Title: Alumina-Mediated Soft Propargylic C-H Activation in Unactivated Alkynes

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General Information

All chemicals and solvents were purchased in reagent grade from commercial suppliers (Acros®, SigmaAldrich® or Fluka®, Fluorochem®, Merck®, ChemPur®) and used as received unless otherwise specified. Al_2O_3 (activated, neutral, for column chromatography, 50-200 micron, 185-225 m^2/g) was purchased from Acros Organics®.

Flash column chromatography was performed on Interchim PuriFlash 430 using flash grade silica gel from MacheryNagel 60 M (40-63 mm, deactivated).

NMR spectra were recorded on a Agilent Technologies 400 MHz VNMRS operating at 400 MHz (^{1}H NMR), 100 MHz (^{13}C NMR) and 377 (^{19}F NMR) or on a Agilent Technologies 500 MHz DD2, operating at 500 MHz (^{1}H NMR), 125 MHz (^{13}C NMR) and 470 MHz (^{19}F NMR)at room temperature. The signals were referenced to residual solvent peaks (in parts per million (ppm) ^{1}H: ^{1}H: $CDCl_3$, 7.27 ppm, ^{13}C: $CDCl_3$, 77.00 ppm). Coupling constants were assigned as observed. The obtained spectra were evaluated with the program MestReNova.

High resolution APPI MS spectra were recorded on a Bruker ESI TOF maXis4G instrument. The data was evaluated with the program Bruker Compass DataAnalysis 4.2.

TLC analyses were carried out with TLC sheets coated with silica gel with fluorescent indicator254 nm from Machery-Nagel (ALUGRAM® SIL G/UV254) and visualized via UV-light of 254 nm or 366 nm.

Optimization of alumina loading

Searching for the optimal conditions we have studied how the amount of alumina influence the outcome of the reaction. For this purpose, we have exposed 100 mg (0,77 mmol) of **1a** to different quantities of activated γ-Al_2O_3 (see Table S1) at 40°C for 6h. The optimal loading was found to be 10 g of γ-alumina (weight prior to activation) to 100mg of **1a**. We have additionally tried to scale the procedure up. Thus, we have successfully converted 1g of **1a** using 100 g of activated γ-Al_2O_3 in 82% yield at 40°C within 48h.

Table S1. Optimization of alumina loading.

m(Al_2O_3), g	Conversion of **1