200	-1.16712900
H	0.00734100	3.15220900	-0.62054900
C	-3.86062000	3.41062000	-0.79282500
H	-1.71063700	0.75108900	-2.59340500
C	-3.07318600	4.47648700	-1.23163900

H	-1.05744800	5.21069400	-1.50804400
H	-4.95178600	3.48137600	-0.83387200
H	-3.54365200	5.38444200	-1.62077200
C	-1.47913300	-0.36583800	-0.15451100
C	-0.64001000	-1.32393500	0.64467200
C	-2.36489700	-0.79707700	-1.23913600
C	-3.18811300	-1.92808100	-1.10927400
C	-2.37338700	-0.10716400	-2.46392200
C	-4.00361900	-2.34526600	-2.15980500
H	-3.20979800	-2.47912500	-0.16462000
C	-3.18755100	-0.52375200	-3.51244100
H	-3.87739000	1.41985400	0.04927900
C	-4.00980900	-1.64313000	-3.36506700
H	-4.64190800	-3.22474700	-2.03245400
H	-3.17287100	0.02520600	-4.45888600
H	-4.64860500	-1.97099500	-4.19050400
C	0.21002700	-0.41793400	1.50031600
C	1.25726800	-0.84973900	2.40021400
C	0.06658400	-2.35426400	-0.20363500
C	2.08390800	-1.90515100	2.20708700
H	1.44788300	-0.20825000	3.26815800
C	1.08181800	-3.24553000	0.21404400
H	-0.54211800	-2.70540800	-1.04569100
C	2.13344800	-2.82406200	1.06698400
H	2.87593600	-2.05776300	2.94824800
H	1.22618000	-4.16823200	-0.35915600
H	2.99316100	-3.50336600	1.09150400
B	-1.56484500	-2.01130700	1.75278900
O	-1.30518600	-3.24589800	2.26234200
O	-2.65746800	-1.41104300	2.30241900
C	-2.32346200	-3.55065400	3.21021500
C	-3.12078400	-2.24080700	3.36221700
H	-1.85891300	-3.88046900	4.15270000
H	-2.93949000	-4.37645300	2.81572200
H	-4.20808400	-2.38705400	3.26442900
H	-2.92063400	-1.73701000	4.32304900

TS17

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -2104.064817131112 a.u.

Thermal correction to G: 1190.563 kJ/mol 284.551 kcal/mol 0.453461 a.u.

Optimized atomic Cartesian coordinates:

Pd	-3.17939600	-0.64126100	-0.33544300
O	-3.73576600	1.37986400	-0.00304000

C	-4.65003100	1.79562300	0.76163300
O	-4.76922900	-1.19569000	0.96308300
C	-5.54023300	-0.40939300	1.57896100
C	-5.53159300	0.99936600	1.51765500
H	-6.27067100	1.52386900	2.12679400
C	-4.77433700	3.29807800	0.85257900
H	-4.90918700	3.71542300	-0.16075200
H	-5.60758100	3.62373800	1.49368000
H	-3.83087700	3.71454600	1.24788500
C	-6.56176900	-1.07824100	2.46938700
H	-7.16354700	-1.78278200	1.86876100
H	-6.03765600	-1.67567200	3.23624200
H	-7.23330300	-0.36321300	2.96860600
C	0.37530900	1.11751000	-0.35575400
C	1.38175600	0.93969100	0.64997400
C	0.14711800	2.35642900	-1.11717700
C	1.22632700	3.04738000	-1.69780900
C	-1.14275000	2.89374000	-1.27530700
C	1.02543500	4.22629800	-2.41138600
H	2.23442100	2.63942000	-1.58841200
C	-1.34200800	4.07361200	-1.99392000
H	-1.99847800	2.39611700	-0.80687100
C	-0.26176500	4.74705500	-2.56506900
H	1.88250700	4.74253100	-2.85610500
H	-2.35617300	4.47414100	-2.09783600
H	-0.41961600	5.67446300	-3.12481600
C	2.30545800	1.98258700	1.12179400
C	1.84268700	3.25913900	1.48321200
C	3.68295400	1.72643100	1.22579000
C	2.72173400	4.23969100	1.93883600
H	0.77303000	3.47608100	1.41160000
C	4.56287700	2.70480100	1.68423300
H	1.63082400	0.80552800	3.47158200
C	4.08735300	3.96748200	2.04398100
H	2.33614300	5.22536900	2.21889500
H	5.63222900	2.48107300	1.75589500
H	4.77802200	4.73694000	2.40300800
C	1.35986500	-0.39097900	1.08290500
C	2.09346200	-0.91251500	2.24461900
C	2.74474000	-2.15896000	2.23421100
C	2.14571200	-0.15815300	3.43358800
C	3.42427000	-2.62345600	3.36089100
H	2.73273300	-2.74962800	1.31505400
C	2.82666700	-0.62135900	4.55568300

H	4.05801700	0.74323400	0.92899800
C	3.47295300	-1.85956300	4.52727600
H	3.92942300	-3.59438100	3.32161700
H	2.84693600	-0.01216400	5.46526000
H	4.00770800	-2.22590300	5.40924600
C	-0.27375100	-0.11114800	-0.55134700
C	-1.36268400	-0.32700200	-1.47497600
C	-0.26911400	-2.30984700	0.78216300
C	-2.00365700	-1.55179300	-1.78403600
H	-1.49210400	0.46621800	-2.22120500
C	-1.40924800	-2.90371200	0.34175800
H	0.23335500	-2.79192600	1.62891700
C	-2.26811900	-2.51603000	-0.77119000
H	-2.52420200	-1.64331000	-2.74365800
H	-1.74301300	-3.79482400	0.88503600
H	-2.99942200	-3.28497700	-1.05189900
C	0.37354600	-1.10743500	0.29551200
H	-0.44302100	-4.33476100	-2.03387900
C	0.59551200	-3.98823500	-2.16663100
O	0.62598900	-2.57598700	-2.19412600
C	1.50251800	-4.38756200	-0.99043100
H	0.97454800	-4.37733600	-3.13019300
B	1.58334800	-2.13771600	-1.29840700
O	2.21113200	-3.20632600	-0.66664700
H	0.91876200	-4.72109400	-0.11508600
H	2.22053700	-5.18162900	-1.25793800
I	2.99009300	-0.57906700	-2.05716600

TS17-13

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -2104.041843658026 a.u.

Thermal correction to G: 1185.709 kJ/mol 283.391 kcal/mol 0.451612 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.43817300	-1.61486500	-0.24442100
O	-3.44668500	-0.87360600	-0.02540400
C	-4.37203900	-1.48806700	0.56645800
O	-2.03563700	-3.41758300	0.64413700
C	-3.17797200	-3.64131600	1.13724600
C	-4.29261200	-2.77963500	1.13338700
H	-5.19763500	-3.15660800	1.61477900
C	-0.80391800	1.36748700	-0.59276600
C	-0.00523300	1.44547600	0.56292900
C	0.77959400	0.27918500	0.66595700
C	0.59868300	-0.50651500	-0.52754100

C	1.49054000	-0.14234500	1.88546500
C	2.61188800	0.54732400	2.36818800
C	1.01164100	-1.23935600	2.61901300
C	3.23711800	0.15267400	3.54885000
H	3.01056200	1.38061600	1.78774200
C	1.63693400	-1.63505700	3.80066900
H	0.12482200	-1.77211600	2.26071100
C	2.75327300	-0.94069700	4.26886000
H	4.11603300	0.69875700	3.90540600
H	1.24567600	-2.48977600	4.36119600
H	3.24637000	-1.25155000	5.19522500
C	-0.52677200	0.14308600	-1.28129300
C	-0.86158000	-0.07581700	-2.67002000
C	0.54955000	-1.98154700	-0.58568100
C	-0.47742300	-1.11558700	-3.46806800
H	-1.48699500	0.70079900	-3.12435200
C	0.64043900	-2.69669600	-1.84637100
H	1.04163400	-2.49879400	0.24598400
C	0.22569400	-2.30626800	-3.09081600
H	-0.79127300	-1.06391500	-4.51724000
H	1.05693700	-3.70881600	-1.77237200
H	0.39243400	-3.02659600	-3.90071300
B	2.26781000	0.24078200	-1.37446300
O	2.40942800	1.59935800	-1.06124500
O	2.19541000	0.07295700	-2.75636800
C	2.58779000	2.30513800	-2.27167700
C	2.04813800	1.35090100	-3.33716100
H	3.66318900	2.52281200	-2.42403300
H	2.03977400	3.26179800	-2.23021000
H	0.98051600	1.54043400	-3.55545500
H	2.61217100	1.39584100	-4.28449800
I	3.94900800	-1.12599000	-0.56274100
C	-0.08120600	2.53772800	1.55319700
C	1.00521700	3.39569800	1.77352400
C	-1.26447500	2.75459500	2.27344000
C	0.91646600	4.43370400	2.70056100
H	1.91429900	3.25289500	1.18355500
C	-1.35520900	3.79132700	3.20073300
H	-2.11869900	2.09351500	2.09754600
C	-0.26299600	4.63293000	3.41968700
H	1.77322400	5.09644300	2.85817300
H	-2.28493200	3.94300100	3.75798900
H	-0.33288200	5.44699700	4.14784400
C	-1.71519300	2.41584200	-1.07042400

C	-1.28901100	3.74961200	-1.17987900
C	-3.03869900	2.10011400	-1.42173000
C	-2.15625800	4.73887700	-1.63864900
H	-0.26093000	4.00372800	-0.90642600
C	-3.90494300	3.09270700	-1.87796300
H	-3.38642200	1.07127700	-1.28405600
C	-3.46774600	4.41369500	-1.99145800
H	-1.80548900	5.77220700	-1.72291000
H	-4.93584300	2.83301800	-2.13923400
H	-4.14970000	5.19117300	-2.34969200
C	-3.32833500	-4.99458500	1.79434300
H	-4.32995200	-5.15785800	2.22044300
H	-3.11842400	-5.78565000	1.05299500
H	-2.57422000	-5.09591300	2.59470300
C	-5.68838200	-0.74934500	0.65714100
H	-6.07409500	-0.56884400	-0.36218800
H	-6.45119700	-1.29216800	1.23611200
H	-5.51735200	0.24004700	1.11610000

TS17-15

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -2104.052894900710 a.u.

Thermal correction to G: 1187.809 kJ/mol 283.893 kcal/mol 0.452413 a.u.

Optimized atomic Cartesian coordinates:

Pd	2.16474700	-0.85065400	-0.17023700
O	3.15844700	0.96274600	-0.80337100
C	4.34245400	1.05590800	-1.22209000
O	3.96908400	-1.86861800	-0.61170000
C	5.02955400	-1.36189300	-1.07241900
C	5.25961500	-0.00494700	-1.37510200
H	6.24865800	0.25102700	-1.76126100
C	4.79576000	2.45366300	-1.57902300
H	4.74963300	3.09064900	-0.67757200
H	5.81757400	2.48648700	-1.98745000
H	4.09552400	2.88631500	-2.31467100
C	6.15423400	-2.34417100	-1.31059400
H	6.39535900	-2.85854300	-0.36367400
H	5.81500100	-3.11907800	-2.02041000
H	7.06559100	-1.86928800	-1.70501100
C	0.38939900	0.11489200	0.78179200
C	-0.27784500	1.13646100	-0.00108500
C	0.84504100	0.26824300	2.18681300
C	1.85816000	1.16831600	2.55754900
C	0.25164600	-0.50579100	3.19824400

C	2.25292100	1.29728400	3.88726500
H	2.36320100	1.74629800	1.78283400
C	0.65508800	-0.38637300	4.52775600
H	-0.54859000	-1.19996900	2.93043500
C	1.65424800	0.52030400	4.88145400
H	3.04698100	2.00446500	4.14748700
H	0.17494300	-1.00253000	5.29474900
H	1.96830400	0.61930100	5.92520900
C	-0.23743800	2.58759400	0.25699500
C	0.97489900	3.29482400	0.18996900
C	-1.41305700	3.30953600	0.51465600
C	1.01057800	4.67356900	0.39424300
H	1.88441600	2.74480500	-0.07504700
C	-1.37848000	4.68879100	0.71539300
H	-0.14371900	2.65158500	-2.44008600
C	-0.16541500	5.37746000	0.66136800
H	1.96529600	5.20630200	0.33042900
H	-2.30819800	5.23081700	0.91693900
H	-0.13788700	6.46038300	0.81896000
C	-0.99787000	0.51880700	-1.02274900
C	-1.72903800	1.22816800	-2.08421000
C	-3.01308000	0.82557100	-2.49076000
C	-1.14837000	2.33394100	-2.73103000
C	-3.69124800	1.51031900	-3.49928400
H	-3.48445100	-0.02944500	-1.99907400
C	-1.82699700	3.01696100	-3.73713800
H	-2.36326400	2.76983700	0.55561700
C	-3.10507900	2.61026000	-4.12649000
H	-4.69319900	1.18150700	-3.79408200
H	-1.35079100	3.87301900	-4.22593100
H	-3.63932700	3.14696600	-4.91680700
C	0.06824500	-1.15422700	0.17111100
C	0.85602200	-2.30345200	0.51310600
C	-1.02349800	-1.79613300	-2.06541300
C	0.85153600	-3.56881600	-0.21069800
H	1.14260900	-2.39631900	1.56961400
C	-0.56847100	-3.06559800	-2.25515800
H	-1.62171500	-1.37449600	-2.88154200
C	0.25768900	-3.88081500	-1.39165900
H	1.45994200	-4.35450400	0.25288200
H	-0.85694300	-3.54249700	-3.19930600
H	0.44263400	-4.89587500	-1.76522200
C	-0.85168200	-0.91595100	-0.93384900
B	-2.77987000	-1.69560400	0.19159300

O	-2.33003500	-2.89207700	0.69773800
O	-3.71276700	-1.86341700	-0.81423900
I	-3.20036100	-0.07094600	1.62913200
C	-2.97204400	-3.94175300	-0.00552600
C	-3.79958900	-3.24890500	-1.10569900
H	-3.60994300	-4.50598000	0.69881700
H	-2.21171300	-4.62358400	-0.41815600
H	-3.39060800	-3.43763400	-2.11173200
H	-4.86032900	-3.55313800	-1.09188300

TS17-16-2

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -2104.030823565562 a.u.

Thermal correction to G: 1187.121 kJ/mol 283.729 kcal/mol 0.452150 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.97612700	0.02916400	-0.25694300
O	3.45941000	-0.76611900	-1.65663700
C	4.62228800	-0.32614700	-1.85575400
O	3.49046800	1.51605900	0.24058600
C	4.64576200	1.61839200	-0.24744400
C	5.22555000	0.78542100	-1.22873500
H	6.24731400	1.02442500	-1.53278000
C	5.43674300	-1.08923100	-2.87911400
H	4.89721900	-1.09416500	-3.84272600
H	6.44364600	-0.67098400	-3.03231400
H	5.52885800	-2.14181000	-2.55731200
C	5.47832400	2.76137000	0.29496100
H	5.60059600	2.63661500	1.38569700
H	6.47301600	2.83418500	-0.17148300
H	4.93516100	3.71036500	0.14007800
C	0.25183100	-1.11377100	-0.14684400
C	0.14900600	0.03013300	0.76502000
C	0.52833200	-2.51847200	0.25319500
C	1.43445900	-3.29111900	-0.49354400
C	-0.08319400	-3.11017300	1.36849200
C	1.70329000	-4.61441000	-0.14842400
H	1.96213500	-2.82355400	-1.33040400
C	0.19521900	-4.43072100	1.72125400
H	-0.78640200	-2.52440400	1.96303200
C	1.08429000	-5.19196900	0.96224000
H	2.41504600	-5.19507700	-0.74405500
H	-0.29229700	-4.86885900	2.59817200
H	1.30089800	-6.22854800	1.23918800
C	0.17245700	-0.03449900	2.24655300

C	-0.91830500	0.44646000	2.98632400
C	1.25679300	-0.58600800	2.94467600
C	-0.92547200	0.37730400	4.37858300
H	-1.77301000	0.87312900	2.45416300
C	1.24916600	-0.66334000	4.33569900
H	2.11912800	-0.94734700	2.37463100
C	0.15695600	-0.18123700	5.06011800
H	-1.78727700	0.75912700	4.93506100
H	2.10657000	-1.09819100	4.85876400
H	0.15141500	-0.23747900	6.15315500
C	-0.46312900	1.11556300	0.02156500
C	-0.39974600	2.51250900	0.47855900
C	-1.30709500	3.50260500	0.06161900
C	0.64111700	2.91024500	1.34419400
C	-1.19745200	4.81877600	0.50680300
H	-2.13118700	3.22951000	-0.59227800
C	0.75175200	4.22387800	1.78516400
H	1.39652400	2.18014300	1.63843100
C	-0.17087700	5.18868700	1.37433800
H	-1.92738000	5.56158400	0.17001600
H	1.57730300	4.49894500	2.44877900
H	-0.08334700	6.22301900	1.72100100
C	-0.48752500	-0.77494100	-1.36440100
C	-0.72707600	-1.63548400	-2.40162800
C	-1.00814400	1.49094300	-2.41087600
C	-1.31990600	-1.36156400	-3.67190000
H	-0.39572600	-2.66856300	-2.24934600
C	-1.28769900	1.15037200	-3.70088500
H	-0.79810300	2.55206700	-2.23421900
C	-1.55662700	-0.14567500	-4.25097700
H	-1.53649400	-2.24476900	-4.28467800
H	-1.30959900	1.97881500	-4.41945000
H	-1.94087400	-0.15560300	-5.27789100
C	-0.95922600	0.64275200	-1.23139700
B	-3.11729300	0.42770600	-0.74633700
O	-3.71747000	0.28172600	-1.98707100
O	-3.54111500	1.59047500	-0.11105100
I	-3.23711800	-1.41930200	0.50973400
C	-4.38172000	1.49583200	-2.27915200
C	-4.55631400	2.16580100	-0.91288600
H	-5.34050000	1.28223100	-2.78051500
H	-3.75687200	2.10571100	-2.95630700
H	-4.43287100	3.26184200	-0.95110000
H	-5.54429900	1.94374600	-0.46708500

TS17-16-3

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -2104.059933063205 a.u.

Thermal correction to G: 1193.214 kJ/mol 285.185 kcal/mol 0.454471 a.u.

Optimized atomic Cartesian coordinates:

Pd	-3.07851100	-0.60322200	-0.34371600
O	-3.31273200	0.63977100	1.35793500
C	-4.02265100	1.67826500	1.42932500
O	-4.60222200	0.53721500	-1.28699500
C	-5.14311200	1.57900800	-0.82026100
C	-4.90606700	2.15984400	0.44084100
H	-5.45468600	3.07498200	0.67349300
C	-3.88296100	2.46017700	2.71431300
H	-4.53998500	3.34223400	2.75875500
H	-4.10136500	1.79805000	3.57015900
H	-2.83257200	2.78427700	2.82196700
C	-6.13931700	2.24879200	-1.73870000
H	-6.93429500	1.52870000	-2.00136500
H	-6.59796900	3.14635900	-1.29654300
H	-5.63423400	2.52782700	-2.68034000
C	0.99103100	0.91210900	-1.05627300
C	1.25186100	0.98613200	0.34829200
C	1.59536400	1.77613300	-2.08281800
C	0.80307900	2.45228400	-3.02688900
C	2.98719300	1.96913700	-2.13606500
C	1.37861400	3.27603800	-3.99446900
H	-0.28460500	2.34531400	-2.98151300
C	3.56307300	2.79462800	-3.09860000
H	3.61821100	1.45004600	-1.41000100
C	2.76221400	3.45118600	-4.03595000
H	0.73792400	3.79350700	-4.71583700
H	4.65000500	2.92389900	-3.12062300
H	3.21483700	4.09987600	-4.79243600
C	2.14934400	1.95174100	0.99877500
C	2.09949400	3.32102300	0.68574800
C	3.08961300	1.52925700	1.95407700
C	2.95413500	4.23206800	1.30310100
H	1.36900300	3.67177300	-0.04870600
C	3.94273800	2.43940800	2.57480500
H	-0.03702500	1.93369400	2.72130000
C	3.88131600	3.79657300	2.25224900
H	2.89262400	5.29394500	1.04362600
H	4.66827000	2.08400500	3.31376900

H	4.55306000	4.51152600	2.73765700
C	0.53581800	-0.03459400	0.99202800
C	0.37890400	-0.16834500	2.44773300
C	0.49417400	-1.40167400	3.11230900
C	0.07753700	0.96858100	3.22246600
C	0.32238400	-1.49003900	4.49425900
H	0.74217600	-2.29313100	2.53045300
C	-0.08904400	0.87975100	4.60156600
H	3.15077600	0.46505500	2.19621300
C	0.03285600	-0.35257400	5.24825800
H	0.42408100	-2.46218700	4.98811200
H	-0.32570600	1.78067200	5.17706400
H	-0.10035400	-0.42464200	6.33227600
C	0.10611700	-0.15675700	-1.29024500
C	-0.46545200	-0.48112300	-2.56476100
C	-1.30131200	-1.64004600	0.29990800
C	-1.56177300	-1.24317000	-2.82767600
H	0.00770900	0.00022000	-3.42790400
C	-2.10077700	-2.41102100	-0.57969400
H	-1.35773800	-1.94245200	1.35183400
C	-2.41912500	-1.95587100	-1.88960800
H	-1.88243700	-1.30392900	-3.87381200
H	-2.69099900	-3.23342400	-0.15823600
H	-3.23816700	-2.50464300	-2.37115700
C	-0.14277400	-0.81343600	-0.01625900
H	-0.69920600	-4.41841900	0.76277500
C	0.31353600	-4.51816600	0.33467800
O	1.11019800	-3.41819400	0.73447800
C	0.30720200	-4.45537000	-1.20222000
H	0.75955900	-5.45107400	0.71890700
B	1.30095800	-2.59878500	-0.37059900
O	0.79276300	-3.16568300	-1.51984900
H	0.97954100	-5.21376500	-1.64502900
H	-0.69931600	-4.59115800	-1.63042800
I	3.31671900	-1.68225600	-0.50434900

Int18

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -1552.304134814651 a.u.

Thermal correction to G: 1041.075 kJ/mol 248.823 kcal/mol 0.396525 a.u.

Optimized atomic Cartesian coordinates:

Pd	-2.82552900	-0.50084400	-0.67199500
O	-3.05557800	1.22070300	0.60523000
C	-3.70935600	1.28066200	1.68097500

O	-4.17428200	-1.50756700	0.65666900
C	-4.67684900	-1.04367500	1.71613900
C	-4.49587000	0.25319500	2.24069100
H	-5.00408900	0.47909500	3.18067600
C	-3.61371900	2.59664500	2.41925500
H	-3.92941900	3.41457000	1.74793100
H	-4.22204500	2.62515700	3.33638800
H	-2.55761900	2.78660000	2.68096400
C	-5.55719000	-2.00409300	2.48478900
H	-6.37696500	-2.34996700	1.83056600
H	-4.96703200	-2.89645300	2.75918200
H	-5.98614100	-1.56236700	3.39729200
C	0.99337800	0.89796200	-0.71703300
C	2.14109100	0.21709900	-0.22244600
C	0.81985800	2.35388500	-0.80980100
C	1.84631900	3.18071400	-1.30543300
C	-0.37772200	2.97290400	-0.40124500
C	1.68913300	4.56217200	-1.38416500
H	2.78066600	2.72080400	-1.63907100
C	-0.53659300	4.35645600	-0.48905100
H	-1.19071300	2.36386100	0.00928000
C	0.49425100	5.16090100	-0.97664100
H	2.50575100	5.17841200	-1.77470300
H	-1.47798400	4.80979600	-0.16010700
H	0.36934700	6.24654200	-1.03955100
C	3.33821500	0.85033500	0.34846000
C	3.23329100	1.88088300	1.30052800
C	4.63042200	0.44827900	-0.03608000
C	4.36684000	2.48553500	1.83952800
H	2.23891300	2.20242900	1.62251700
C	5.76542400	1.04821100	0.50543100
H	3.14904600	-1.36379800	2.04442900
C	5.64174700	2.07275100	1.44631100
H	4.25352400	3.28423900	2.57993100
H	6.75820700	0.71591100	0.18457400
H	6.53281000	2.54582600	1.87065000
C	1.93197400	-1.17872200	-0.36933500
C	2.83383500	-2.24015600	0.09671700
C	3.16810900	-3.33406400	-0.72332900
C	3.40180300	-2.19808800	1.38439800
C	4.02399300	-4.34070100	-0.27676600
H	2.76234400	-3.37790200	-1.73838900
C	4.26371600	-3.19722300	1.82888900
H	4.73730800	-0.34480200	-0.78158100

C	4.57993300	-4.27779300	1.00173600
H	4.26726800	-5.17749700	-0.93980400
H	4.68786800	-3.13656700	2.83653600
H	5.25516700	-5.06475800	1.35177200
C	0.07258500	-0.07710000	-1.18484100
C	-1.15367600	0.22332900	-1.87524600
C	-0.01003400	-2.63962600	-1.07999000
C	-2.01643900	-0.66450800	-2.56604500
H	-1.27603600	1.27953700	-2.14463100
C	-1.26992200	-2.91180100	-1.53910000
H	0.56004900	-3.50214600	-0.71507300
C	-2.24063900	-1.99649600	-2.10763400
H	-2.68374700	-0.25142900	-3.33131800
H	-1.60499800	-3.95308500	-1.47413000
H	-3.10533400	-2.49480700	-2.56486600
C	0.64493500	-1.37844500	-0.94848200

Product

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1079.051427221565 a.u.

Thermal correction to G: 807.485 kJ/mol 192.993 kcal/mol 0.307555 a.u.

Optimized atomic Cartesian coordinates:

C	0.18808300	1.14443400	-0.53628800
C	0.00000000	0.00000000	0.27993500
C	0.47651800	2.50788900	-0.06206200
C	-0.27964800	3.60594900	-0.50338100
C	1.51404500	2.74181100	0.85601300
C	-0.00372900	4.89508200	-0.04804300
H	-1.11011300	3.44088500	-1.19629700
C	1.78716900	4.02804300	1.31410400
H	2.11422700	1.89821000	1.20831200
C	1.03003200	5.11130600	0.86316500
H	-0.60863600	5.73561900	-0.40185300
H	2.60162100	4.18742100	2.02740800
H	1.24461700	6.12179600	1.22367500
C	0.00000000	0.00000000	1.75206200
C	-0.73955500	0.95368600	2.46902500
C	0.73955500	-0.95368600	2.46902500
C	-0.74325100	0.95051800	3.86201600
H	-1.32438700	1.69886800	1.92306900
C	0.74325100	-0.95051800	3.86201600
H	1.32438700	-1.69886800	1.92306900
C	0.00000000	0.00000000	4.56382300
H	-1.33147400	1.69702900	4.40418300

H	1.33147400	-1.69702900	4.40418300
H	0.00000000	0.00000000	5.65798100
C	-0.18808300	-1.14443400	-0.53628800
C	-0.13035500	-0.73080900	-1.88668900
C	-0.47651800	-2.50788900	-0.06206200
C	0.27964800	-3.60594900	-0.50338100
C	-1.51404500	-2.74181100	0.85601300
C	0.00372900	-4.89508200	-0.04804300
H	1.11011300	-3.44088500	-1.19629700
C	-1.78716900	-4.02804300	1.31410400
H	-2.11422700	-1.89821000	1.20831200
C	-1.03003200	-5.11130600	0.86316500
H	0.60863600	-5.73561900	-0.40185300
H	-2.60162100	-4.18742100	2.02740800
H	-1.24461700	-6.12179600	1.22367500
C	0.13035500	0.73080900	-1.88668900
C	0.36043100	1.54387200	-2.99490700
C	-0.36043100	-1.54387200	-2.99490700
C	0.31858700	1.22210700	-4.35322000
H	0.60937800	2.58611400	-2.76522900
C	-0.31858700	-1.22210700	-4.35322000
H	-0.60937800	-2.58611400	-2.76522900
C	0.00000000	0.00000000	-4.95010600
H	0.54804400	2.04277400	-5.04067600
H	-0.54804400	-2.04277400	-5.04067600
H	0.00000000	0.00000000	-6.04619500

Int3-Me4

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1423.924768520953 a.u.

Thermal correction to G: 1008.807 kJ/mol 241.111 kcal/mol 0.384234 a.u.

Optimized atomic Cartesian coordinates:

C	-1.15519000	-0.63973800	-0.08581900
C	-1.24685700	0.68723800	0.27433100
C	-2.17992000	-1.32803400	-0.90875500
C	-2.23604800	1.58582800	0.78207800
Pd	0.47626600	0.80752200	-0.47704400
B	0.07942300	-1.41582400	0.50284900
C	-2.44770200	-2.69448200	-0.73373100
C	-2.93294400	-0.61690600	-1.85845200
C	-1.96458200	2.96918200	0.82616400
C	-3.47039100	1.10222100	1.26802200
O	0.59688200	-1.19477300	1.76115500
O	0.64162300	-2.50513700	-0.11223500

C	-3.44521000	-3.32589800	-1.47426100
H	-1.86773100	-3.26814900	-0.00680700
C	-3.93129400	-1.24703800	-2.59603100
H	-2.71717700	0.44300400	-2.02653100
C	-2.91332300	3.84790800	1.33511400
H	-0.99225100	3.32226700	0.46932800
C	-4.41545400	1.98751400	1.76712400
H	-3.66991000	0.02757500	1.24221400
C	1.78442200	-2.00146900	1.87454900
C	1.49716800	-3.15387900	0.84620700
C	-4.19292100	-2.60565400	-2.40647600
H	-3.63973500	-4.39169300	-1.32057300
H	-4.50365500	-0.67494800	-3.33253800
C	-4.13772200	3.35889000	1.79915700
H	-2.70292800	4.92029800	1.37281400
H	-5.37355600	1.61410300	2.13922100
C	1.93258800	-2.45583800	3.31462400
C	2.96726300	-1.12674200	1.47163500
C	0.69750100	-4.30388800	1.44827000
C	2.72448400	-3.68103300	0.12605100
H	-4.97357100	-3.10292200	-2.98983200
H	-4.88451900	4.05328800	2.19586300
H	1.02490700	-2.96165900	3.67725900
H	2.11728500	-1.58050900	3.95973600
H	2.78799900	-3.14479500	3.41895600
H	3.92416000	-1.66161600	1.58802200
H	2.98659400	-0.23429000	2.11946700
H	2.87089400	-0.78557900	0.42768400
H	1.30311700	-4.89761900	2.15252700
H	0.36177100	-4.96766700	0.63400500
H	-0.19561200	-3.93311500	1.97880300
H	2.42578300	-4.47365600	-0.58039500
H	3.44343500	-4.11222900	0.84327200
H	3.22616700	-2.88554000	-0.44541000
C	2.42559600	3.09072700	-0.29892700
C	2.76995400	4.44866000	0.25830200
C	3.37021800	2.43095100	-1.10352000
O	1.27721100	2.66364300	0.02647800
H	2.69812800	4.41874900	1.35953400
H	2.02567700	5.18440100	-0.09387500
H	3.77596100	4.78745800	-0.03063000
C	3.21203800	1.17322600	-1.72056700
H	4.31795800	2.94595300	-1.27028500
C	4.35270700	0.62246100	-2.53780400

O	2.19028400	0.43338000	-1.65185300
H	4.69850300	-0.32121800	-2.07921200
H	3.99034900	0.37388500	-3.55021300
H	5.20230700	1.31719700	-2.61468800

TS4-Me4

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1423.912552125832 a.u.

Thermal correction to G: 1009.109 kJ/mol 241.183 kcal/mol 0.384349 a.u.

Optimized atomic Cartesian coordinates:

C	0.67835300	-0.33355600	0.68241400
C	-0.01283800	0.87213900	0.60903100
C	0.14567200	-1.44781100	1.51820900
C	0.34268600	2.25232300	0.74661900
Pd	-1.44153300	-0.05233500	-0.16786300
B	2.04854800	-0.44356500	-0.05031400
C	0.36653900	-2.79645000	1.18130600
C	-0.55750700	-1.16999900	2.70878600
C	-0.52793800	3.25747800	0.27509100
C	1.54498900	2.62552700	1.38538600
O	2.48167100	0.49736800	-0.94360400
O	2.93353000	-1.47172100	0.11201400
C	-0.11297000	-3.82120100	1.99180300
H	0.91358900	-3.03480300	0.26646600
C	-1.04315800	-2.19906200	3.51133300
H	-0.70794900	-0.12786400	3.00806500
C	-0.19087300	4.59726400	0.41985900
H	-1.47063500	2.95619300	-0.19043900
C	1.88042200	3.96602800	1.51839700
H	2.20480200	1.84639500	1.77557900
C	3.85893400	0.20163400	-1.24109600
C	3.94390500	-1.32881500	-0.90863000
C	-0.82490400	-3.53172400	3.15830200
H	0.06746600	-4.86191200	1.70505600
H	-1.58710600	-1.95529900	4.42918200
C	1.01445600	4.95167500	1.03366400
H	-0.86680800	5.37466900	0.05297300
H	2.81641200	4.25069800	2.00715700
C	4.71027300	1.06142800	-0.31295700
C	4.13767700	0.55510100	-2.68964100
C	3.51950900	-2.21508500	-2.07411700
C	5.27813200	-1.78762100	-0.35224500
H	-1.20128900	-4.34043500	3.79161000
H	1.27891000	6.00777700	1.14300900

H	5.78583800	0.94152600	-0.52189800
H	4.44158100	2.12032200	-0.46390000
H	4.52849400	0.81088600	0.74594100
H	5.16100400	0.25628600	-2.97352600
H	4.04754800	1.64561600	-2.82748100
H	3.42430900	0.06498500	-3.36925500
H	3.40626500	-3.25033000	-1.71138600
H	2.55090600	-1.89042300	-2.49032000
H	4.26968000	-2.20962300	-2.88159400
H	5.52752600	-1.26647000	0.58432200
H	6.08498900	-1.60850200	-1.08318800
H	5.23976500	-2.86956200	-0.14189100
C	-4.21493200	0.94415400	-0.68485000
C	-5.25485200	2.01718600	-0.48239400
C	-4.54509300	-0.17712000	-1.46162000
O	-3.10749100	1.17603400	-0.10846800
H	-5.43217600	2.15324100	0.59869200
H	-4.86798600	2.97620300	-0.86960800
H	-6.20837700	1.78574200	-0.97977200
C	-3.70749700	-1.27647100	-1.75133500
H	-5.55477800	-0.20553300	-1.87524900
C	-4.26084000	-2.39812700	-2.59390700
O	-2.51512300	-1.42209100	-1.36758600
H	-3.62264000	-2.53146300	-3.48490600
H	-4.21242300	-3.33979400	-2.01935100
H	-5.29870900	-2.22340100	-2.91430300

TS4-cis-Me4

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1423.919416805093 a.u.

Thermal correction to G: 1011.090 kJ/mol 241.656 kcal/mol 0.385104 a.u.

Optimized atomic Cartesian coordinates:

Pd	-1.11023800	0.32960400	0.38827800
C	0.57386300	1.03528600	-0.13566500
O	-2.32903300	1.71849100	-0.49354800
C	1.38277900	-0.04450000	0.08947200
C	0.90233700	2.40744300	-0.47631600
C	-3.59275500	1.74971600	-0.36452100
C	2.77335900	0.11740000	0.59074300
B	0.85438400	-1.49017500	-0.20266200
C	0.13283400	3.48551600	-0.00186900
C	1.99730000	2.67600400	-1.32199800
C	-4.25510200	2.86521100	-1.13249600
C	-4.39462400	0.87988000	0.38992600

C	3.82039800	-0.67725200	0.09694700
C	3.07827800	1.09111100	1.55610500
O	-0.17049900	-1.77731300	-1.07718600
O	1.43672800	-2.61781600	0.30414300
C	0.46139300	4.79296300	-0.34702600
H	-0.72155000	3.28040200	0.64646400
C	2.31583000	3.98248900	-1.67332600
H	2.59320500	1.84136700	-1.70103600
H	-5.34309600	2.90223600	-0.97485500
H	-3.80808000	3.82871900	-0.83228500
H	-4.04931200	2.73630200	-2.20957400
C	-3.95812500	-0.21690500	1.16643500
H	-5.46905300	1.07091300	0.37201500
C	5.12907400	-0.48951800	0.53765300
H	3.60725500	-1.44522400	-0.65080900
C	4.38504100	1.27684000	1.99993200
H	2.27073100	1.70455900	1.96654700
C	-0.43086400	-3.19587800	-0.98816900
C	0.93609600	-3.74086300	-0.44810300
C	1.55082100	5.04479900	-1.18350800
H	-0.13816400	5.62365300	0.03661800
H	3.16685400	4.17738800	-2.33252500
C	-4.99177000	-1.03846900	1.89426600
O	-2.76386000	-0.59166100	1.31439500
C	5.41832200	0.48850900	1.49018900
H	5.93086400	-1.11430600	0.13210100
H	4.59754800	2.04002100	2.75490400
C	-0.82348600	-3.70241500	-2.36334100
C	-1.57985200	-3.38895500	-0.00742800
C	0.82385000	-4.94040000	0.47315000
C	1.94773800	-4.01560100	-1.55568800
H	1.80435400	6.07332100	-1.45764800
H	-4.74494900	-1.06450200	2.96984200
H	-4.94619800	-2.07952300	1.52834400
H	-6.01503000	-0.65576400	1.76507800
H	6.44538900	0.63211800	1.83899700
H	-1.78706200	-3.25468200	-2.65871100
H	-0.07504800	-3.43562400	-3.12452400
H	-0.94417200	-4.79900600	-2.35272900
H	-1.32370000	-3.01593500	0.99748400
H	-2.45160600	-2.81417000	-0.35877800
H	-1.86494000	-4.45101900	0.06859900
H	1.82937100	-5.24048300	0.81254300
H	0.21708000	-4.71181400	1.36201200

H	0.37039900	-5.79551500	-0.05615200
H	2.93516400	-4.19494100	-1.09876200
H	2.03761900	-3.15357200	-2.23802200
H	1.67208700	-4.90391300	-2.14721800

Int5-Me4

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1423.940622807471 a.u.

Thermal correction to G: 1009.800 kJ/mol 241.348 kcal/mol 0.384612 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.71676300	-0.22382900	-0.21689000
C	-0.06467000	0.59163400	-0.31884500
O	2.66216400	1.52023100	0.21415900
C	-0.90967900	-0.46210400	-0.24738900
C	-0.36386200	2.01969400	-0.37855800
C	3.88813300	1.63875100	0.53106400
C	-0.07877200	-1.70738600	-0.28296100
B	-2.44055900	-0.46957200	-0.02004600
C	0.08605400	2.90726200	0.61282700
C	-1.12074000	2.52933900	-1.44685600
C	4.30218700	3.05432300	0.83816700
C	4.84235300	0.61661200	0.61753300
C	-0.09303000	-2.66808400	0.76091500
C	0.74767800	-1.94971600	-1.41286400
O	-3.14017700	-1.62781700	0.19242700
O	-3.23043500	0.64516200	0.02390300
C	-0.23118000	4.26146200	0.54568400
H	0.68401400	2.52125100	1.44032800
C	-1.42426200	3.88670700	-1.51874200
H	-1.47351100	1.84353000	-2.22212900
H	4.06509500	3.69866800	-0.02599100
H	3.70891100	3.42867000	1.69099500
H	5.37247100	3.14156300	1.07631300
C	4.62230800	-0.75468900	0.35966800
H	5.85270800	0.91065500	0.90710200
C	0.68270000	-3.80784000	0.67588400
H	-0.73672200	-2.49443700	1.62722900
C	1.53305700	-3.12254300	-1.48003000
H	0.62907100	-1.32811100	-2.30635200
C	-4.54137400	-1.28938200	0.18121900
C	-4.51323500	0.23811500	0.53541400
C	-0.98266700	4.75795100	-0.52147100
H	0.11595900	4.93827300	1.33260300
H	-2.01535100	4.26669900	-2.35777000

C	5.78022500	-1.70954300	0.50171500
O	3.52934300	-1.27540900	0.01152300
C	1.50538700	-4.03630500	-0.44557600
H	0.65942400	-4.54148800	1.48728800
H	2.15278900	-3.30103400	-2.36292100
C	-5.27089100	-2.16409300	1.18342000
C	-5.05105100	-1.56223900	-1.22973700
C	-5.59559300	1.06888300	-0.12797800
C	-4.49288400	0.49956600	2.03792700
H	-1.22344200	5.82401500	-0.57603700
H	5.94041500	-2.23018300	-0.45854100
H	5.52252200	-2.48167700	1.24762000
H	6.71335900	-1.21136000	0.80385900
H	2.11272800	-4.94442400	-0.49754500
H	-5.22945900	-3.21645500	0.85572700
H	-4.81645700	-2.10013800	2.18368300
H	-6.33152900	-1.86932900	1.25703200
H	-4.85085300	-2.61661700	-1.48329300
H	-6.13592500	-1.38444900	-1.31063600
H	-4.53413900	-0.92896400	-1.97033100
H	-5.48509700	2.12448500	0.17197800
H	-6.59680400	0.72586100	0.18365400
H	-5.52962200	1.01813800	-1.22527600
H	-4.26294500	1.56429500	2.20897400
H	-5.46584900	0.27255100	2.50368800
H	-3.71437300	-0.10157700	2.53722800

Int5-I-Me4

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -1721.828987377348 a.u.

Thermal correction to G: 995.151 kJ/mol 237.847 kcal/mol 0.379033 a.u.

Optimized atomic Cartesian coordinates:

C	-1.05934400	0.56792700	0.35316300
C	-0.16649000	-0.36813000	-0.06349800
C	-0.63093400	1.90614100	0.82623400
C	-0.54573800	-1.75817500	-0.38222100
Pd	1.78008800	-0.17801500	-0.11222300
B	-2.58882900	0.28546500	0.31682500
C	-1.29248100	3.06533600	0.38938600
C	0.43407200	2.06308700	1.72909300
C	-0.39761800	-2.29552400	-1.67189200
C	-1.03495200	-2.59362300	0.63585400
I	1.58301300	1.12911600	-2.38079000
O	-3.47450000	0.84561300	1.20831500

O	-3.22828400	-0.49412600	-0.61373100
C	-0.88920100	4.33162000	0.80907400
H	-2.13148600	2.97186000	-0.30732300
C	0.83741800	3.32788400	2.15591900
H	0.93784300	1.16925500	2.10824500
C	-0.76232300	-3.61227800	-1.94017600
H	0.00200600	-1.65658000	-2.46474300
C	-1.38504200	-3.91627600	0.37014800
H	-1.13146300	-2.18816800	1.64695700
C	-4.80254900	0.59549200	0.72206300
C	-4.58728600	-0.66395600	-0.18616900
C	0.18217700	4.47028200	1.69359300
H	-1.41402800	5.21849500	0.43933700
H	1.67139000	3.42036300	2.85929400
C	-1.25788100	-4.43041600	-0.92088800
H	-0.65545400	-4.00746700	-2.95551400
H	-1.76477600	-4.55005200	1.17825300
C	-5.73459500	0.38129800	1.90032500
C	-5.22686300	1.83022700	-0.06727700
C	-4.65664400	-1.97557500	0.58953500
C	-5.48643300	-0.73258000	-1.40704400
H	0.50060000	5.46368500	2.02491700
H	-1.53566700	-5.46783900	-1.13210400
H	-5.81557800	1.31423900	2.48360500
H	-6.74487300	0.10508100	1.55269200
H	-5.36402900	-0.40834800	2.57138500
H	-4.57048400	1.98747800	-0.93964000
H	-5.14347600	2.71488800	0.58598300
H	-6.26870100	1.75248300	-0.41945800
H	-4.27126300	-2.78601800	-0.05085900
H	-5.69076700	-2.21786200	0.88594100
H	-4.02735100	-1.93981200	1.49418600
H	-5.25277300	-1.64233200	-1.98558000
H	-6.54783800	-0.77748000	-1.10843900
H	-5.34014700	0.13626900	-2.06644100
C	2.90268700	-1.49378500	2.35568200
C	2.65728100	-2.22496000	3.65426700
C	4.22920600	-1.22022600	1.98267900
O	1.84982900	-1.19860300	1.71762600
H	2.01642600	-1.60463800	4.30529600
H	2.09933900	-3.15485000	3.44593800
H	3.58594800	-2.47221400	4.19056900
C	4.66107300	-0.56512900	0.80613400
H	5.00823800	-1.56155600	2.66752500

C	6.14862600	-0.40489900	0.59111200
O	3.93072100	-0.09567100	-0.10362800
H	6.37960800	0.66263900	0.43204500
H	6.43960300	-0.93768100	-0.33147400
H	6.75042900	-0.78592400	1.43022000

Int5-cis-Me4

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1423.950680910865 a.u.

Thermal correction to G: 1015.404 kJ/mol 242.687 kcal/mol 0.386747 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.18802700	-0.26194200	-0.10479600
C	-0.75030500	-0.65885600	-0.10115400
O	1.64730700	-2.18683200	0.16651500
C	-1.59990000	0.41295400	-0.06129600
C	-1.18627400	-2.06314400	-0.04965000
C	2.82484200	-2.66015900	0.24343400
C	-3.07969500	0.33560800	-0.04716600
B	-0.85218000	1.75554000	-0.04608900
C	-0.89943300	-2.94784300	-1.10026300
C	-1.89008100	-2.54739800	1.06340900
C	2.86328600	-4.15233200	0.43835600
C	4.03181700	-1.94892900	0.17081900
C	-3.81768900	1.20421900	0.77428500
C	-3.78980100	-0.56908100	-0.85414200
O	0.51867800	1.71261000	-0.33636100
O	-1.25358600	3.02069000	0.21798900
C	-1.33192000	-4.27056400	-1.05355100
H	-0.33415700	-2.58354800	-1.96308900
C	-2.30557500	-3.87632200	1.11930300
H	-2.11439800	-1.86583800	1.88917500
H	2.34078700	-4.40896400	1.37644200
H	2.30832000	-4.64058800	-0.38130300
H	3.88868200	-4.54839400	0.47397800
C	4.16959000	-0.55571900	0.00636800
H	4.95042500	-2.53170500	0.25684000
C	-5.21041200	1.15167300	0.81031300
H	-3.28658000	1.92793000	1.39901100
C	-5.18152200	-0.61810500	-0.82380400
H	-3.24004800	-1.23929500	-1.51982200
C	1.10406700	2.98917700	0.06077800
C	-0.15373500	3.91691700	-0.06786700
C	-2.03431700	-4.74149700	0.05821400
H	-1.11211100	-4.94360800	-1.88816100

H	-2.85173200	-4.23773000	1.99616000
C	5.55318400	0.03738700	-0.04168700
O	3.21974500	0.26858700	-0.10977400
C	-5.90020800	0.23775200	0.01324400
H	-5.76094600	1.83275200	1.46693700
H	-5.71080400	-1.33096900	-1.46391000
C	2.24611000	3.31916000	-0.87708100
C	1.60071600	2.83260200	1.48981700
C	-0.36740900	4.43702700	-1.48368300
C	-0.18821400	5.05768200	0.93055700
H	-2.36626400	-5.78340200	0.09858200
H	5.64740800	0.80332200	0.74776200
H	5.69390000	0.55129600	-1.00886400
H	6.34609100	-0.71430800	0.08562500
H	-6.99339700	0.19670100	0.03840000
H	3.05468700	2.58594700	-0.72954700
H	2.63409500	4.32903100	-0.66143100
H	1.92887600	3.28006900	-1.92973800
H	0.77759500	2.58152100	2.17964000
H	2.08482600	3.75773600	1.84167200
H	2.34399000	2.01898900	1.51793900
H	-1.36112100	4.91086400	-1.53953700
H	-0.33626700	3.61884700	-2.22239400
H	0.39186100	5.18788200	-1.75559400
H	0.68580400	5.71695000	0.79672200
H	-0.19861600	4.68872500	1.96717600
H	-1.09913800	5.65773200	0.77013200

Int5-cis-I-Me4

Charge = -1 Multiplicity = 1

wB97M-V single point energy: -1721.826892926289 a.u.

Thermal correction to G: 994.361 kJ/mol 237.658 kcal/mol 0.378732 a.u.

Optimized atomic Cartesian coordinates:

I	-0.86711300	0.86030600	-2.66535200
Pd	-0.99972400	0.98222900	-0.03253800
C	0.92617900	0.67666000	0.07694700
C	1.46131500	-0.57343400	0.11952400
C	1.68909000	1.92068900	0.30001400
C	2.92534000	-0.81769300	0.19148700
B	0.52888400	-1.81830300	0.08003400
C	1.68384100	2.98530800	-0.61745200
C	2.40997900	2.08033200	1.49739600
C	3.83799400	-0.11296800	-0.61157600
C	3.44297500	-1.79253300	1.06162900

O	0.87304900	-3.00937700	-0.51206300
O	-0.70443500	-1.88691400	0.67972000
C	2.40086000	4.15212500	-0.36119800
H	1.11044000	2.87816100	-1.54276400
C	3.11161900	3.25453100	1.76063000
H	2.41064400	1.26313300	2.22394600
C	5.20820200	-0.35152900	-0.52854700
H	3.45750000	0.63189200	-1.31566500
C	4.81308100	-2.03340900	1.14936800
H	2.75445500	-2.36475400	1.69175900
C	-0.10186500	-3.99161000	-0.12585100
C	-1.33570400	-3.10275200	0.25595400
C	3.11682600	4.29496700	0.82965900
H	2.39386500	4.96313800	-1.09654600
H	3.66185600	3.35788900	2.70151400
C	5.70564300	-1.31031500	0.35656900
H	5.89518100	0.21385900	-1.16664600
H	5.18689100	-2.79242000	1.84433400
C	-0.33670800	-4.94335300	-1.28444800
C	0.47943700	-4.74542700	1.06631000
C	-2.21712500	-2.75818200	-0.93926800
C	-2.18531800	-3.63374800	1.39671000
H	3.67065600	5.21656700	1.03416600
H	6.78190300	-1.49789900	0.42237400
H	0.58395500	-5.51681000	-1.48601100
H	-1.14174200	-5.65858000	-1.04359800
H	-0.60889000	-4.40040100	-2.20216600
H	1.45614500	-5.16782200	0.77651100
H	0.64150900	-4.06919800	1.92266200
H	-0.17676200	-5.57072600	1.38914400
H	-1.61859800	-2.35487700	-1.77253900
H	-2.92704000	-1.97024000	-0.63796800
H	-2.78725300	-3.63349500	-1.29244600
H	-2.63934600	-4.60389500	1.13111300
H	-2.99728700	-2.91718100	1.60689200
H	-1.59667200	-3.75830500	2.31836600
C	-2.05058300	1.05992600	2.77099300
C	-1.78017700	0.99694700	4.25598300
C	-3.38852700	1.06498500	2.33498800
O	-1.01230200	1.10893200	2.05283400
H	-1.15951900	1.86118100	4.55025400
H	-1.19290800	0.08820600	4.47710600
H	-2.69975200	0.98850600	4.86072200
C	-3.84061800	1.18530900	1.00221700

H	-4.15511000	1.02065700	3.11129100
C	-5.33144400	1.25746200	0.76217900
O	-3.12480100	1.24898900	-0.03136400
H	-5.62518200	0.45514700	0.06285900
H	-5.57437300	2.21629600	0.27097000
H	-5.92267100	1.16797300	1.68630300

TS21

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.146724851254 a.u.

Thermal correction to G: 1194.900 kJ/mol 285.588 kcal/mol 0.455113 a.u.

Optimized atomic Cartesian coordinates:

Pd	0.99655700	0.32997300	1.04707300
O	2.65521300	-0.75467200	0.33788100
C	3.57477800	-1.26819100	1.02955100
O	1.79972600	0.16547000	2.95773300
C	2.85084000	-0.46641600	3.28734900
C	3.71151500	-1.16752400	2.42963300
H	4.56965400	-1.66592700	2.88386600
C	4.59567000	-2.05405500	0.24918700
H	5.03786400	-1.40378300	-0.52544400
H	5.39612000	-2.46816500	0.88038400
H	4.08078500	-2.87515400	-0.28069100
C	3.16529500	-0.43200600	4.76091200
H	3.28478700	0.61764300	5.08195500
H	2.31194500	-0.84669400	5.32543600
H	4.07599700	-0.99402100	5.01595000
C	0.08336700	1.04308000	-0.73103700
C	-0.19292100	-0.36077700	-0.76998800
C	1.03698900	1.75919200	-1.63328900
C	2.40700000	1.88772900	-1.38585100
C	0.52265600	2.30372500	-2.82227400
C	3.24041800	2.53545700	-2.29919100
H	2.83163000	1.46628000	-0.47298500
C	1.35281900	2.94601800	-3.73687800
H	-0.54542800	2.20806300	-3.03628700
C	2.71953900	3.06593200	-3.47769500
H	4.30913200	2.62379200	-2.08208000
H	0.92873800	3.35589000	-4.65862400
H	3.37446600	3.57263000	-4.19289000
C	0.58988300	-1.42724400	-1.43548100
C	0.73521200	-2.67832600	-0.81586100
C	1.15172500	-1.23718900	-2.70329600
C	1.43120200	-3.70640600	-1.44064600

H	0.31548000	-2.83266200	0.18142600
C	1.84547100	-2.27093200	-3.33378600
H	1.04134500	-0.27565500	-3.20834800
C	1.99011900	-3.50672400	-2.70584300
H	1.54152700	-4.67117800	-0.93646900
H	2.27506400	-2.10492600	-4.32631400
H	2.53709300	-4.31539200	-3.20011300
C	-1.60173100	-0.56927500	-0.42090800
C	-2.22214200	0.64957300	-0.25259100
C	-2.23628100	-1.89042300	-0.25005500
C	-2.36314000	-2.78475800	-1.32176300
C	-2.72757300	-2.26944900	1.00645600
C	-2.96627700	-4.02749900	-1.13982200
H	-1.98743500	-2.49885700	-2.30796500
C	-3.32603000	-3.51476000	1.19086700
H	-2.62617700	-1.57693100	1.84773000
C	-3.44627200	-4.39821200	0.11745600
H	-3.06231000	-4.71264200	-1.98756100
H	-3.69982900	-3.79733000	2.17975400
H	-3.91542300	-5.37640400	0.26024700
C	-1.21132300	1.69103900	-0.34302700
C	-1.43458500	3.06208100	-0.51722500
C	-0.37410100	1.48551700	1.84629500
C	-0.55276000	4.02912700	-0.02600500
H	-2.38180200	3.39840200	-0.95707800
C	-0.15141700	2.81757800	2.11156900
H	-0.96953900	0.90964300	2.57597100
C	0.09006500	3.88050800	1.20824100
H	-0.59877700	5.04584900	-0.43301500
H	-0.34601100	3.15738100	3.14344300
H	0.50696600	4.80073500	1.63591200
B	-3.71202000	0.90134600	0.08595100
O	-4.71933100	0.01513000	-0.17503900
O	-4.15983500	2.06718900	0.64706600
C	-5.92652000	0.55552100	0.34269900
C	-5.57905600	2.01056800	0.70694600
H	-6.23375300	-0.03476800	1.22360600
H	-6.72033000	0.48238700	-0.41776200
H	-5.99719700	2.73490100	-0.01341900
H	-5.91687500	2.29159000	1.71723600

Int22

Charge = 0 Multiplicity = 1

wB97M-V single point energy: -1806.162014613726 a.u.

Thermal correction to G: 1190.667 kJ/mol 284.576 kcal/mol 0.453501 a.u.

Optimized atomic Cartesian coordinates:

Pd	1.00928400	0.14900600	1.11666000
O	2.65725600	-0.66123900	0.05596400
C	3.61354000	-1.32917300	0.52833100
O	1.94264300	-0.48906100	2.85421000
C	3.00867100	-1.17592800	2.94796800
C	3.82322100	-1.61221300	1.89458800
H	4.70208600	-2.20445800	2.15503100
C	4.59230000	-1.85267300	-0.48943500
H	5.00626200	-1.00434500	-1.06199200
H	5.41630700	-2.42752800	-0.04083400
H	4.04543100	-2.48707200	-1.20949600
C	3.39338400	-1.53417600	4.36004100
H	3.53080300	-0.60804600	4.94507800
H	2.56717100	-2.09404300	4.83203700
H	4.31400800	-2.13431400	4.41105700
C	0.03516800	1.21666600	-0.52257300
C	-0.17928900	-0.18151400	-0.72141300
C	0.99160400	2.09116400	-1.27047100
C	2.35855100	2.18970700	-0.98824200
C	0.48162500	2.85387500	-2.33603600
C	3.18949300	3.01334100	-1.74707600
H	2.78005400	1.61350000	-0.16414300
C	1.31090100	3.67308500	-3.09839700
H	-0.58283300	2.79176000	-2.57696900
C	2.67285400	3.75700200	-2.80702600
H	4.25382900	3.07412900	-1.50067300
H	0.88764300	4.24967100	-3.92654500
H	3.32688100	4.40186000	-3.40161700
C	0.54894000	-1.09684600	-1.63834200
C	0.75397600	-2.44541500	-1.30868900
C	0.96878600	-0.64559400	-2.89560400
C	1.37070600	-3.31229100	-2.20414000
H	0.45169800	-2.81166000	-0.32575100
C	1.58395700	-1.51557300	-3.79622600
H	0.80862200	0.39631100	-3.17875300
C	1.78958500	-2.85090400	-3.45469800
H	1.52979900	-4.35738800	-1.92195600
H	1.90244800	-1.14203600	-4.77411300
H	2.27389300	-3.53290700	-4.16017200
C	-1.60025600	-0.46788400	-0.41835100
C	-2.28345200	0.70326300	-0.21763500
C	-2.16728700	-1.83036100	-0.37255800

C	-2.93452600	-2.32581900	-1.43233000
C	-1.94141600	-2.64704800	0.74341100
C	-3.46120000	-3.61582900	-1.38138200
H	-3.11244100	-1.69177100	-2.30572400
C	-2.47201300	-3.93429500	0.79740300
H	-1.34458900	-2.26121600	1.57649000
C	-3.23112500	-4.42336600	-0.26725100
H	-4.05558400	-3.99317500	-2.21905400
H	-2.29212300	-4.55988000	1.67688200
H	-3.64497100	-5.43549100	-0.22741200
C	-1.30384500	1.78047800	-0.18702000
C	-1.53088900	3.07252300	0.15874800
C	-0.23915900	0.98314400	2.37329000
C	-0.49417500	3.89373500	0.76579600
H	-2.56008300	3.45351100	0.13777000
C	-0.32741500	2.28488200	2.68250200
H	-0.66650500	0.24310500	3.06764400
C	0.07107500	3.48554300	1.92538700
H	-0.28820700	4.90325000	0.38884600
H	-0.79809400	2.53096800	3.65171100
H	0.73709300	4.19153700	2.44180300
B	-3.78852000	0.84204300	0.13248500
O	-4.58498700	-0.19373800	0.52756900
O	-4.46056600	2.03438700	0.06587900
C	-5.91493100	0.29185600	0.64664700
C	-5.78377000	1.82165600	0.54070400
H	-6.34233400	-0.03575000	1.60760200
H	-6.52507100	-0.13399600	-0.16879000
H	-6.50448900	2.26674300	-0.16354200
H	-5.89750000	2.32135700	1.51831800

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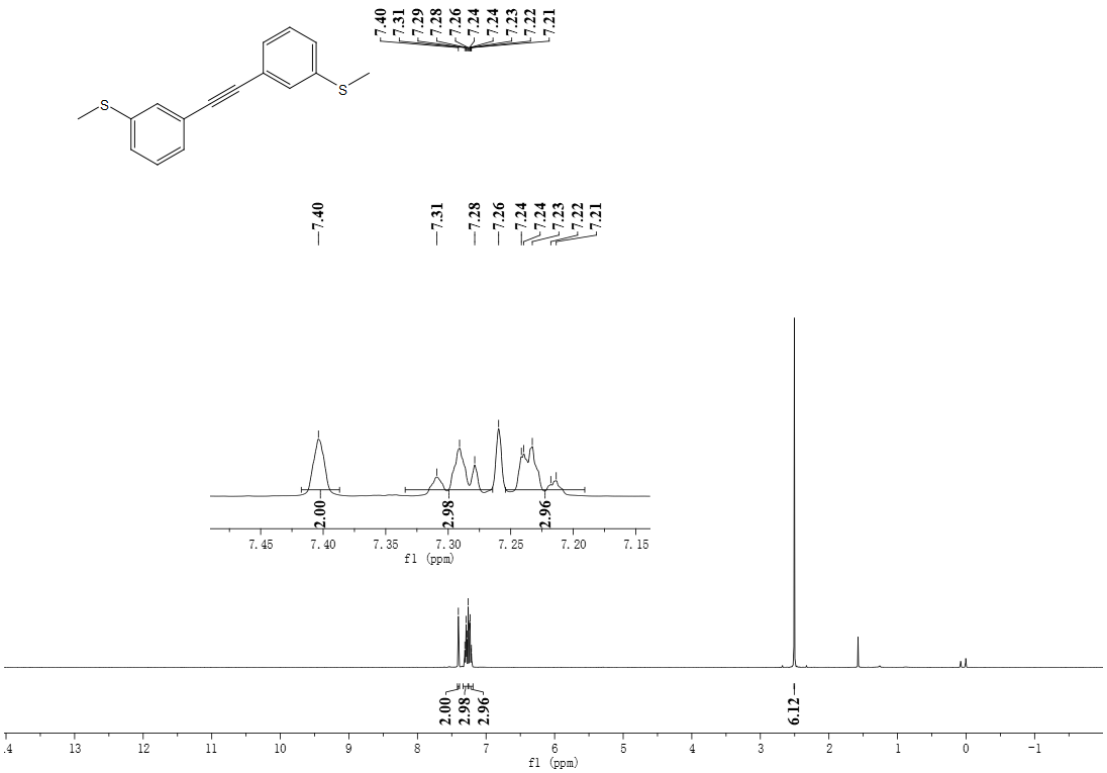
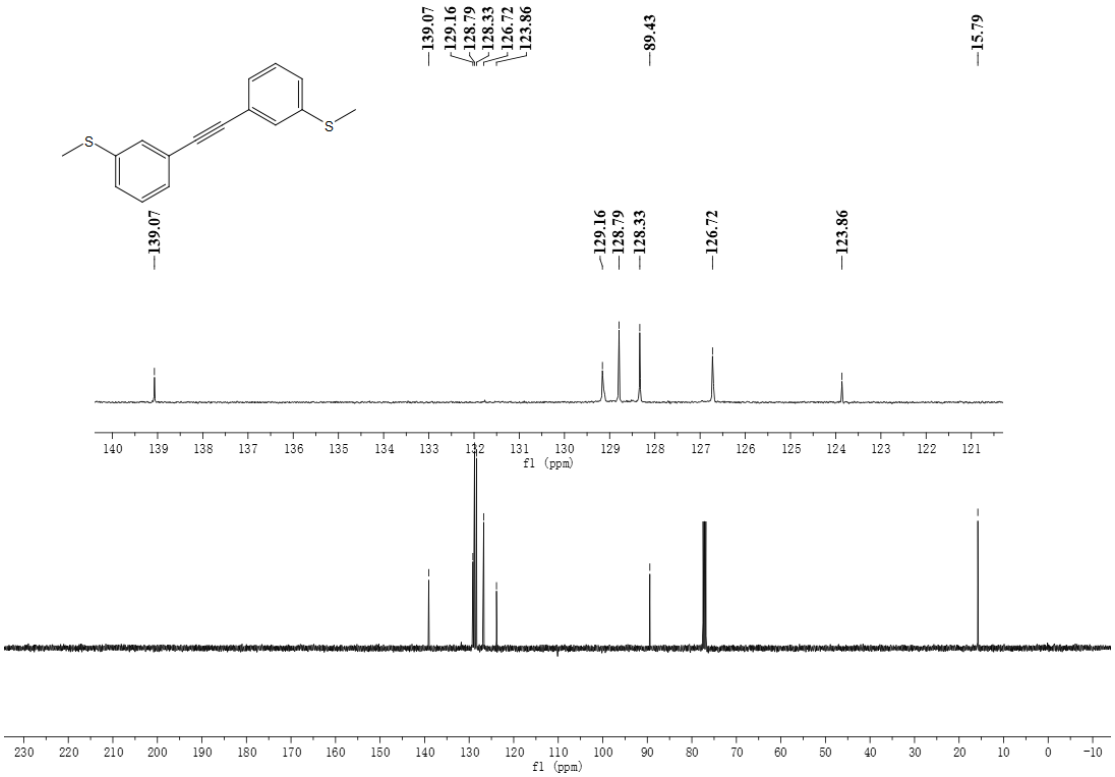
X. Copies of NMR spectra

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



^{13}C NMR ($CDCl_3$, 400 MHz) spectrum of **1g**



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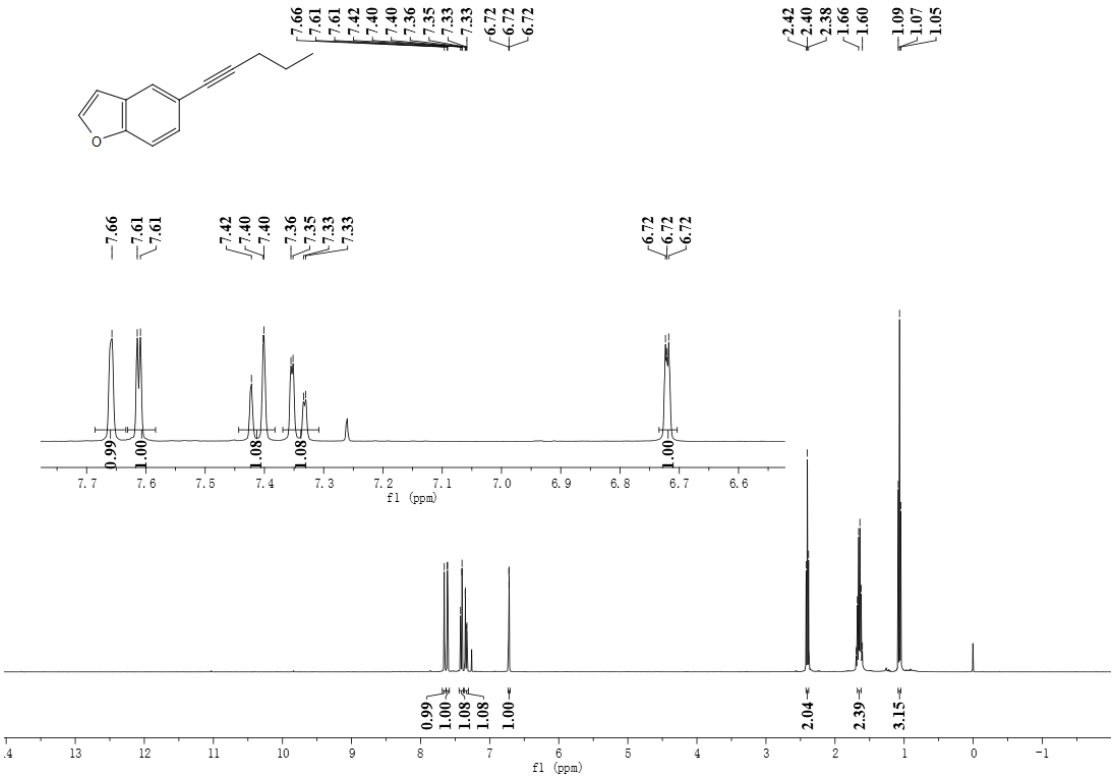

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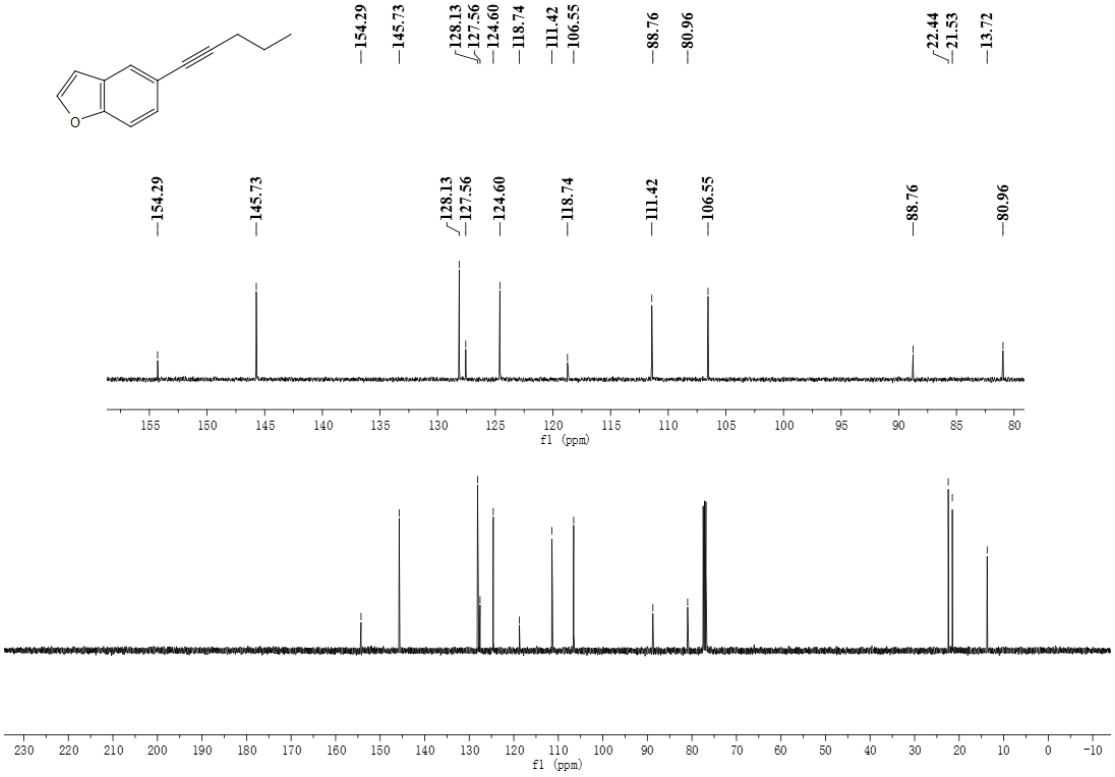

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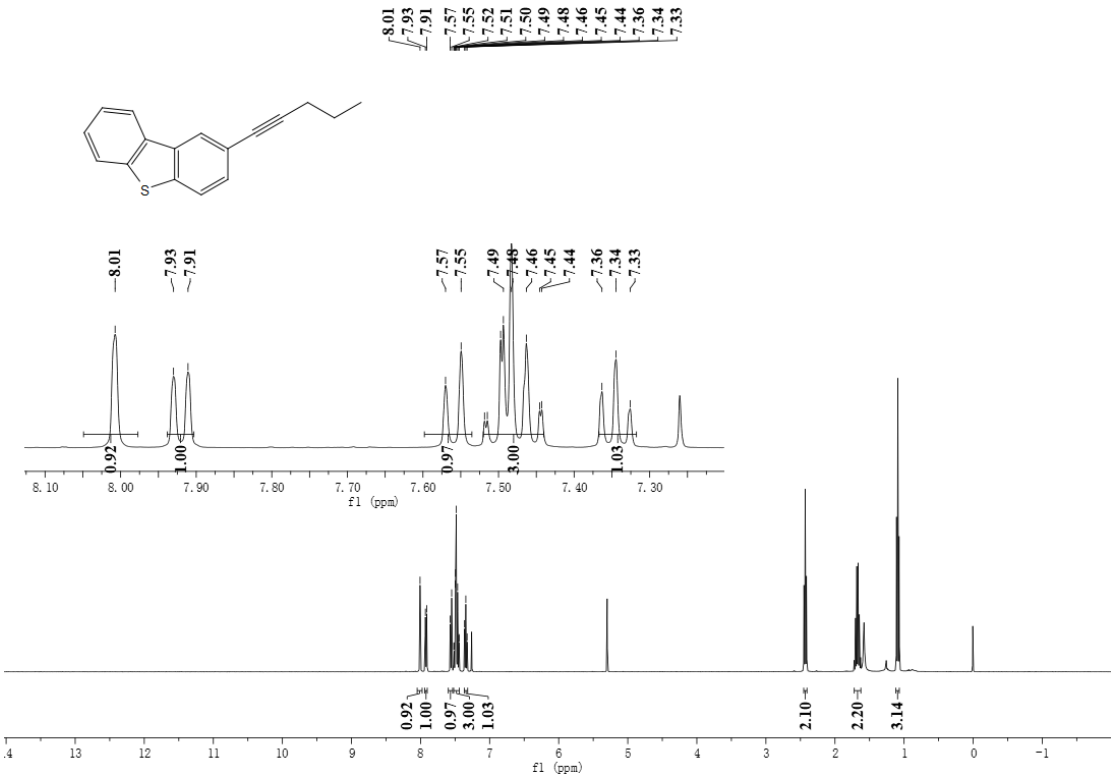

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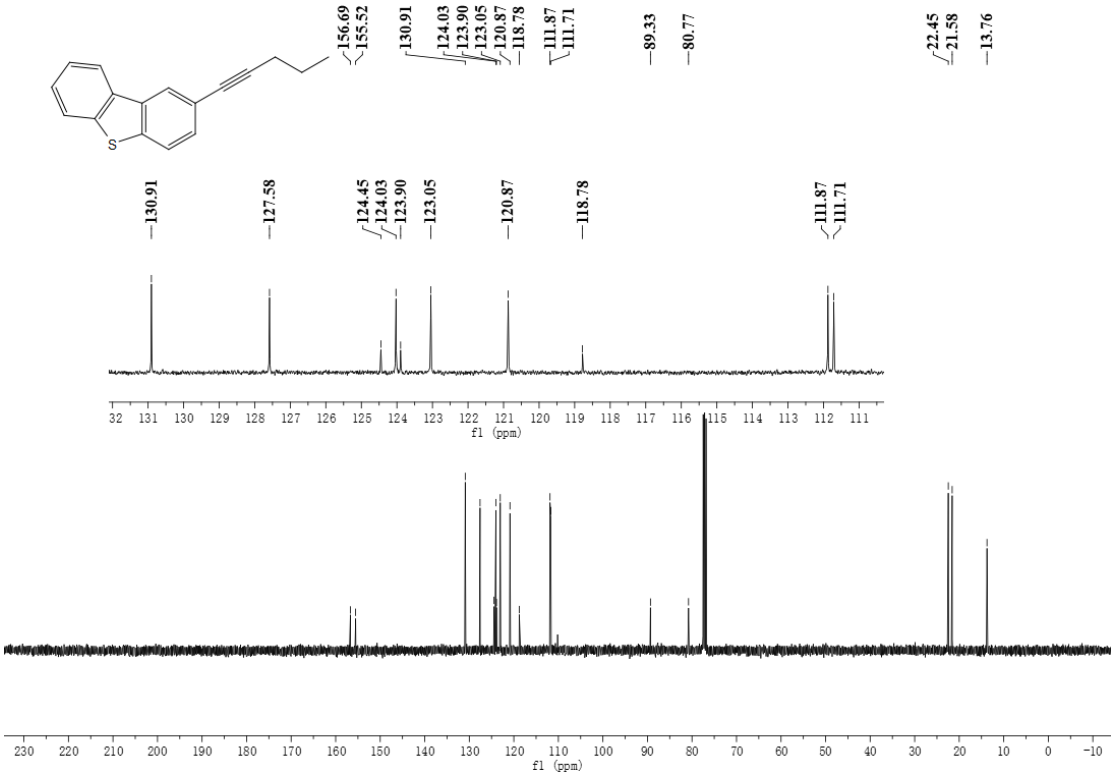

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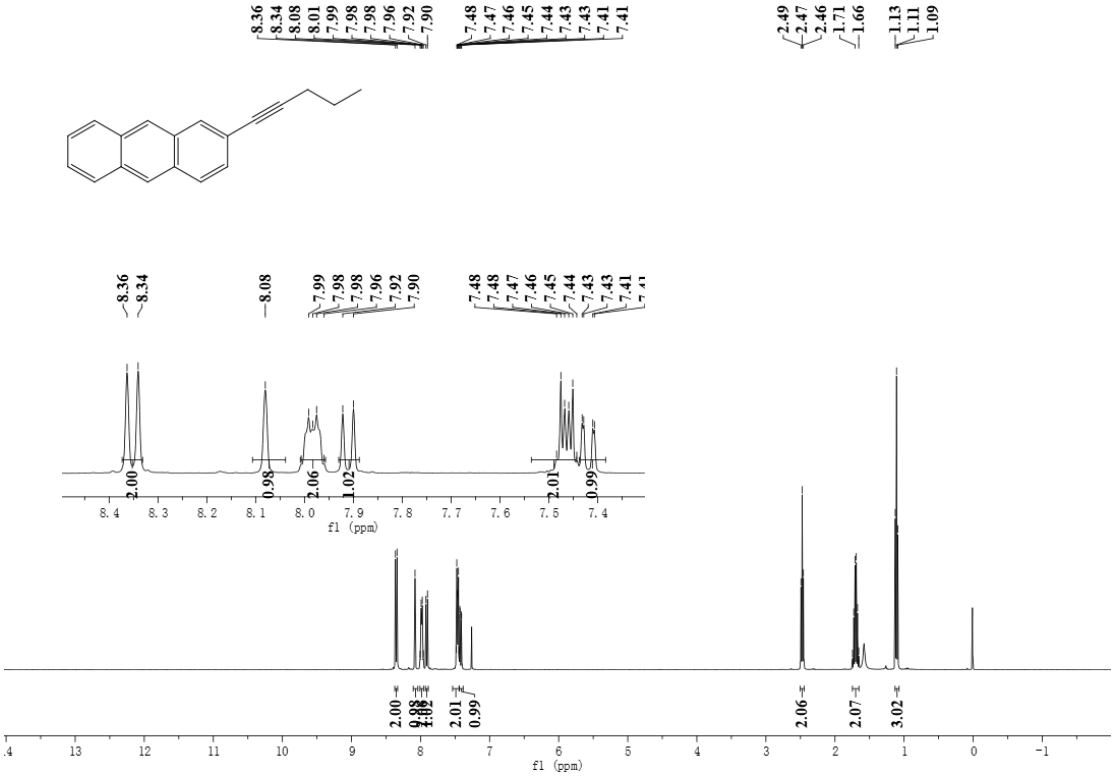

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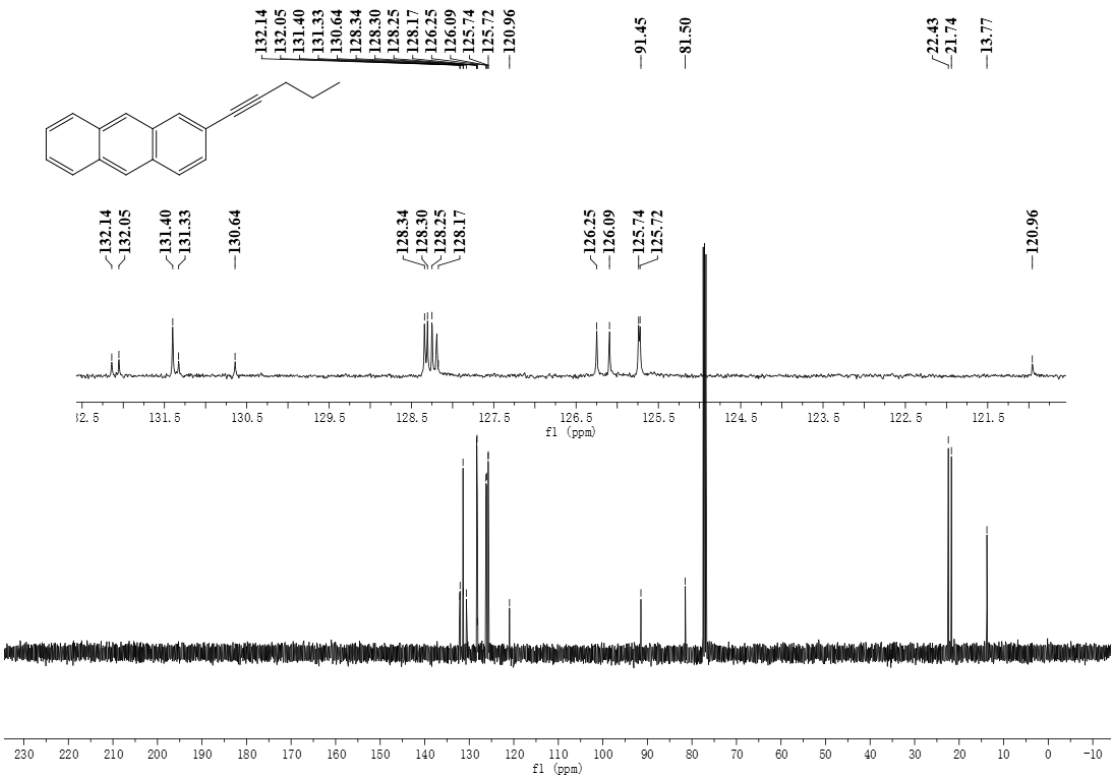

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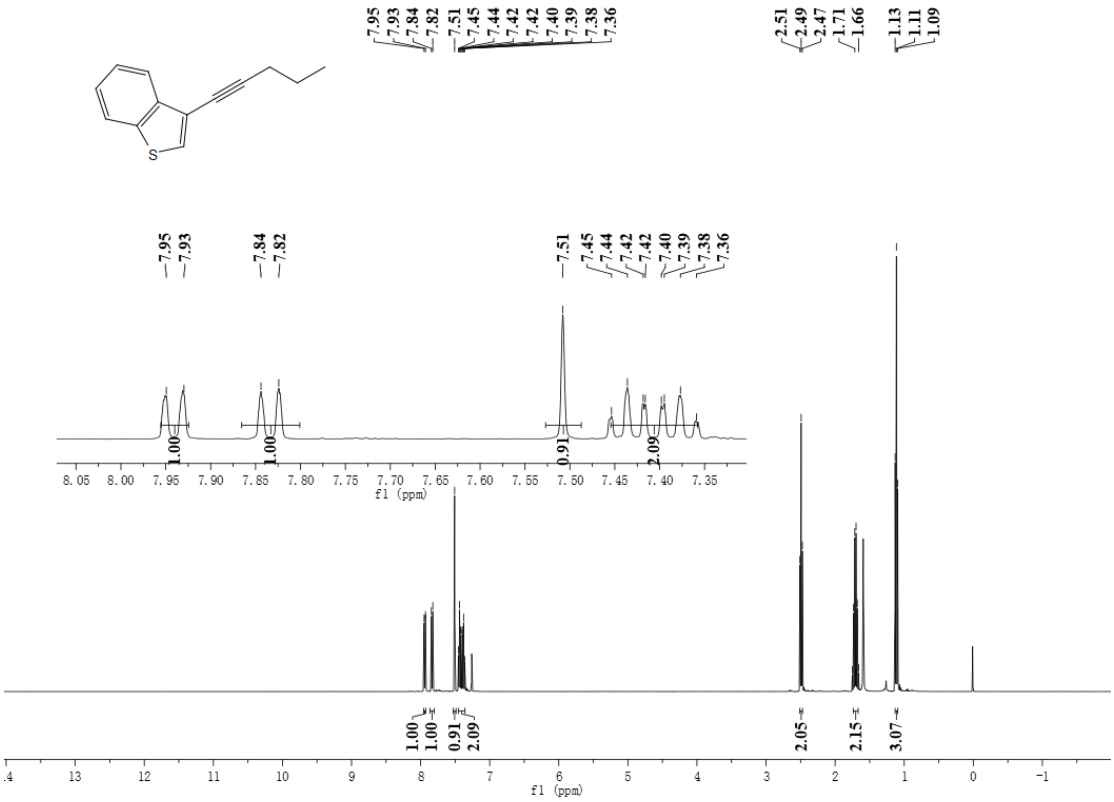

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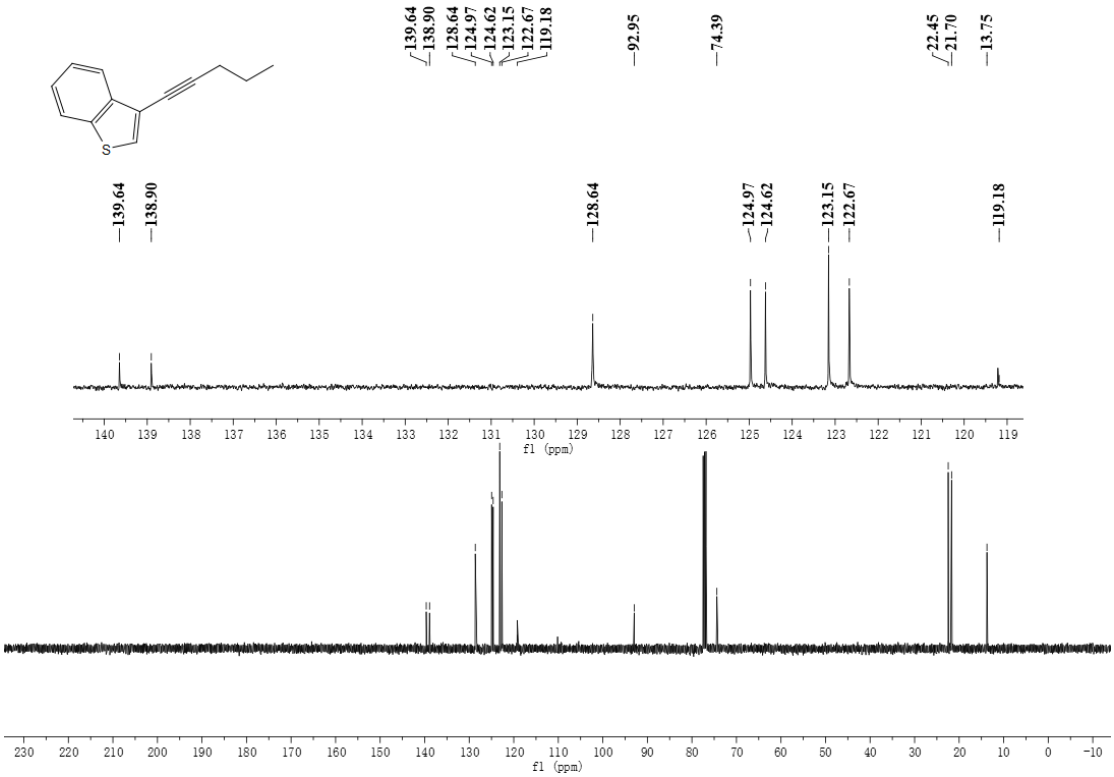
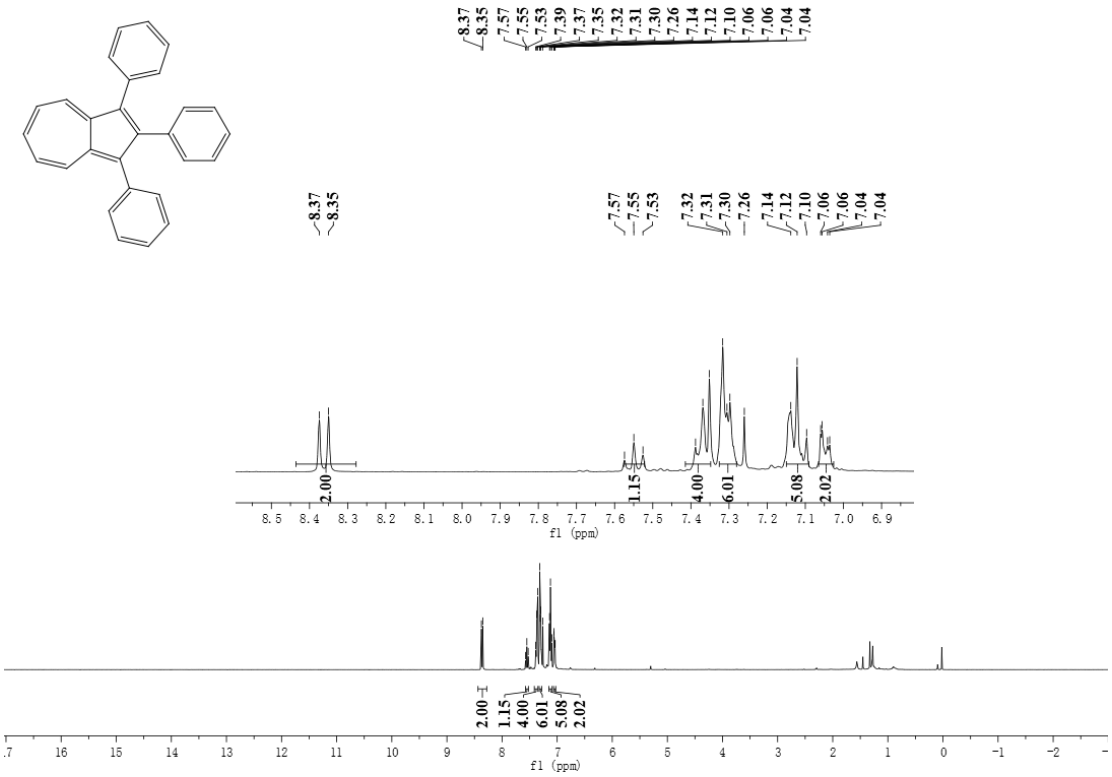


^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **3a**



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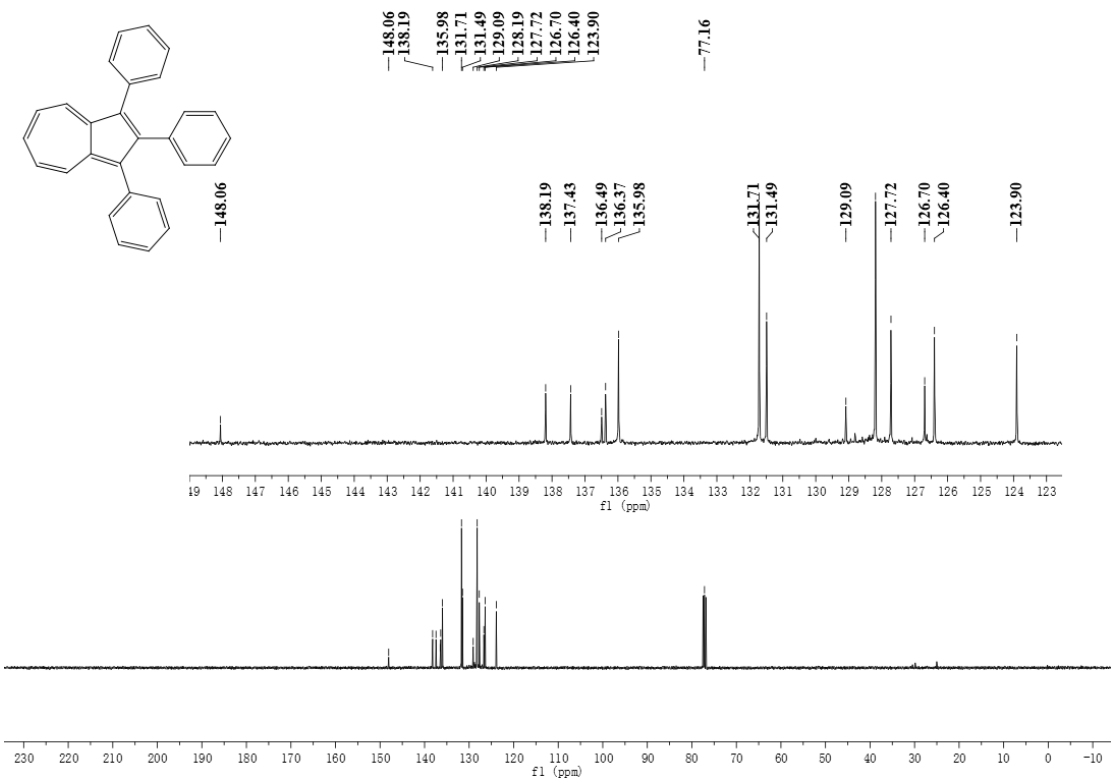

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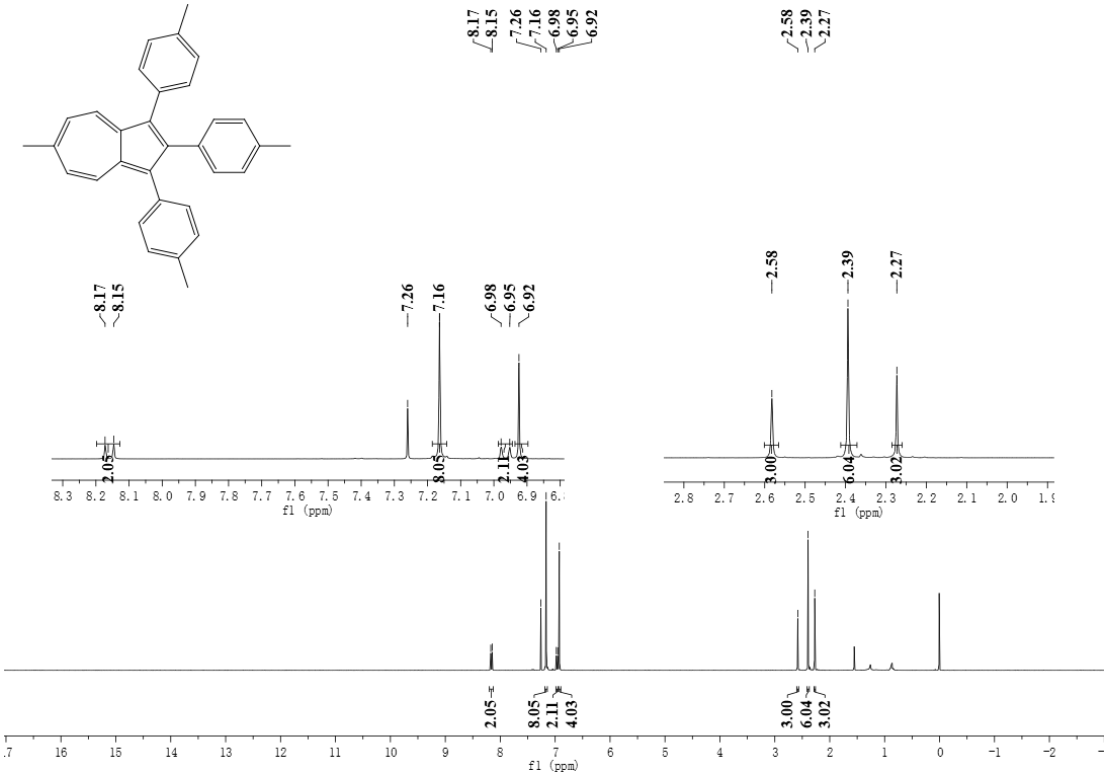

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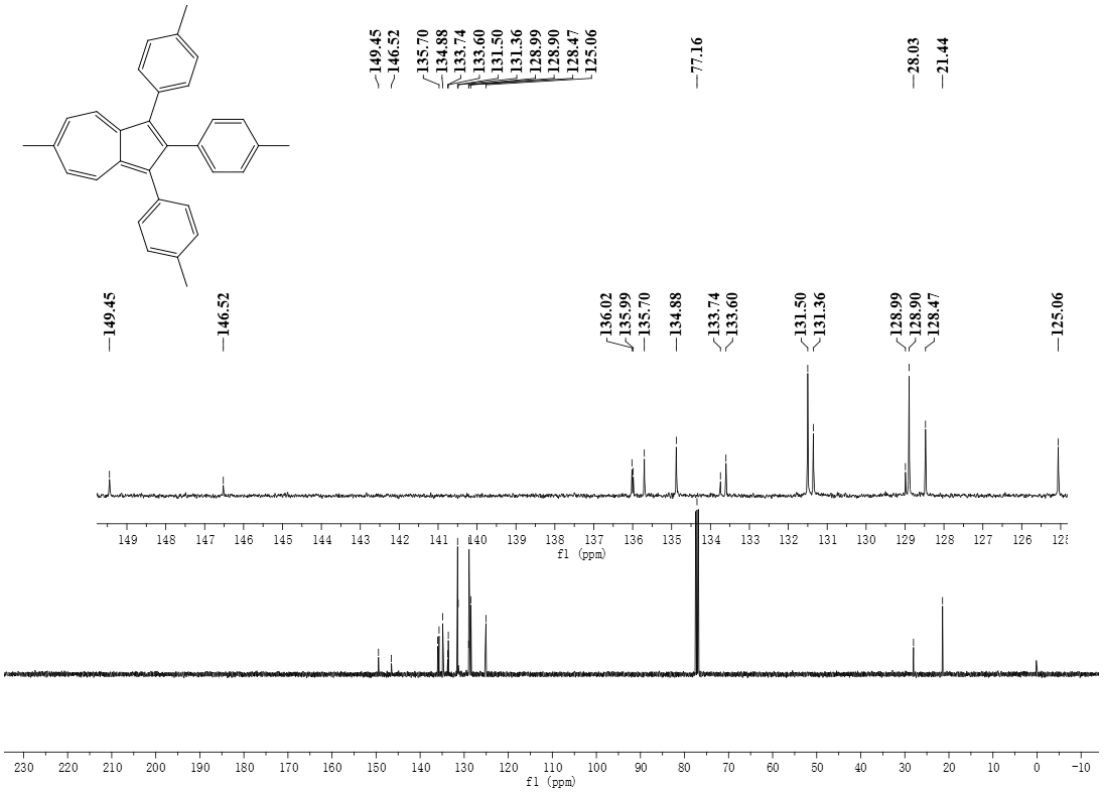

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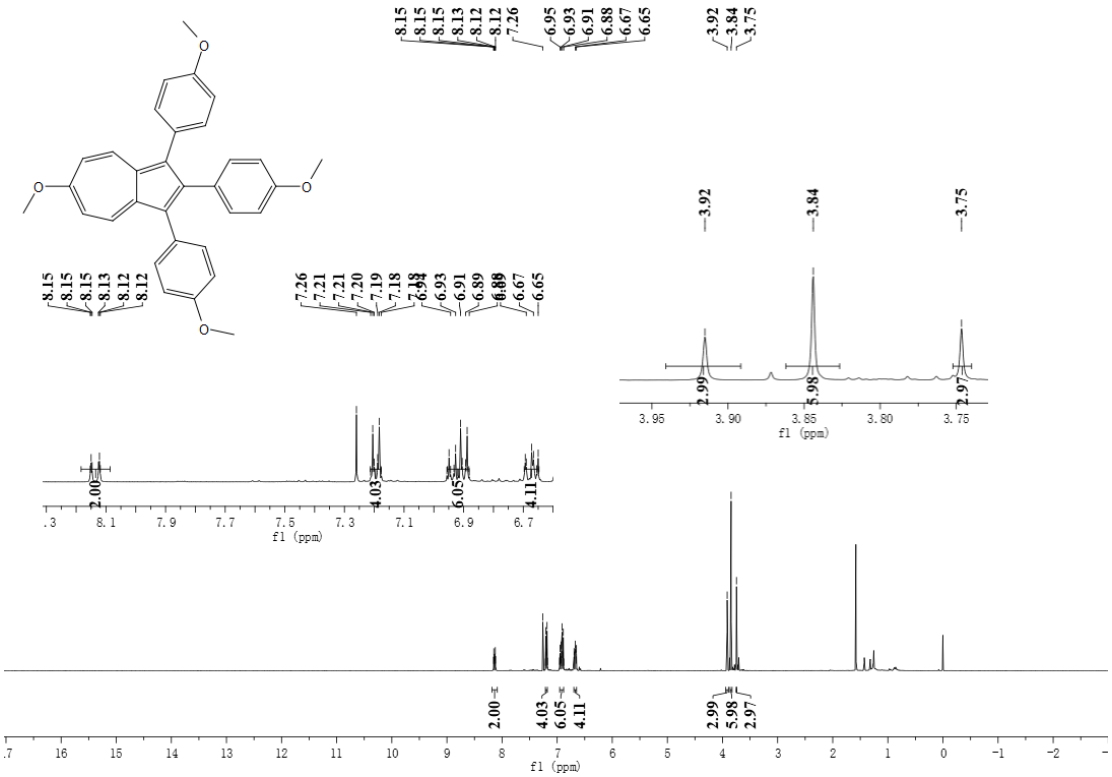

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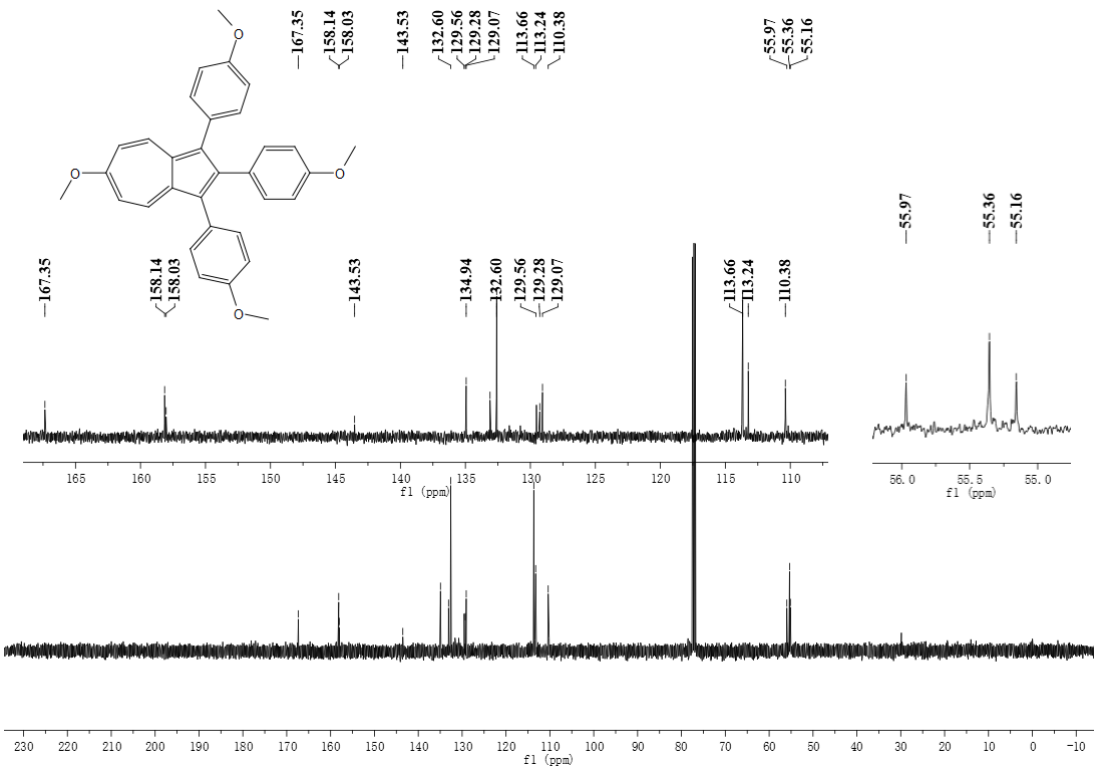

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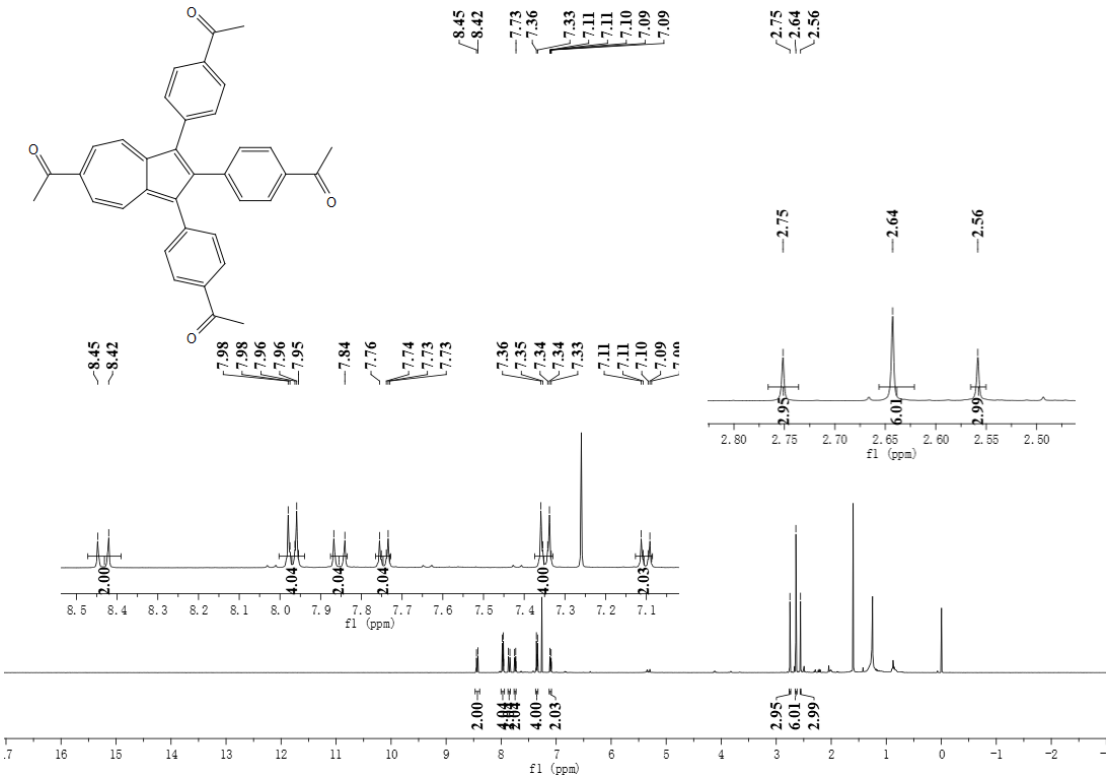

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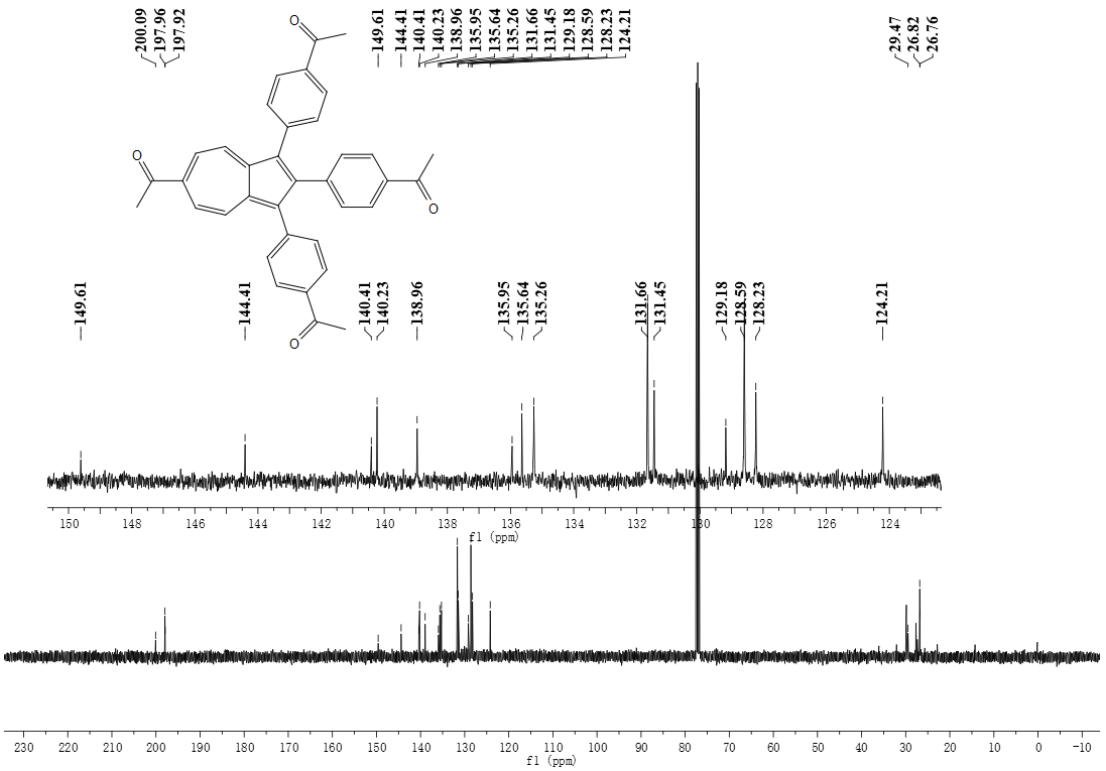

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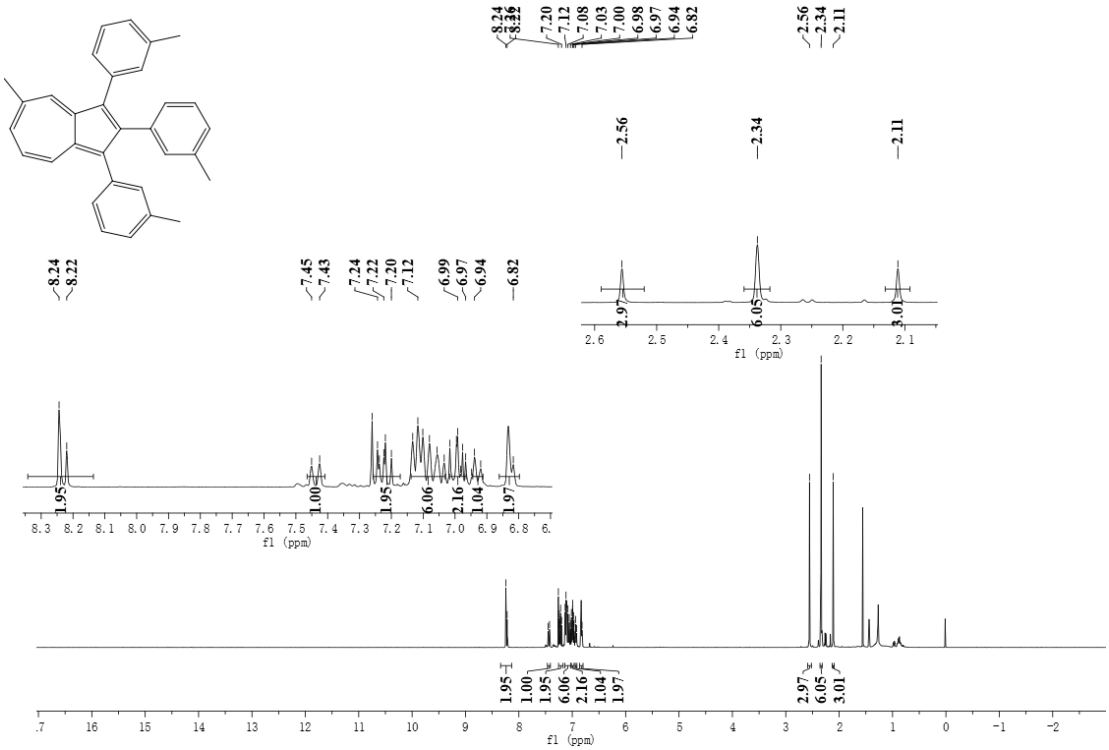

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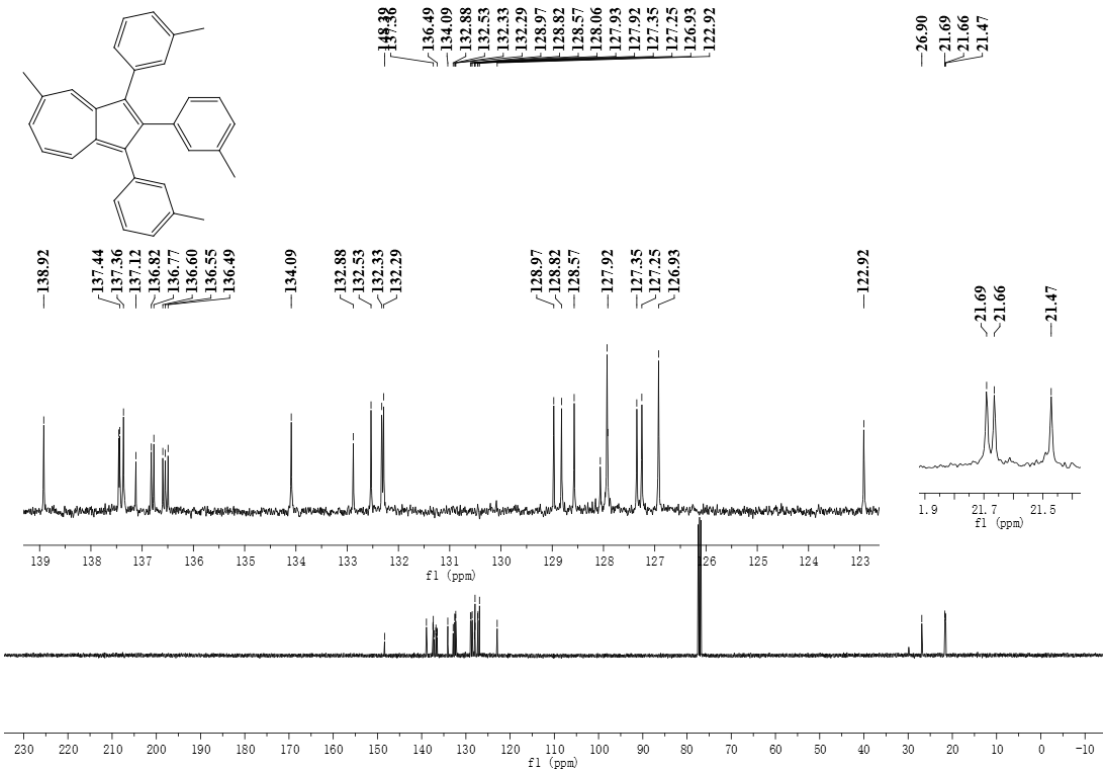

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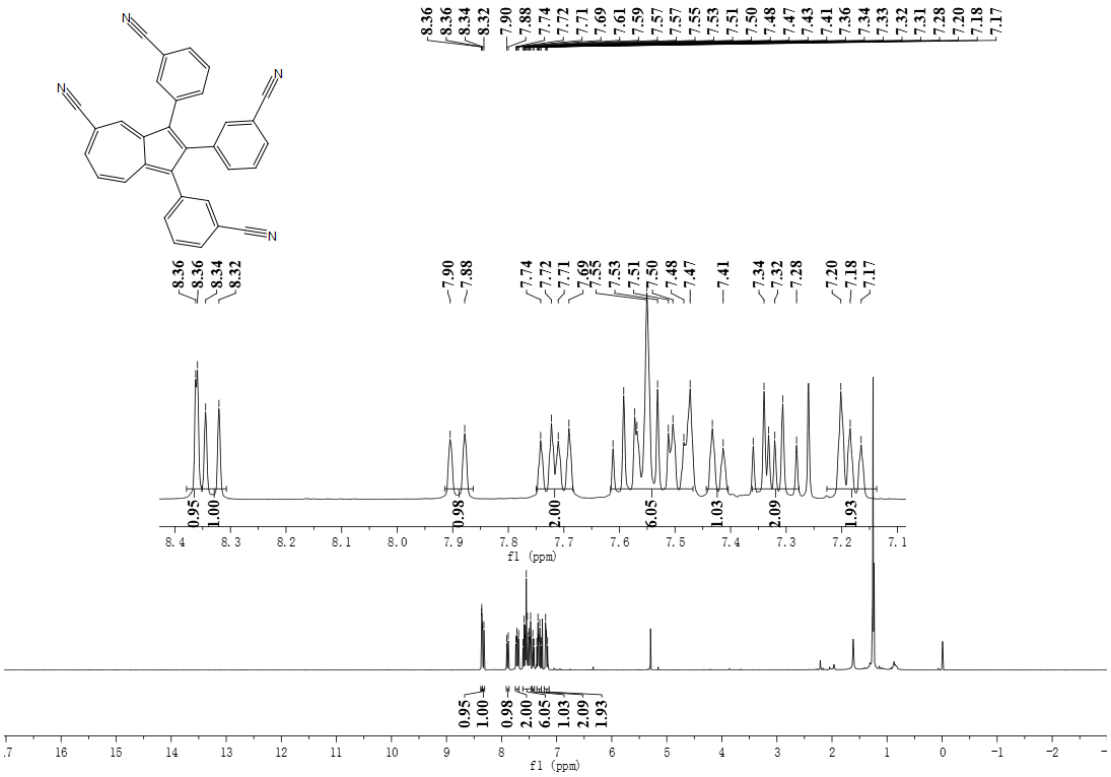

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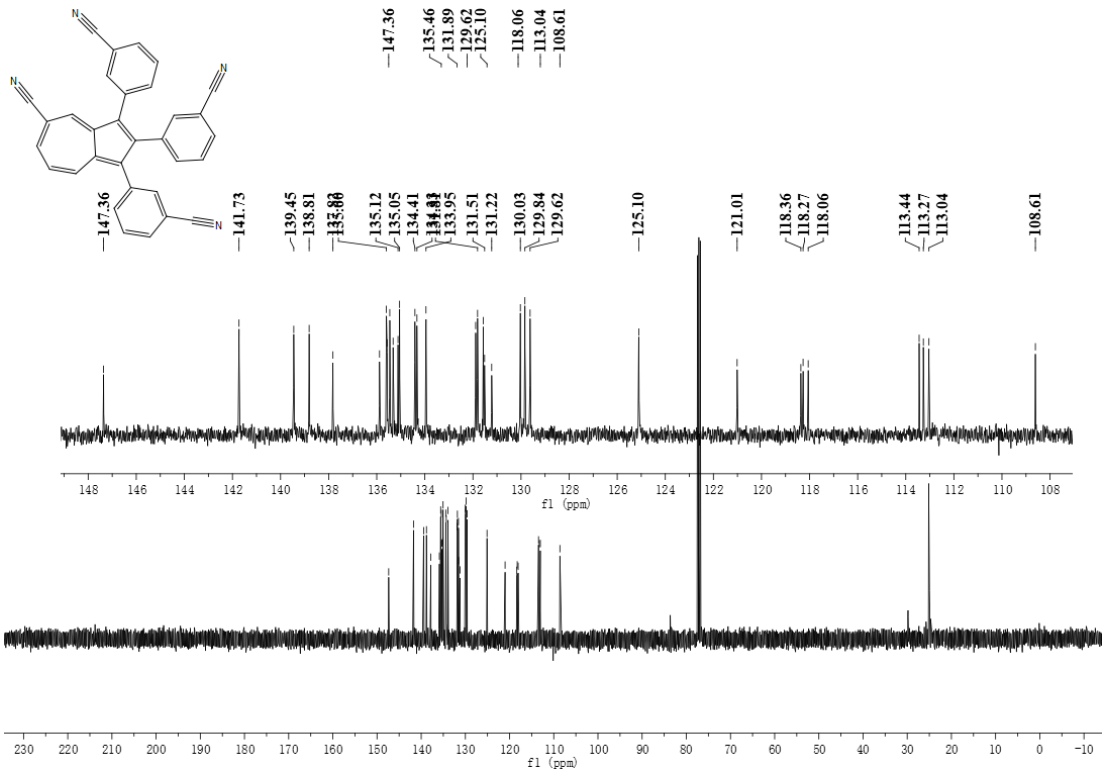

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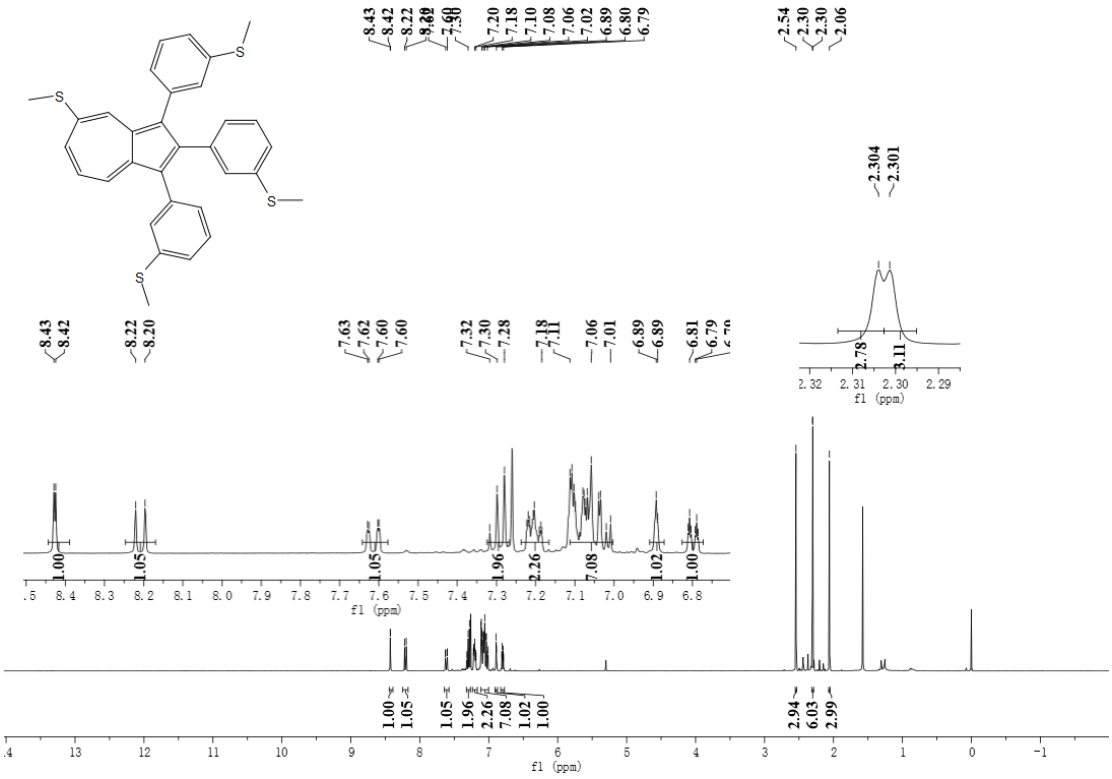

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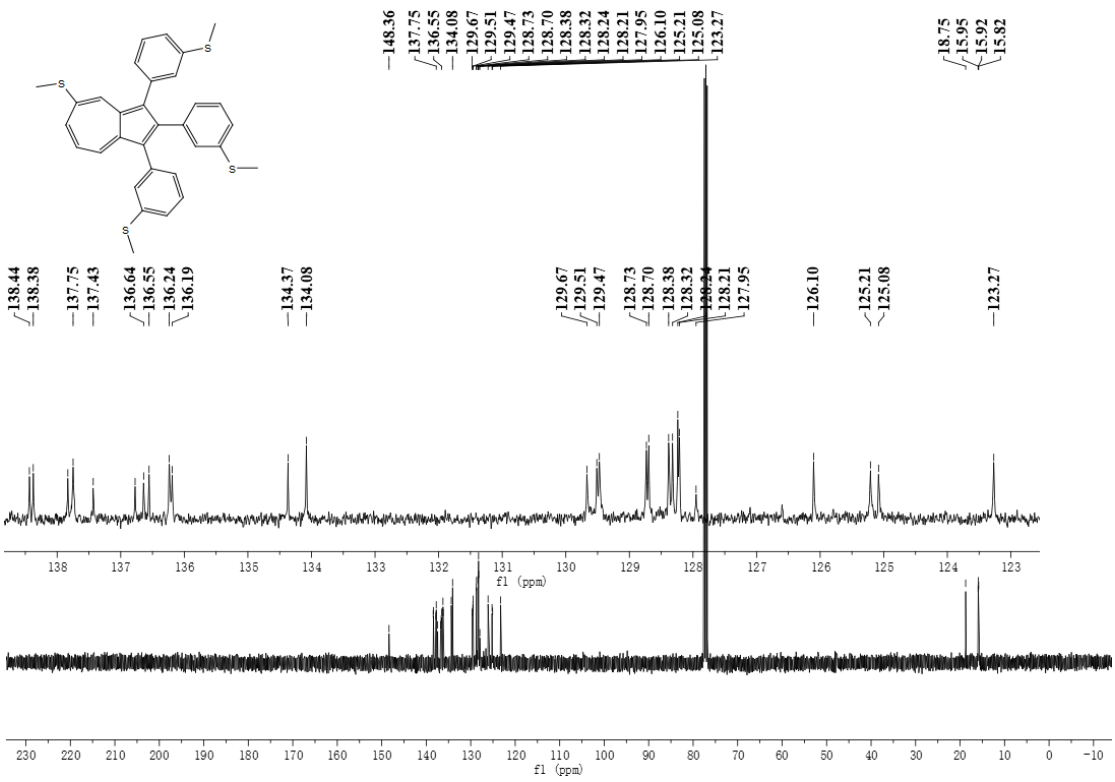

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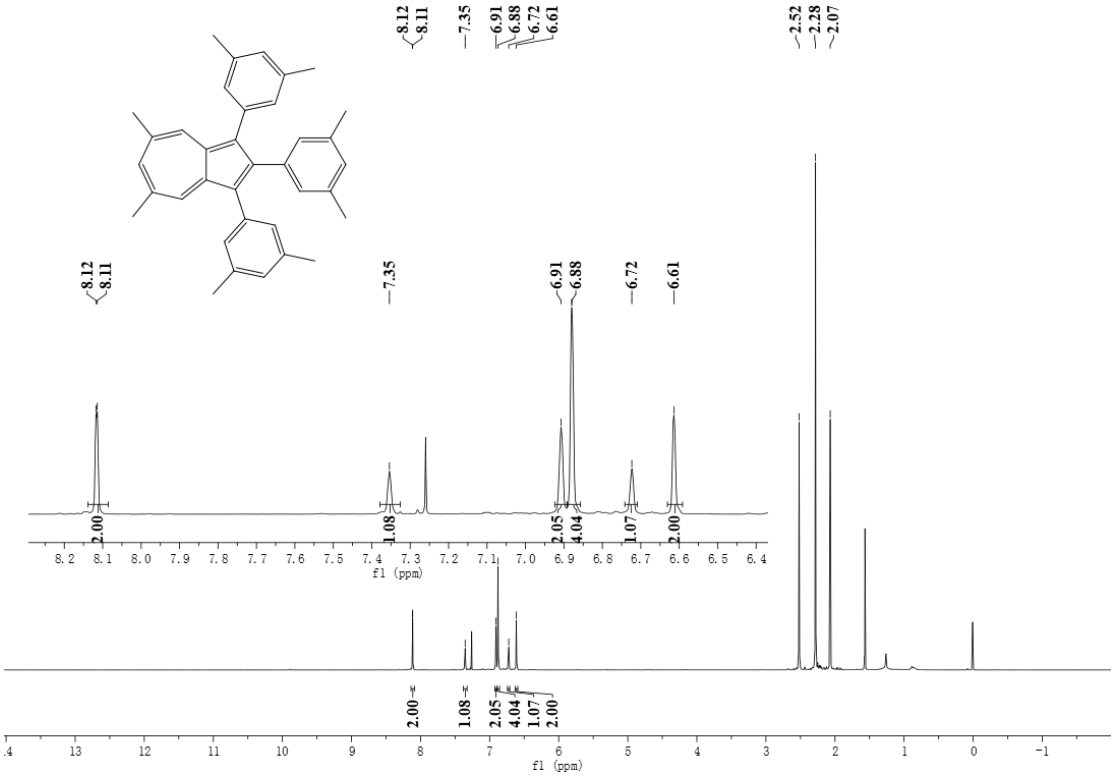

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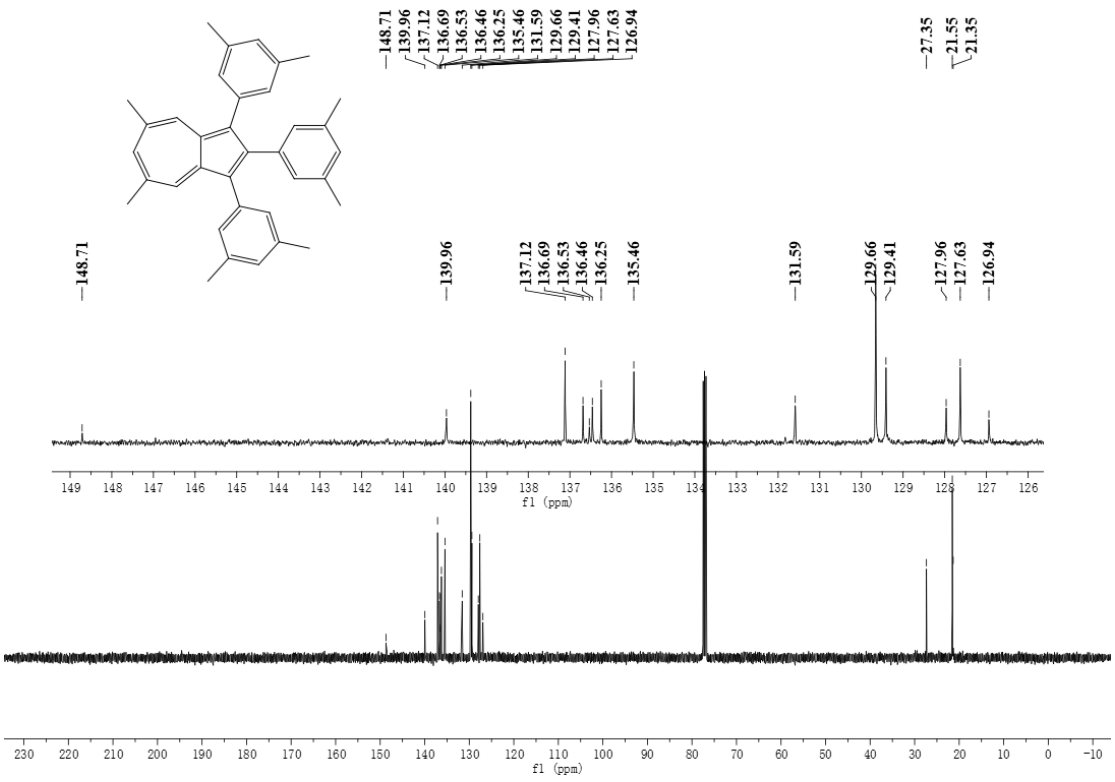

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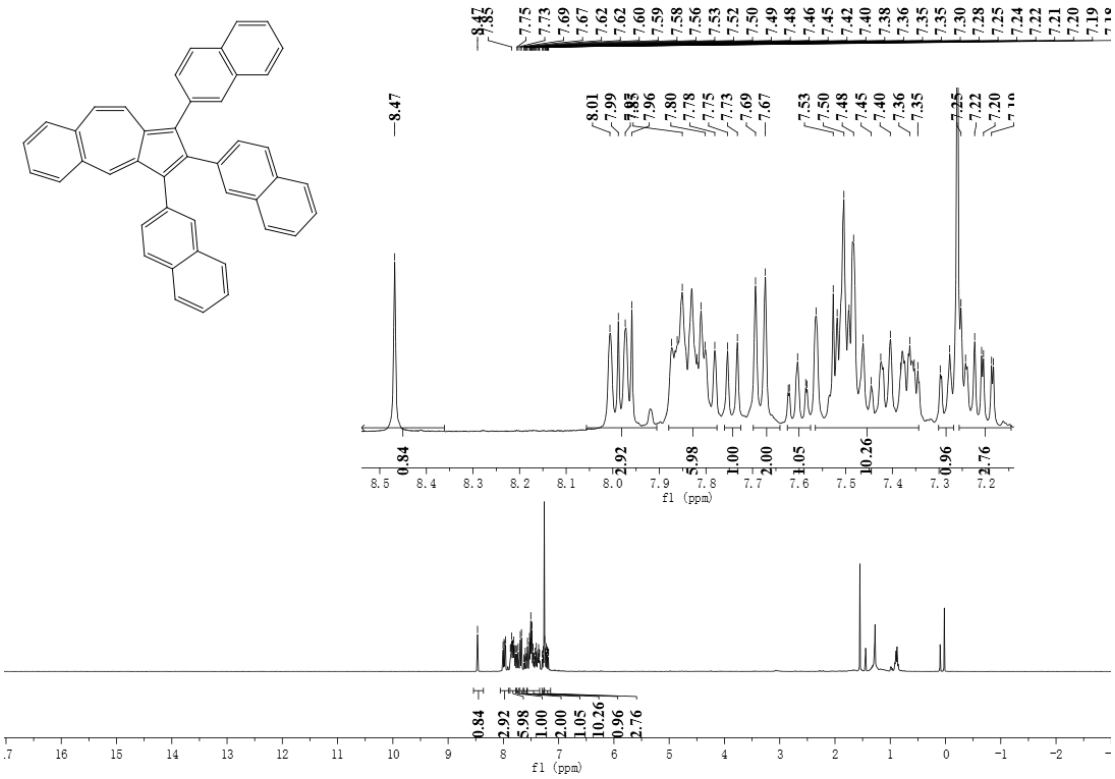

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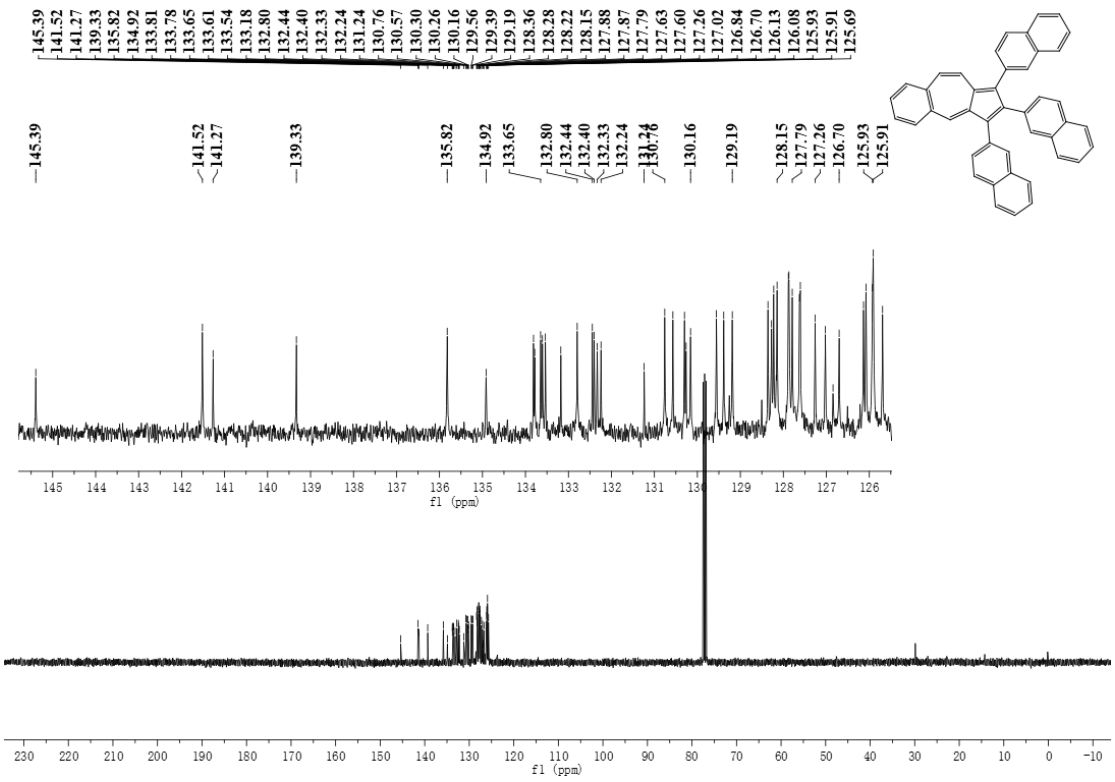

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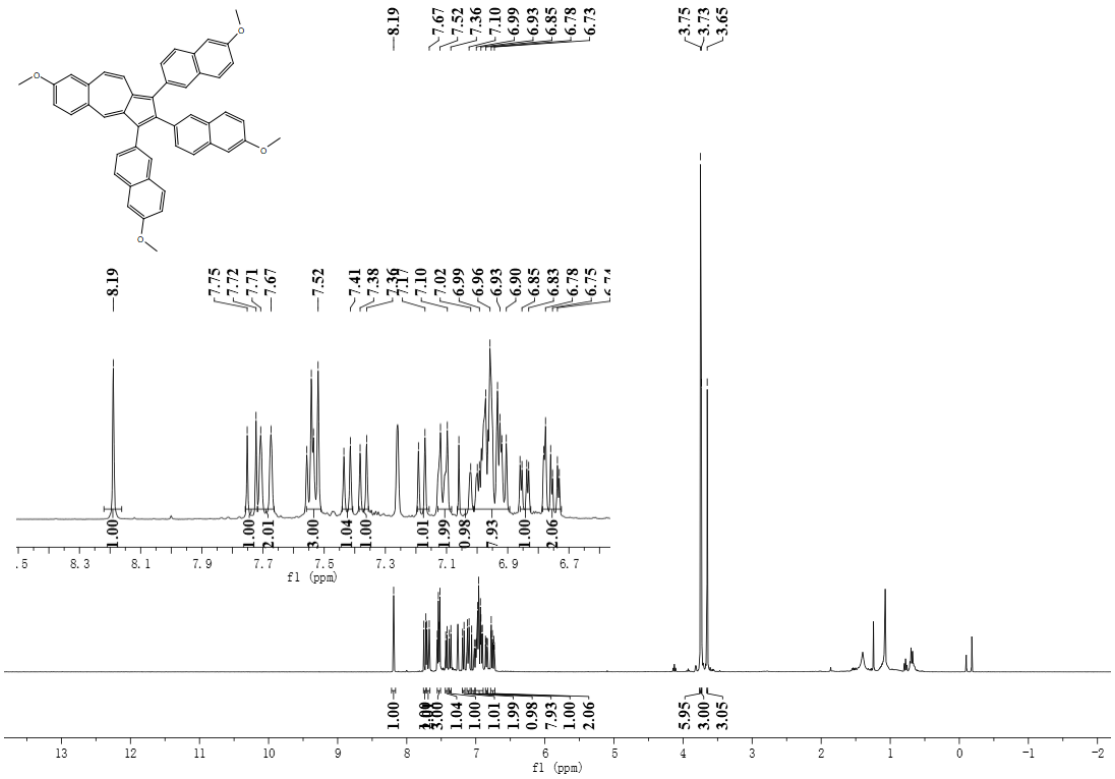

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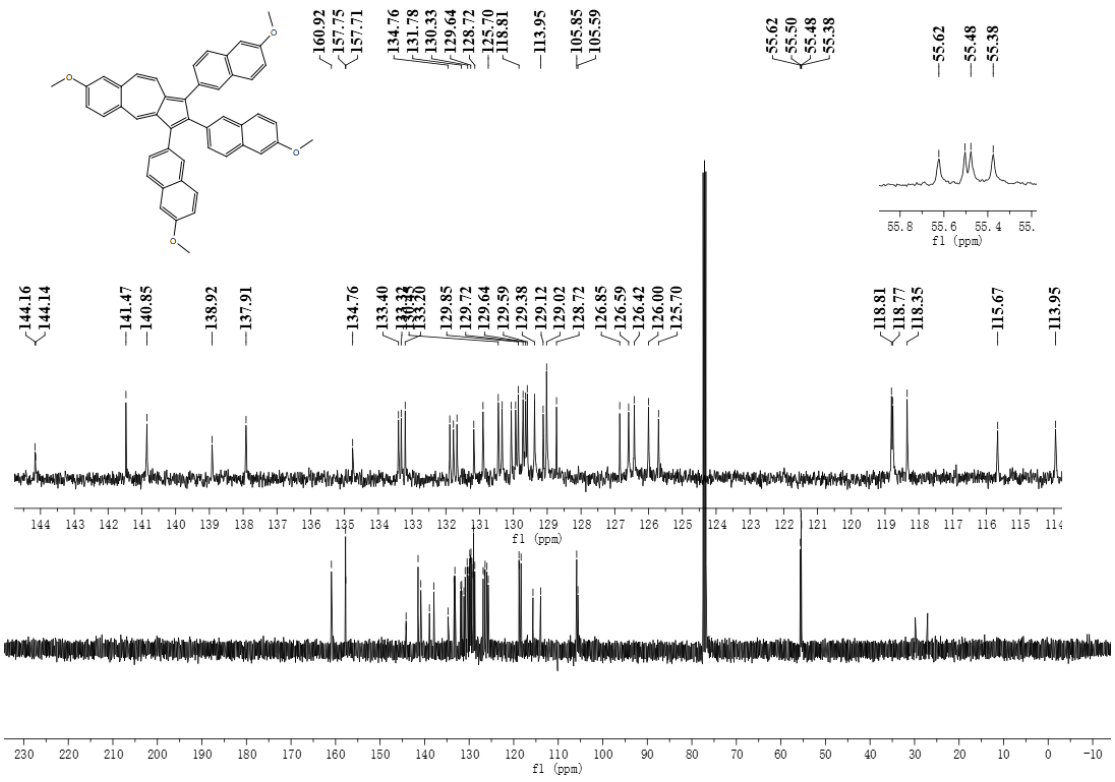

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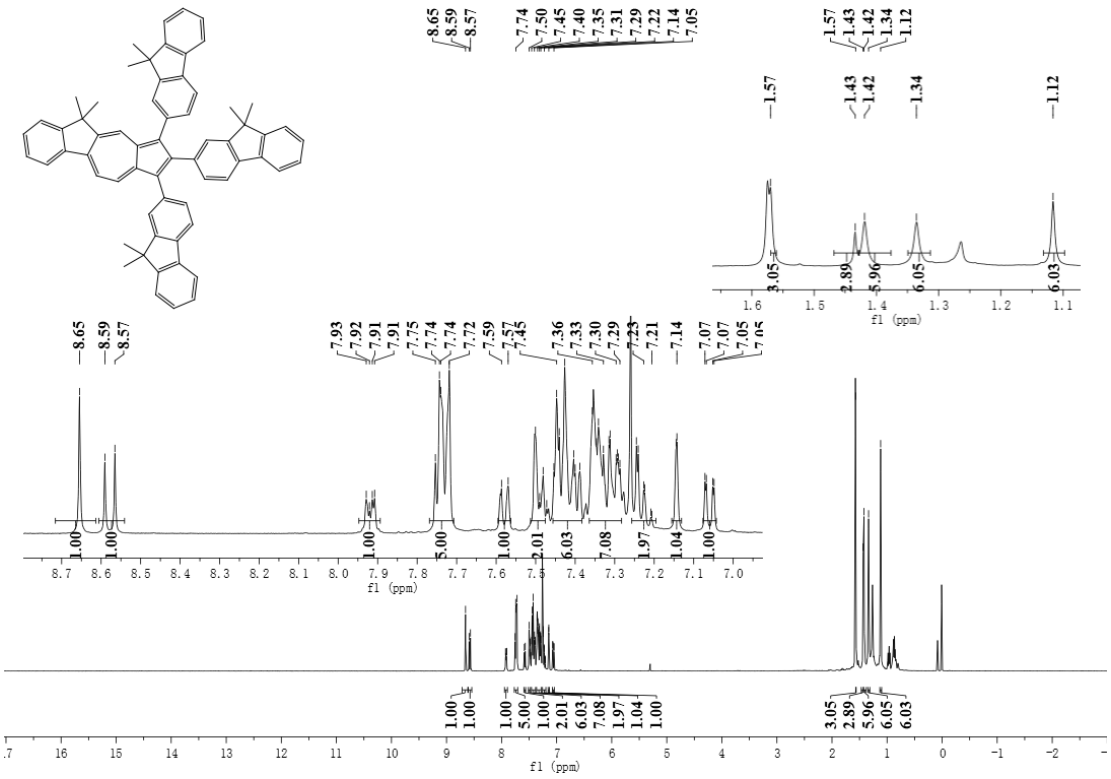

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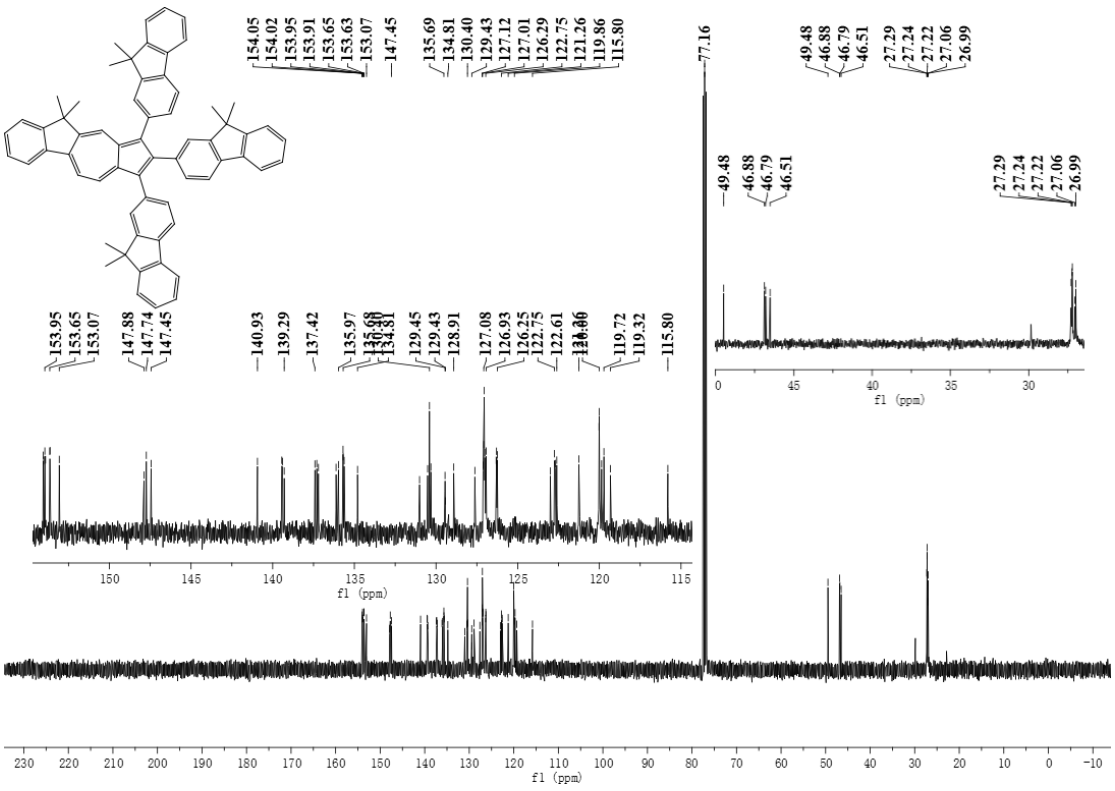

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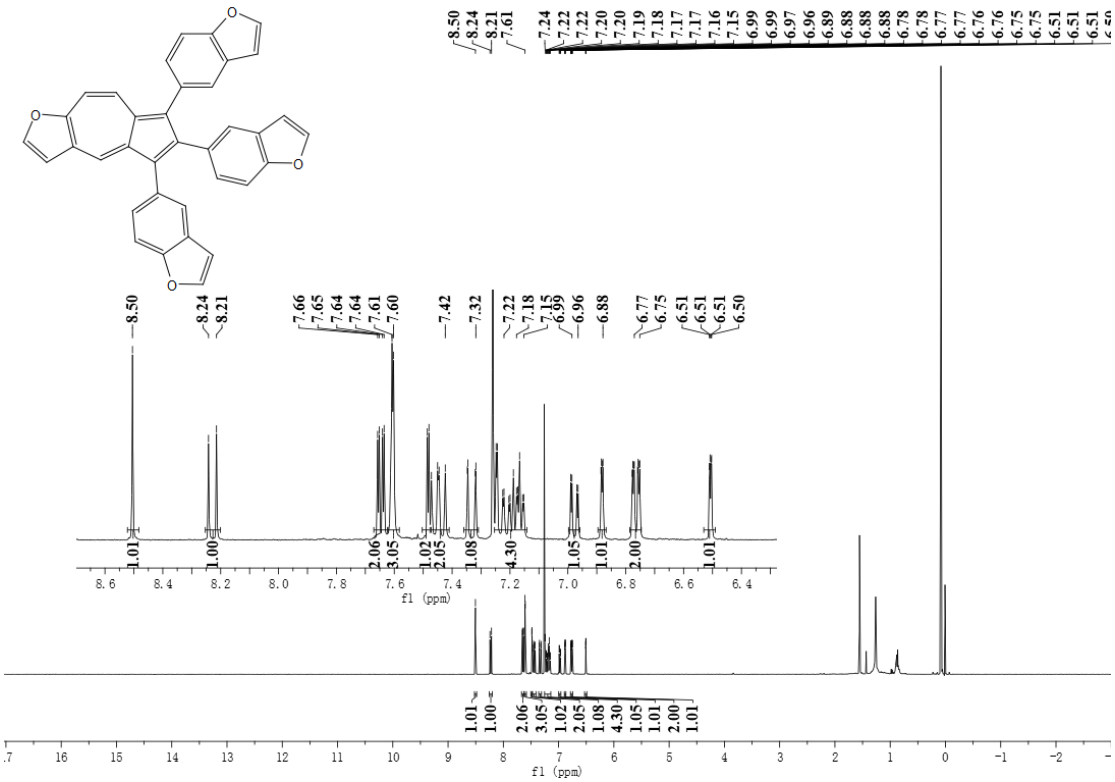

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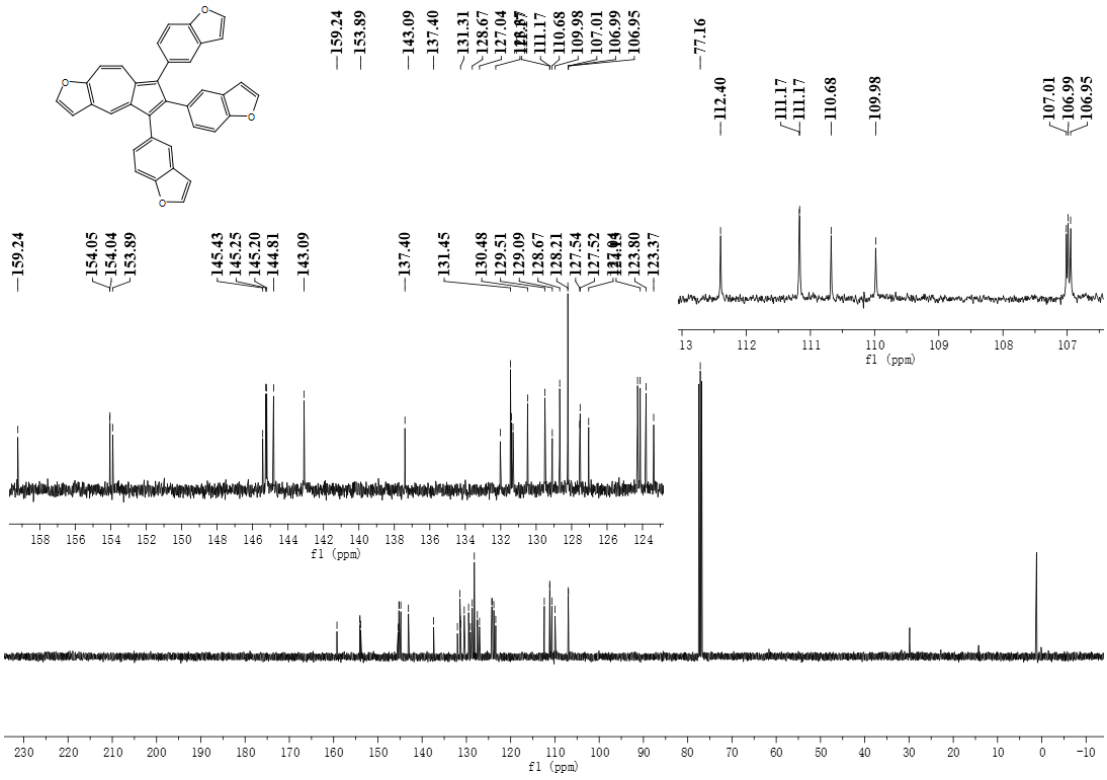

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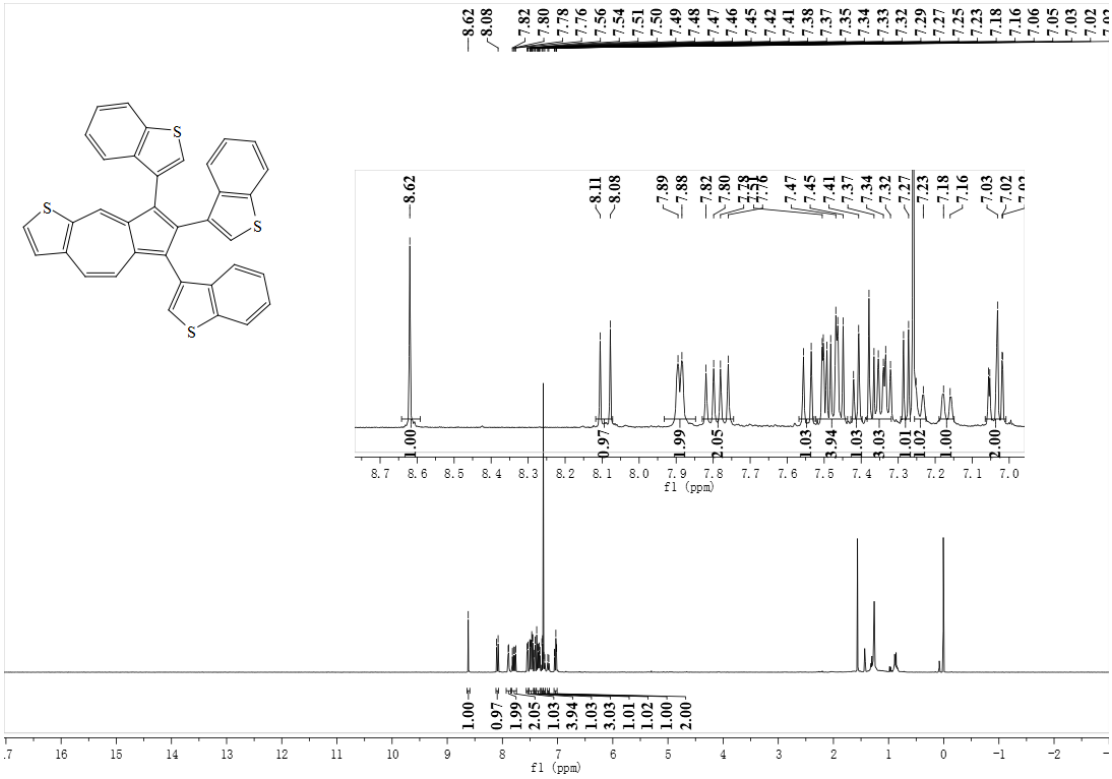

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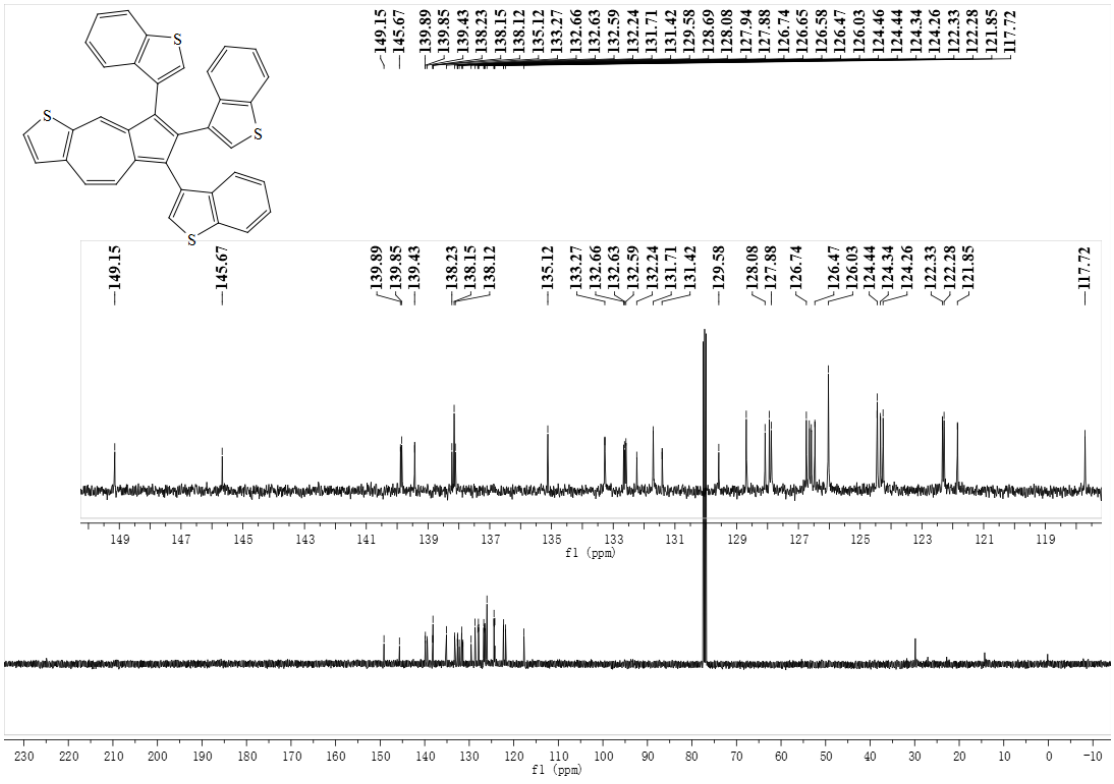

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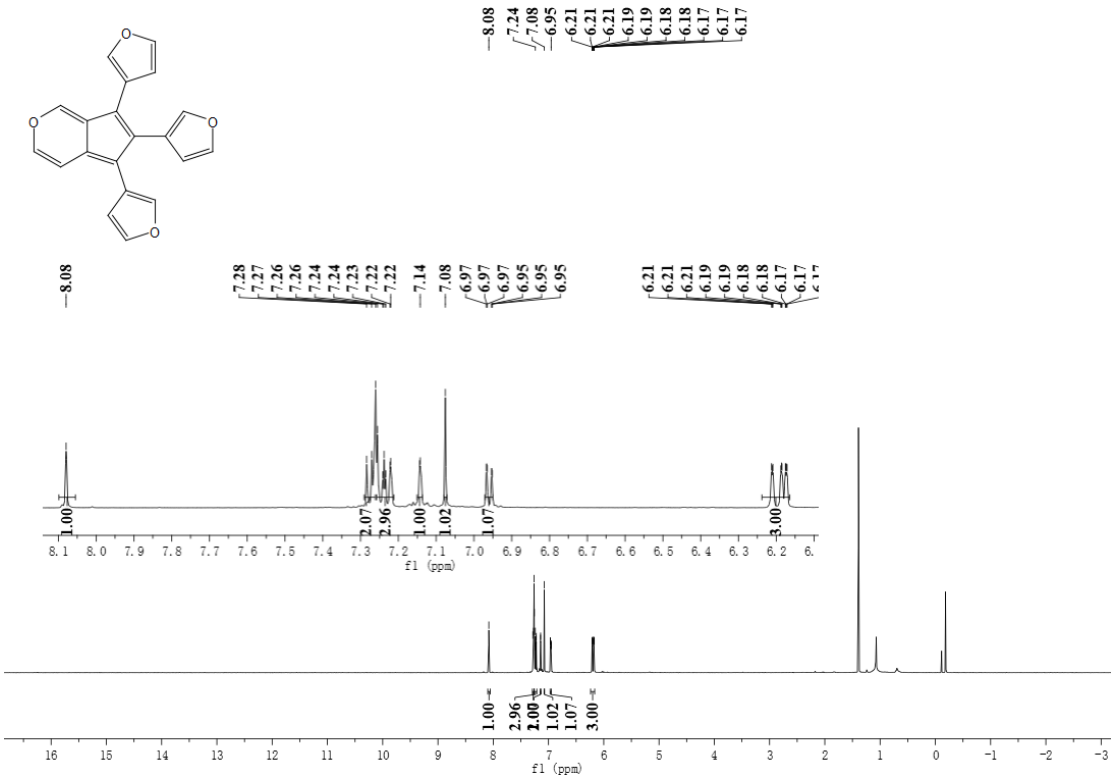

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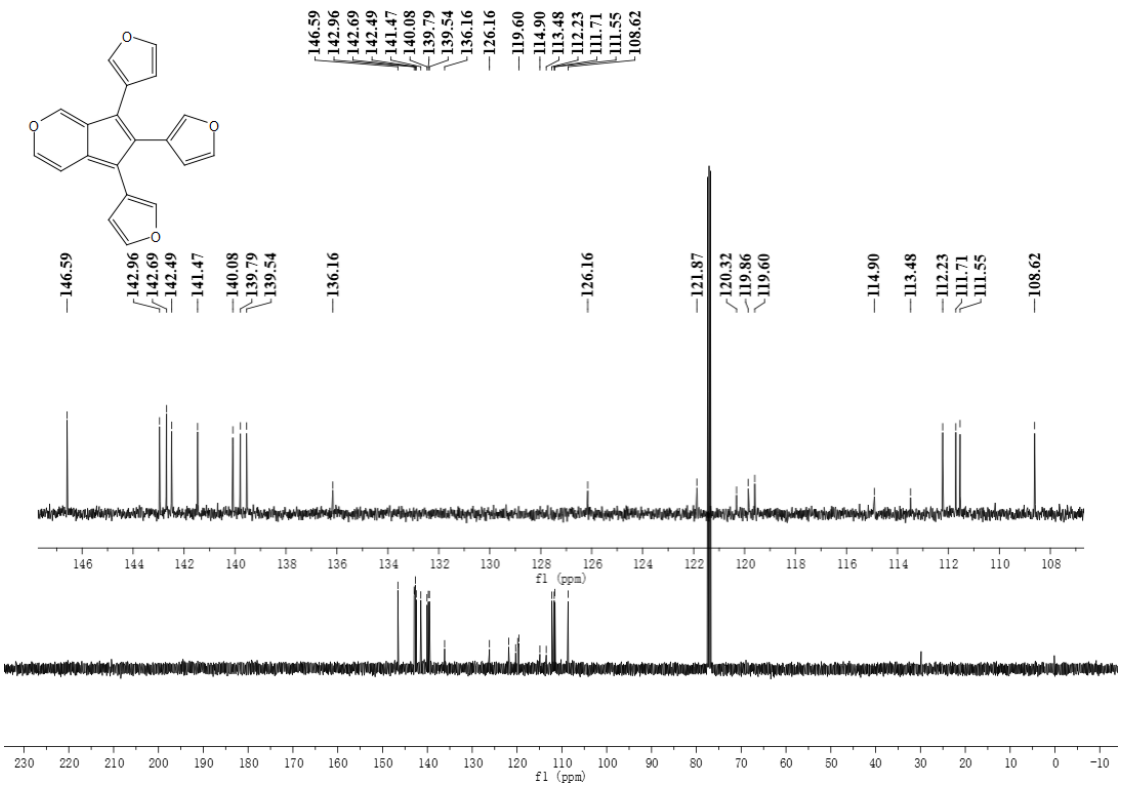

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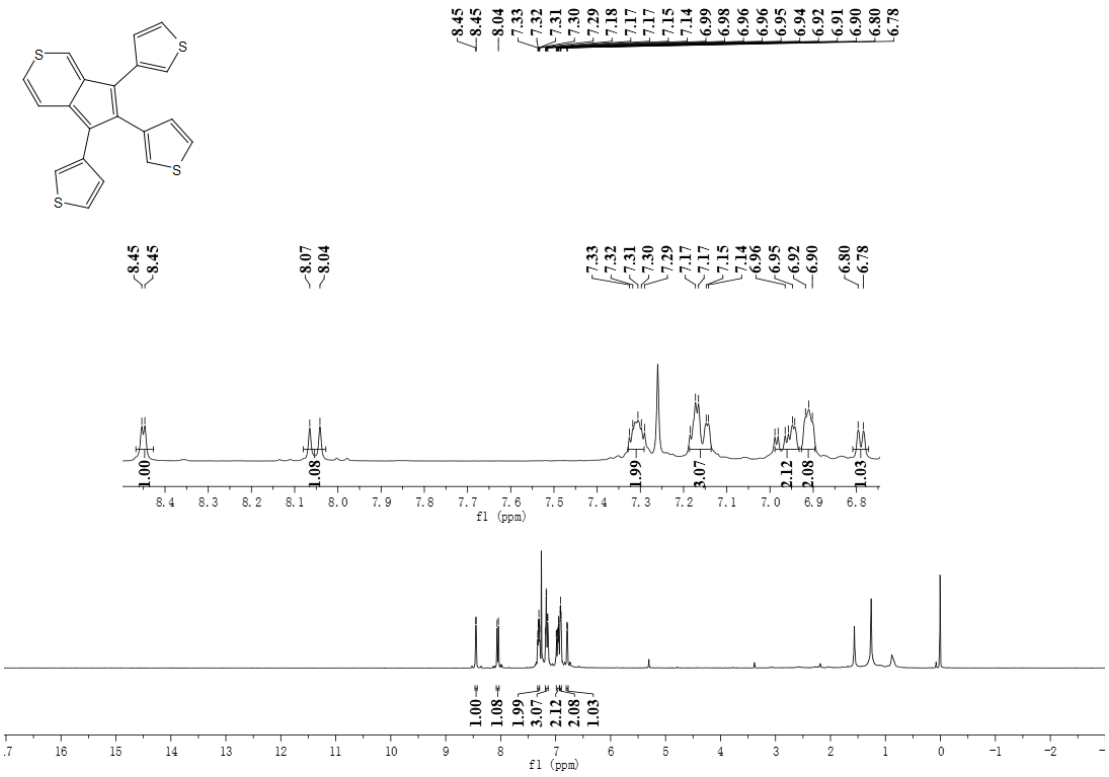

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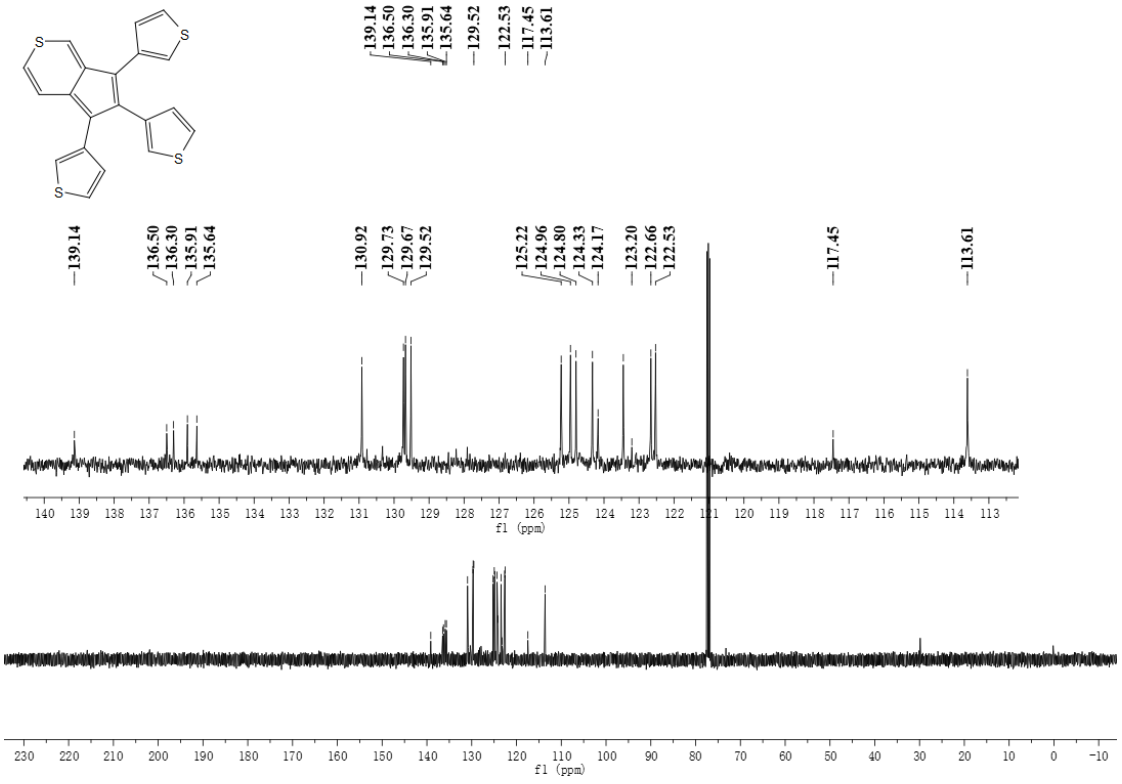

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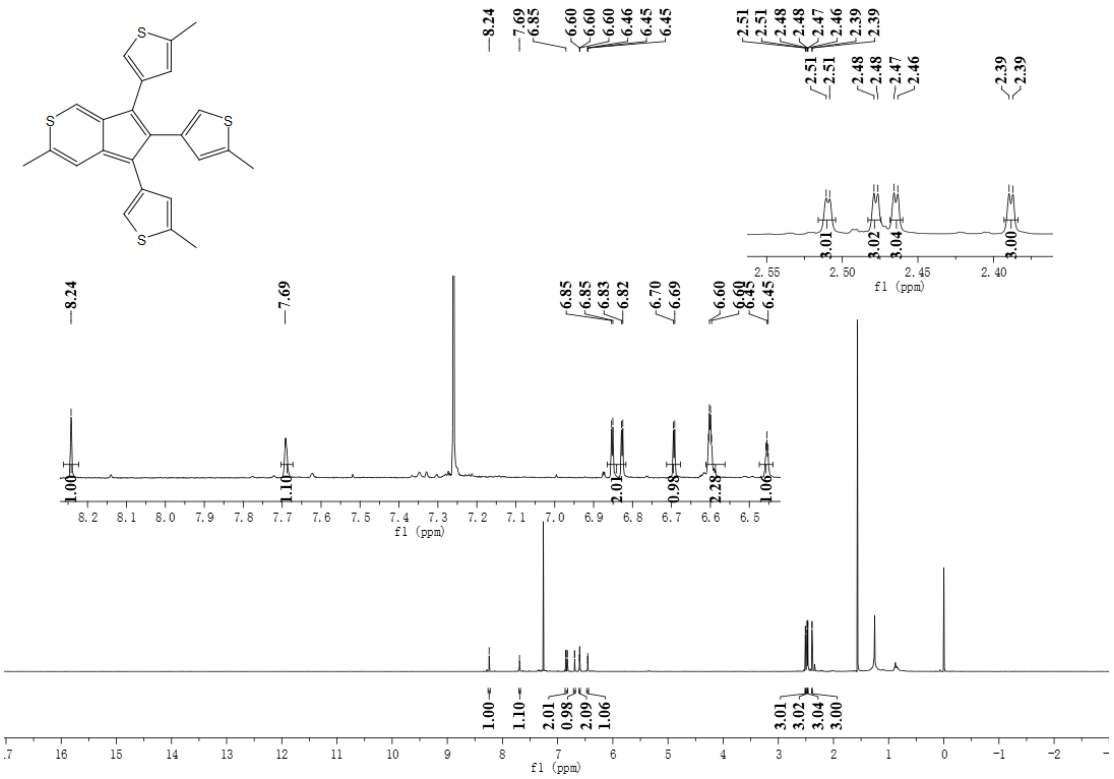

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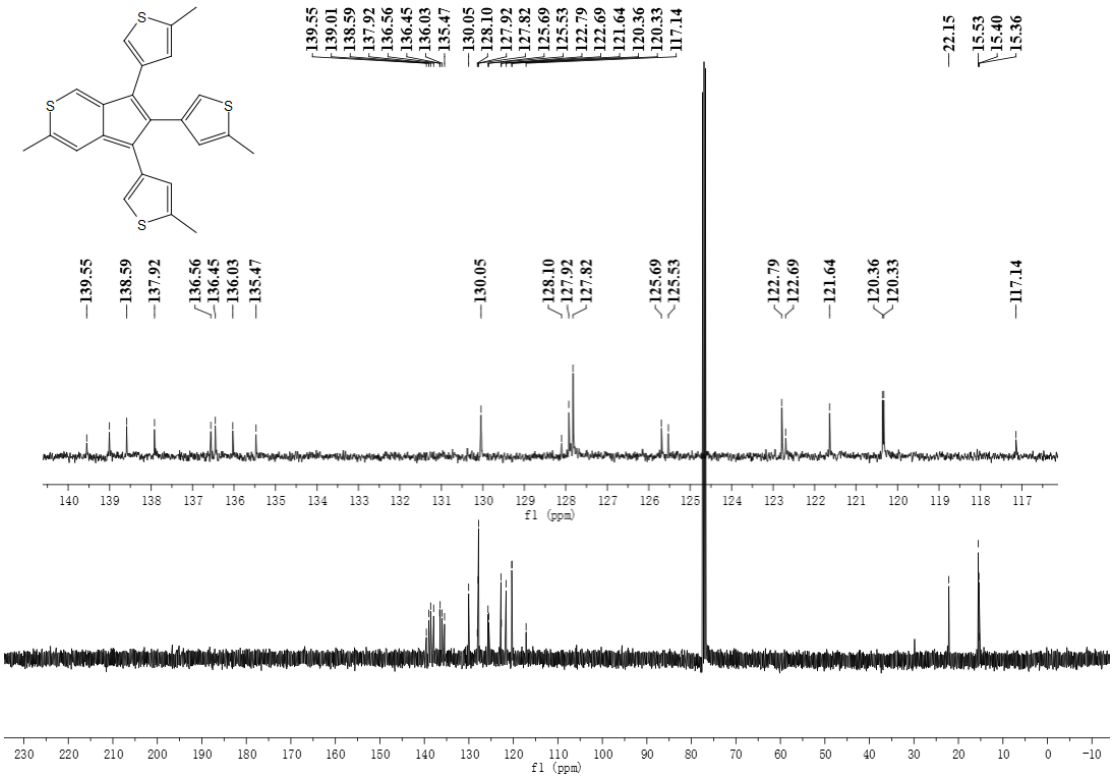

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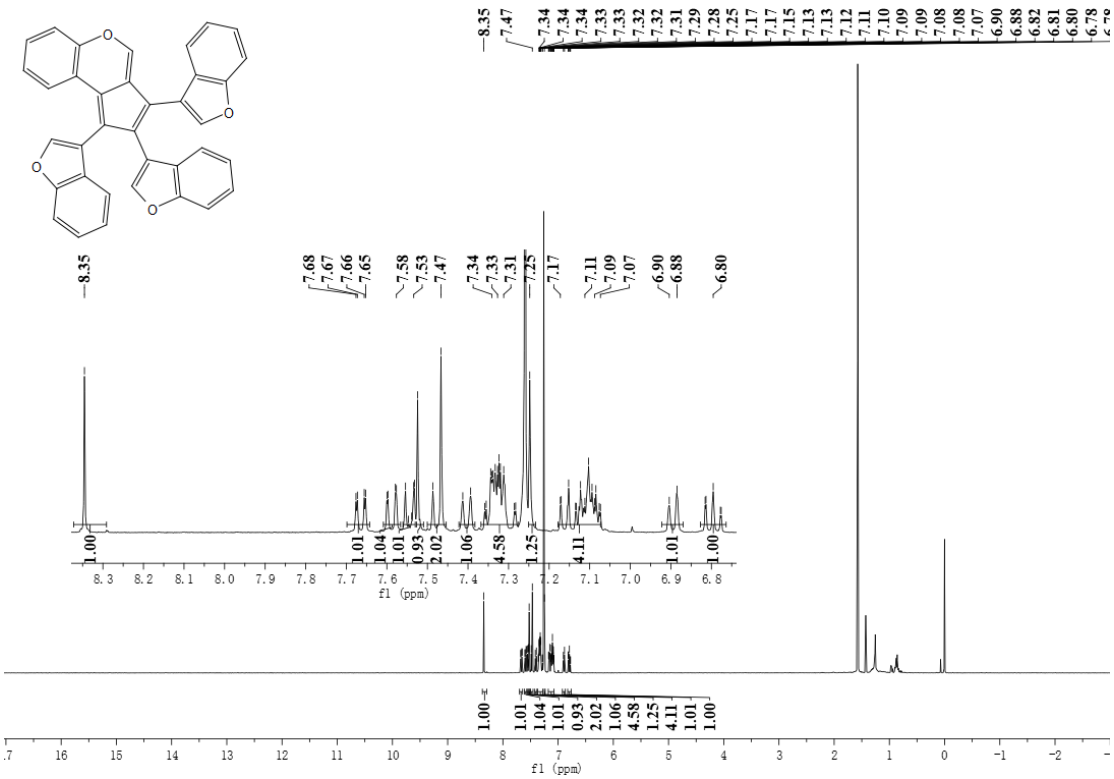

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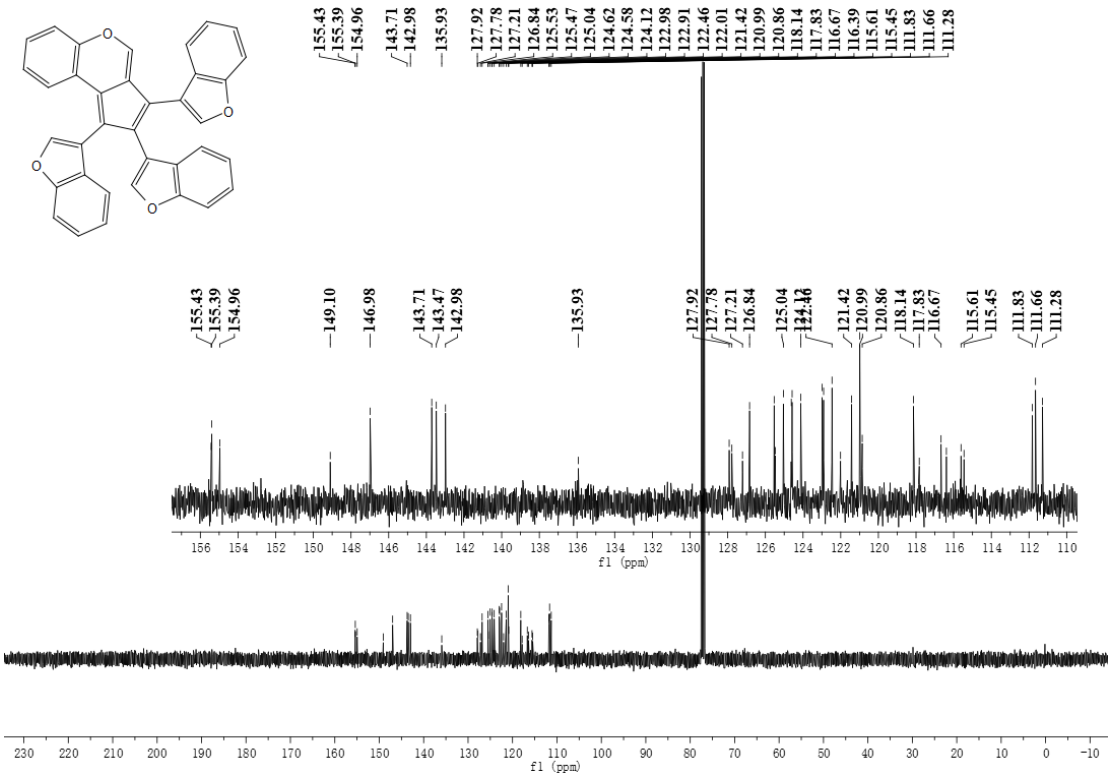

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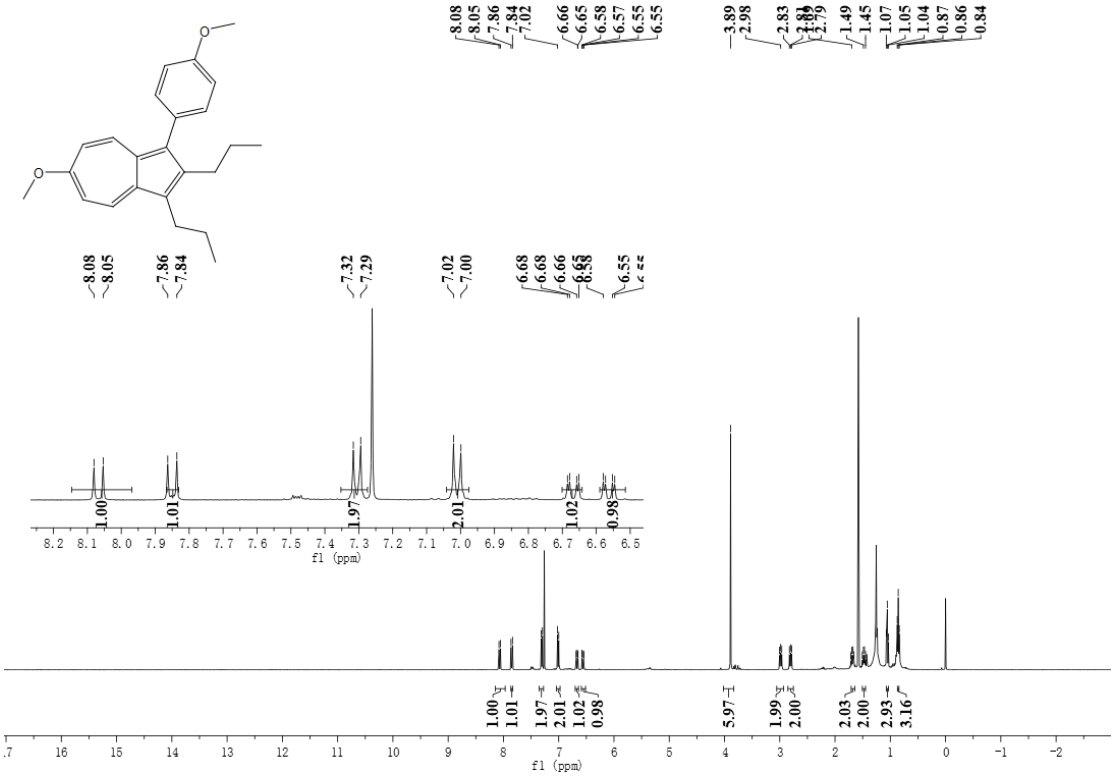
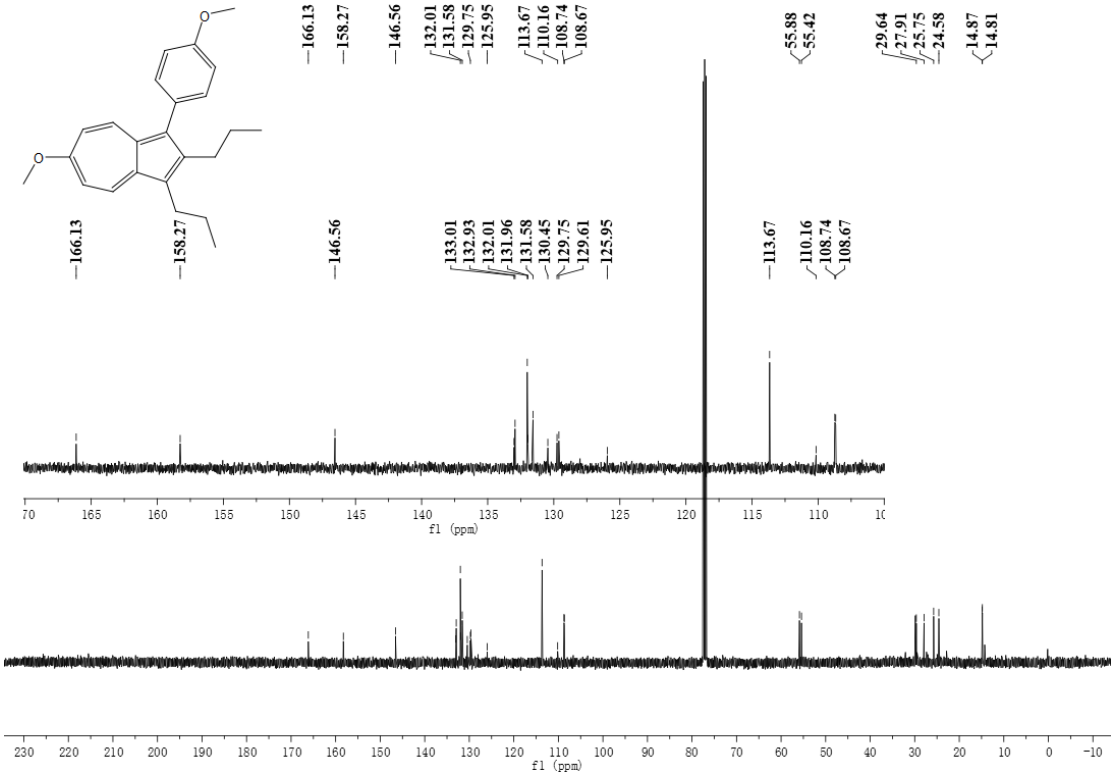
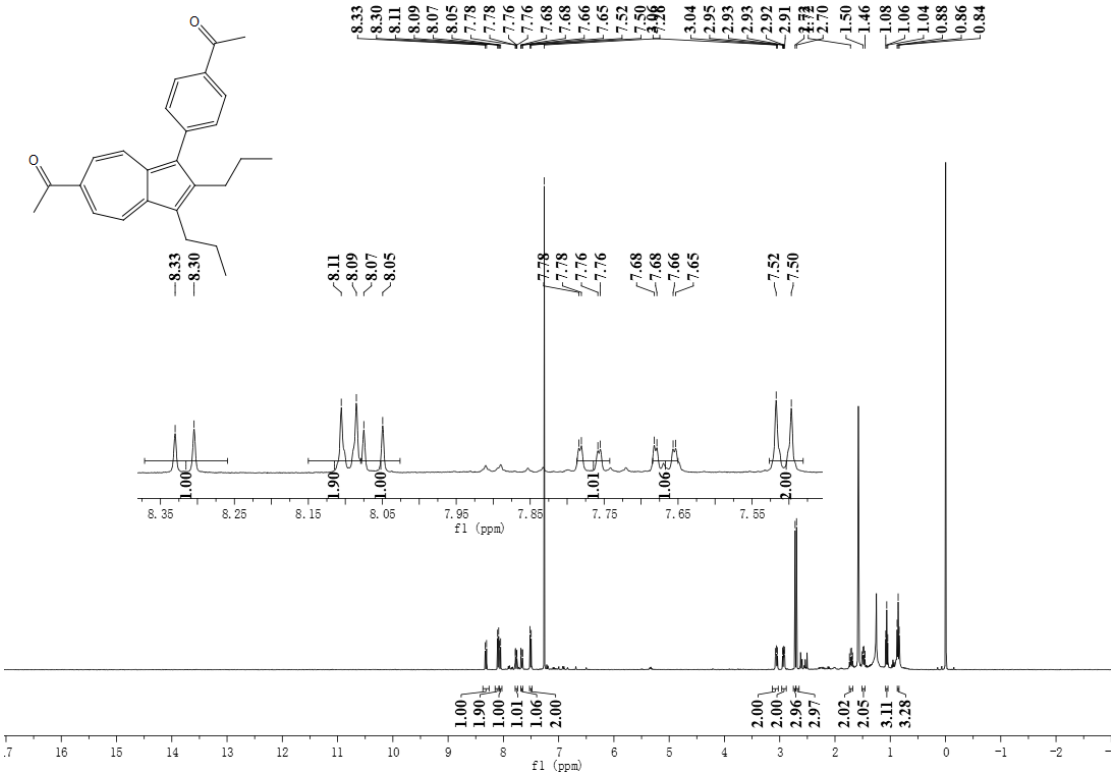


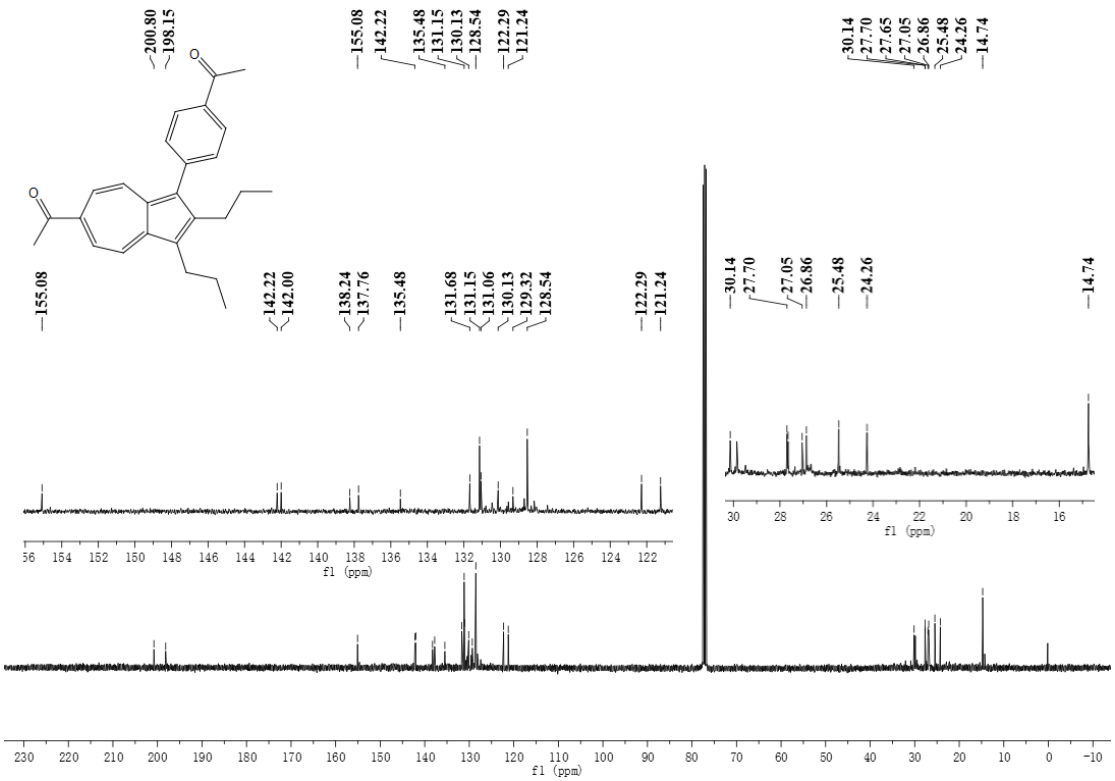
^{13}C NMR ($CDCl_3$, 400 MHz) spectrum of **4a**



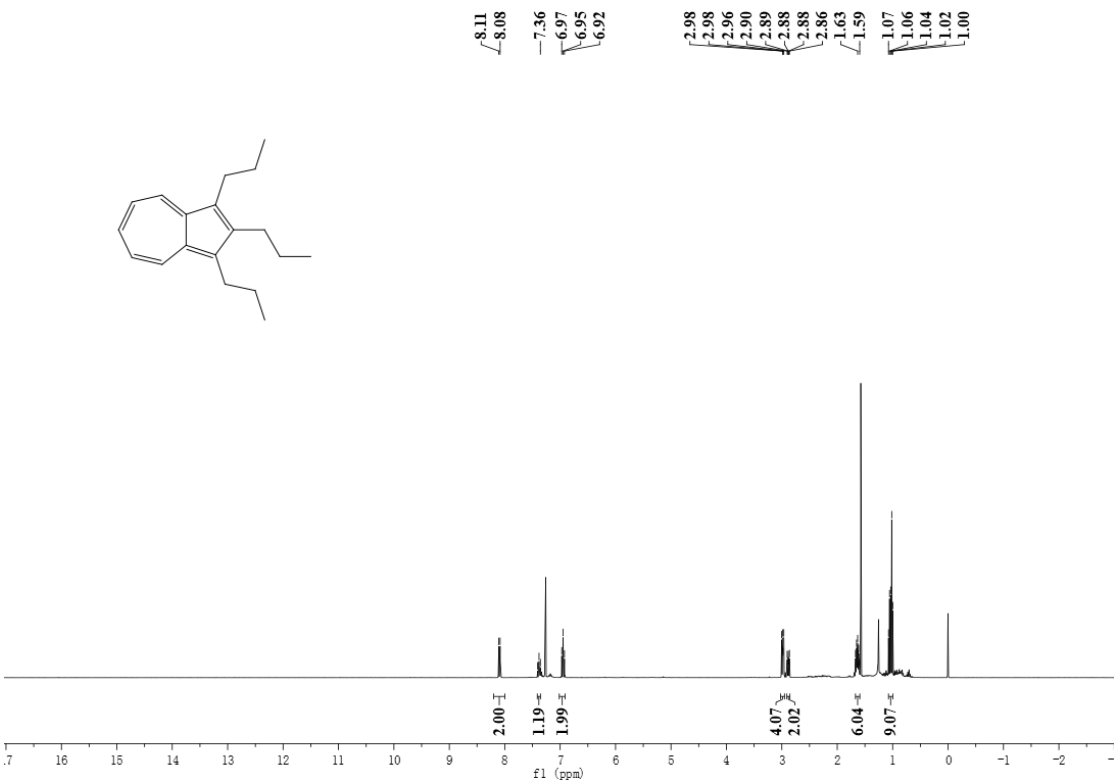
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **4b**



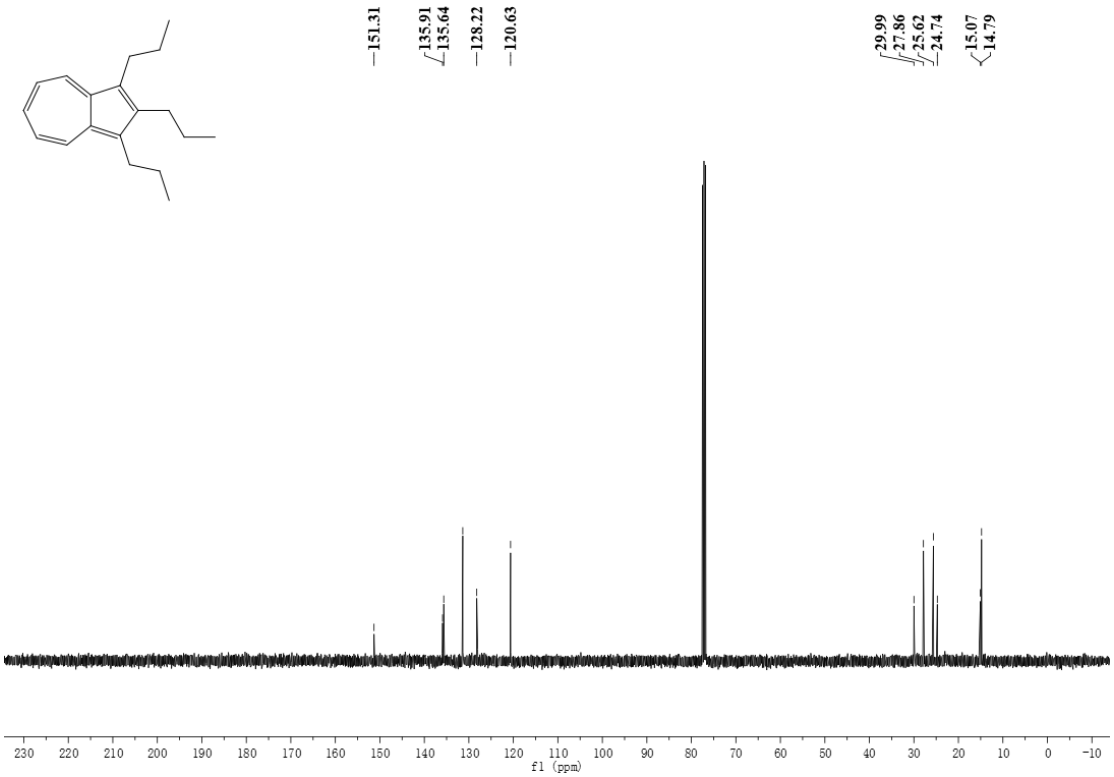
^{13}C NMR ($CDCl_3$, 400 MHz) spectrum of **4b**



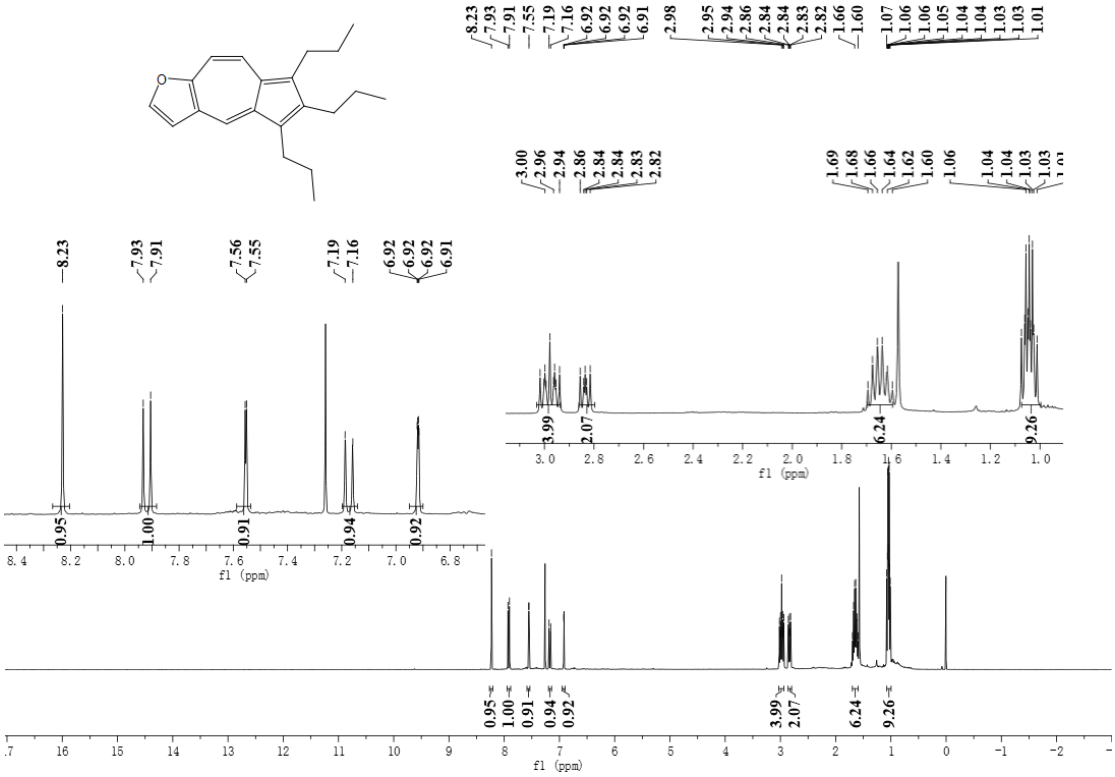
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **4c**



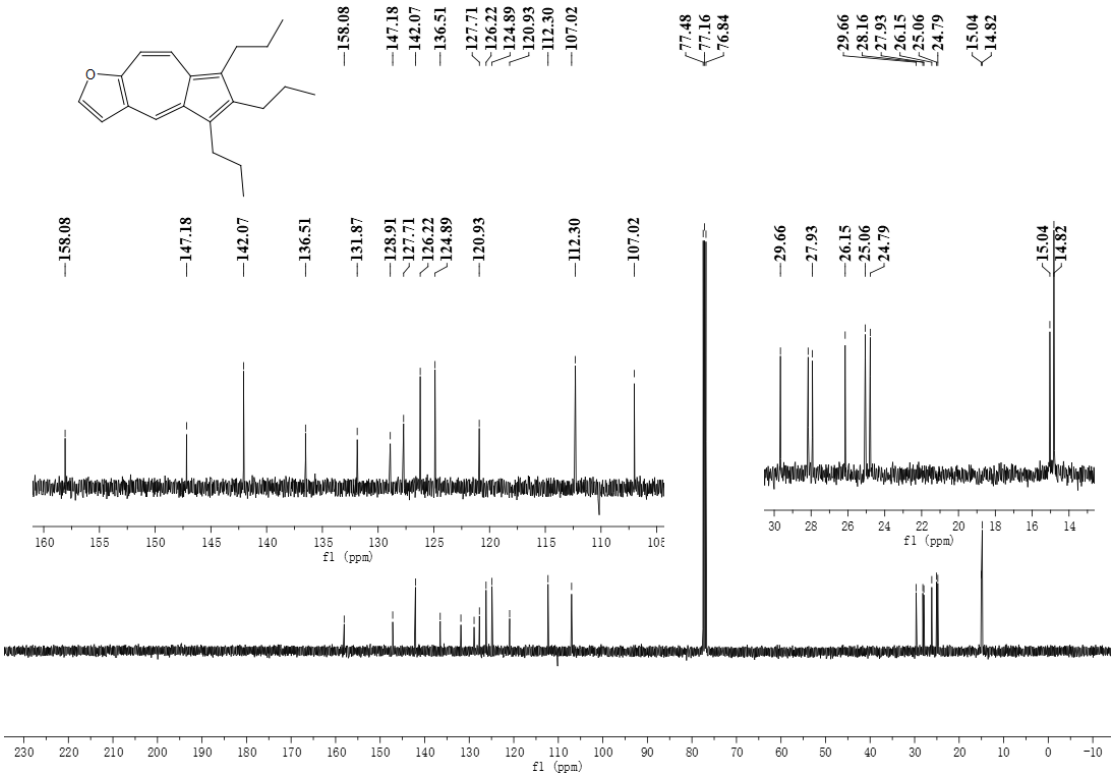
^{13}C NMR ($CDCl_3$, 400 MHz) spectrum of **4c**



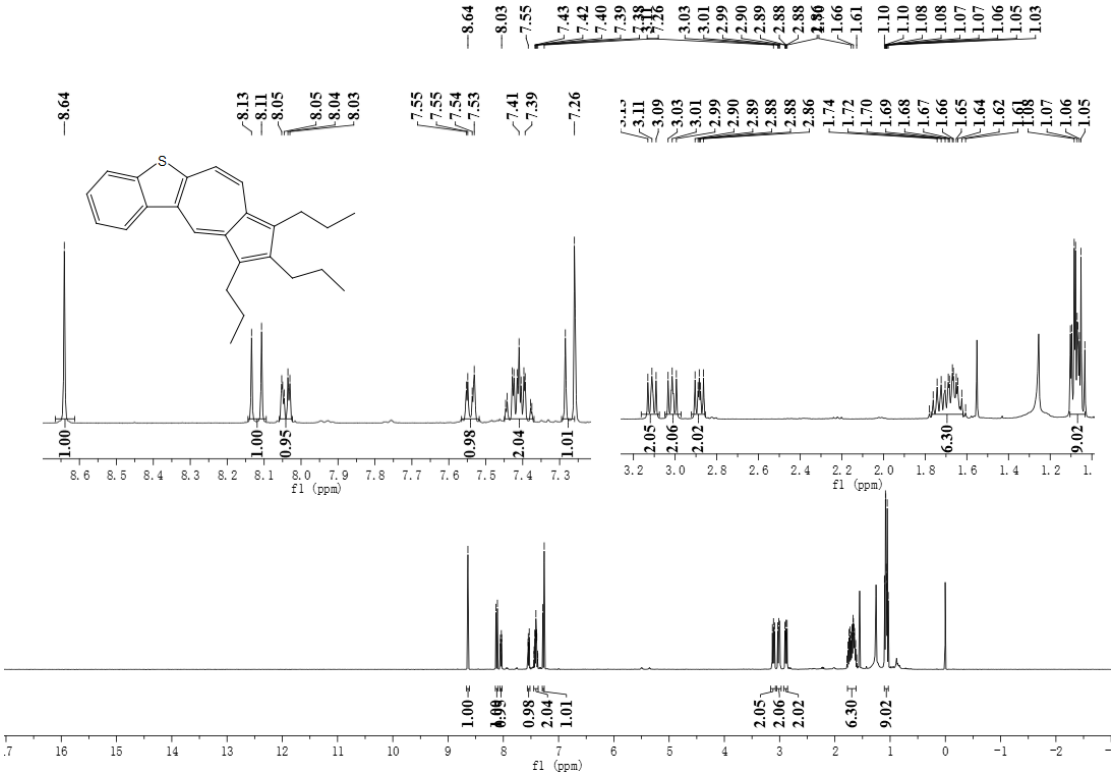
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **4d**



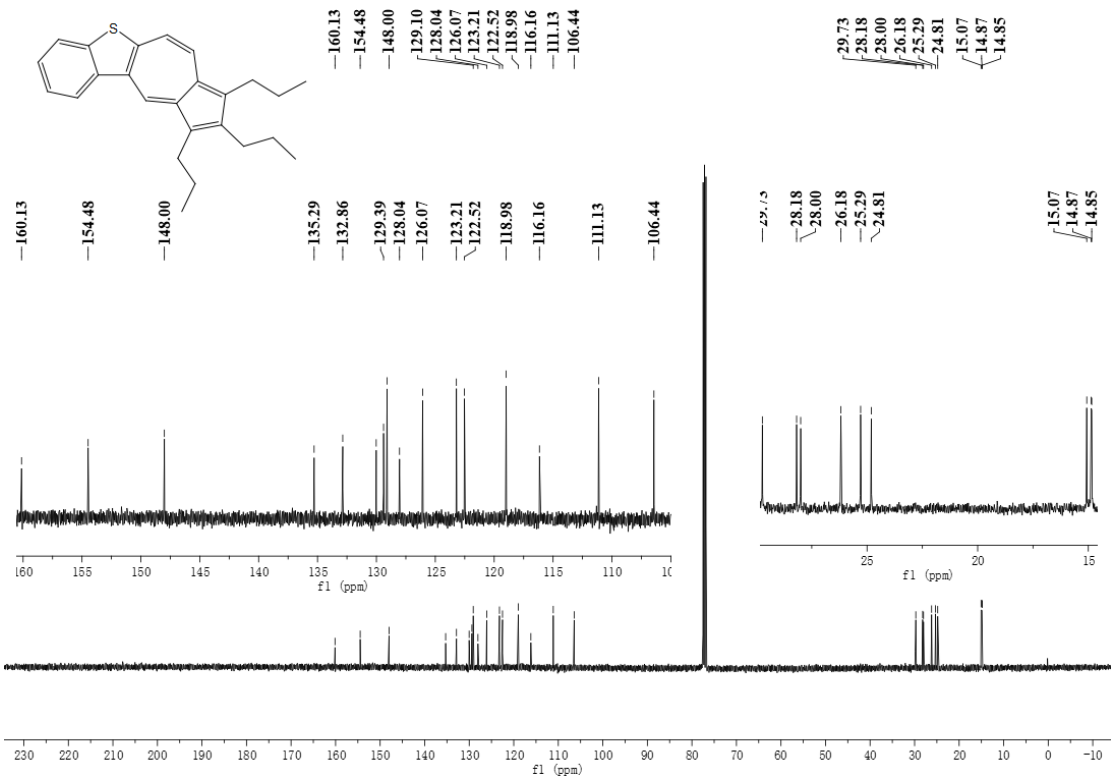
^{13}C NMR ($CDCl_3$, 400 MHz) spectrum of **4d**



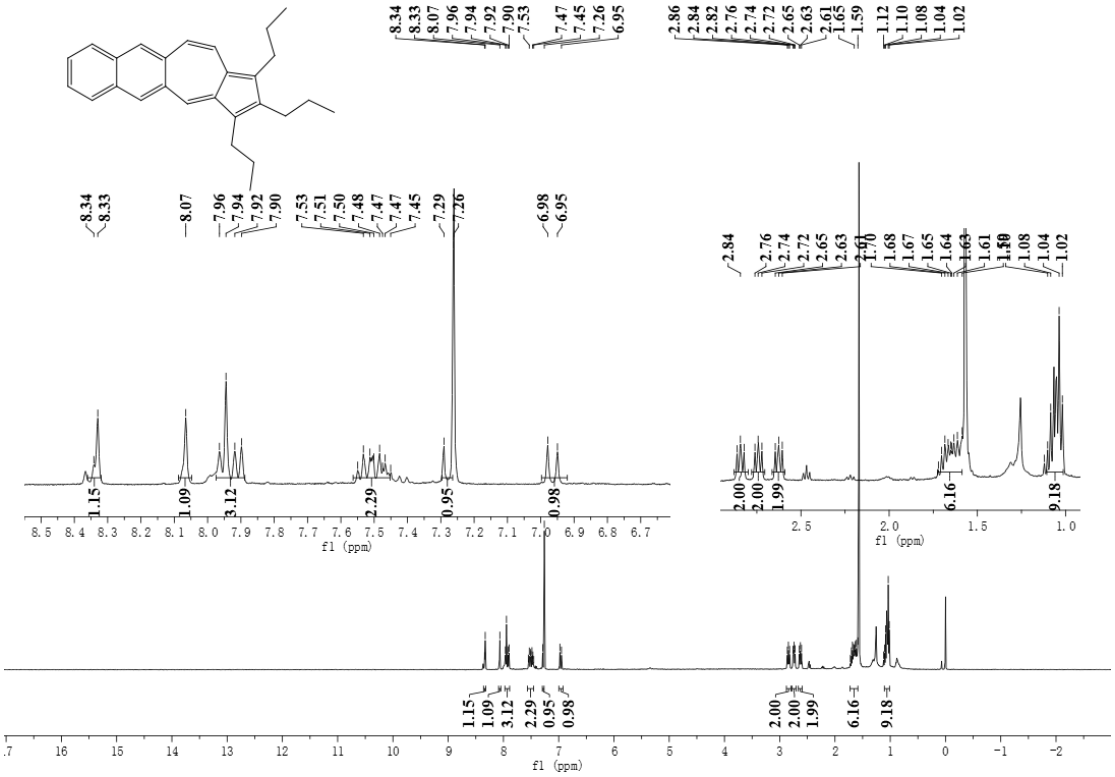
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **4e**



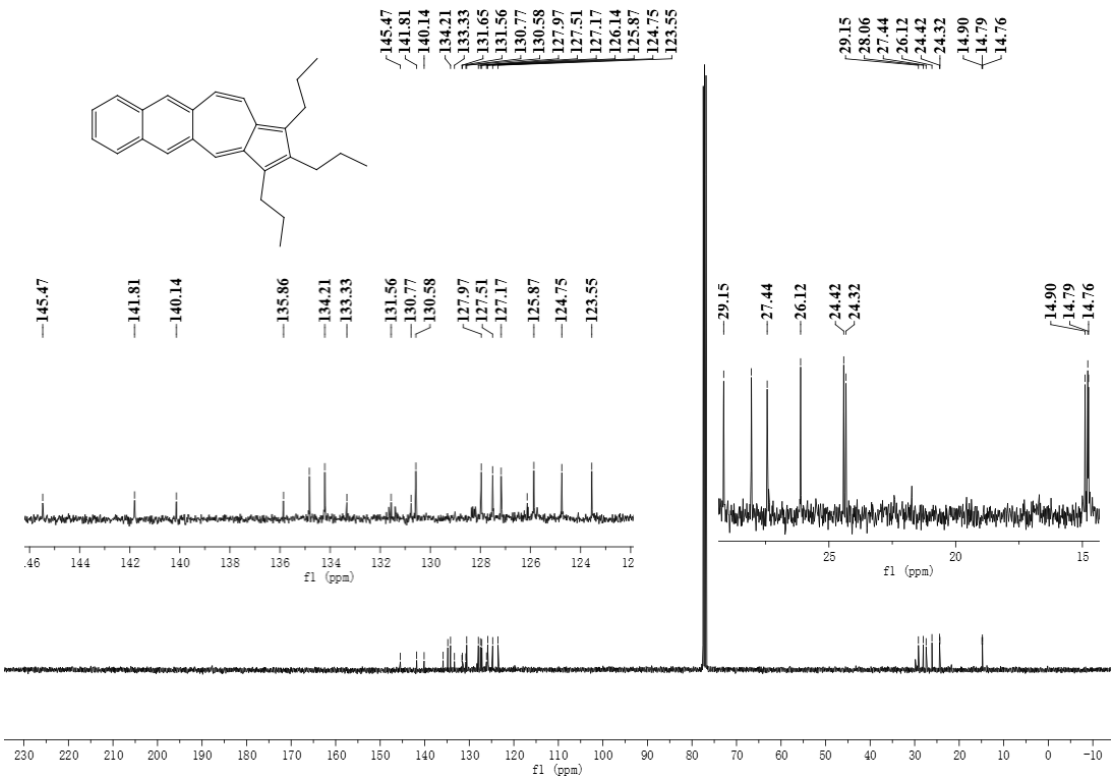
^{13}C NMR ($CDCl_3$, 400 MHz) spectrum of **4e**



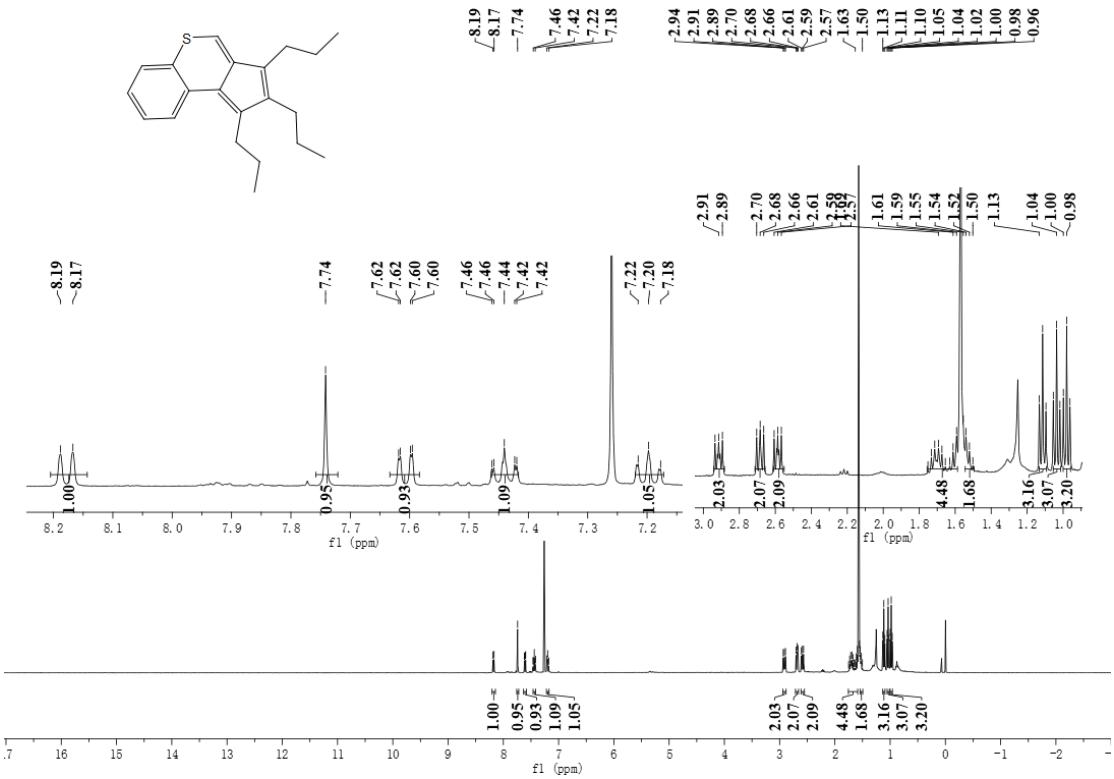
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **4f**



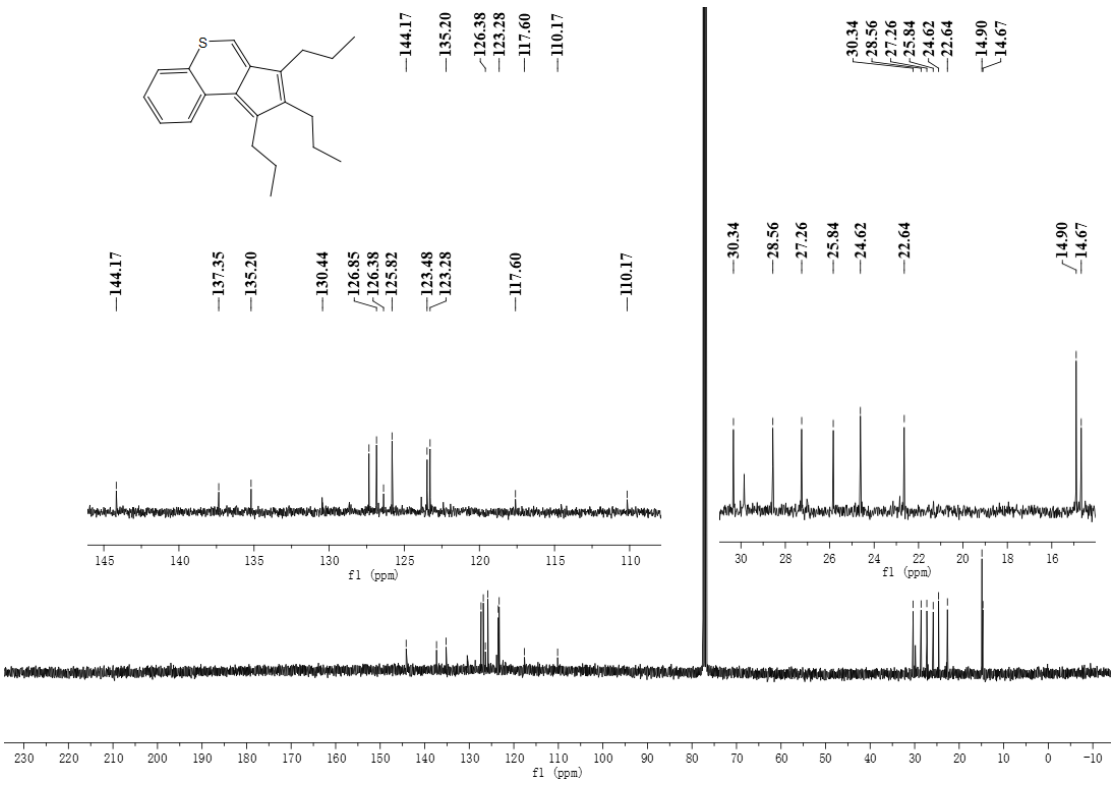
^{13}C NMR ($CDCl_3$, 400 MHz) spectrum of **4f**



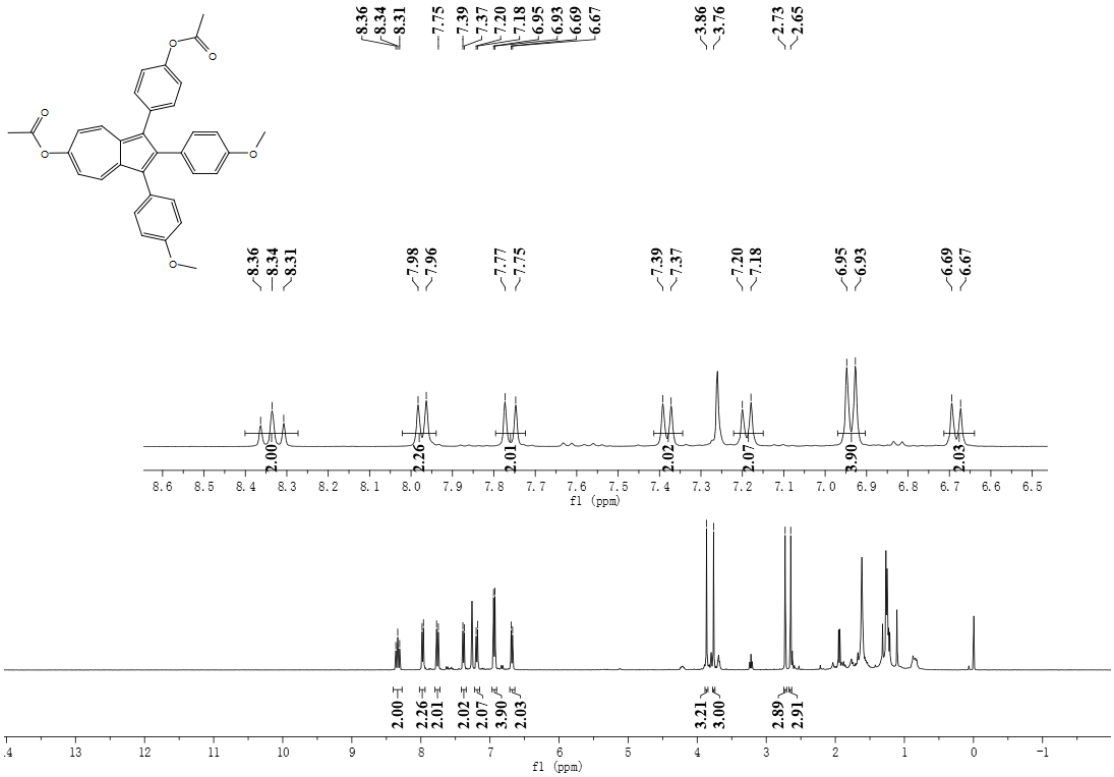
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **4g**



^{13}C NMR ($CDCl_3$, 400 MHz) spectrum of **4g**



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



^{13}C NMR ($CDCl_3$, 400 MHz) spectrum of **3d-1**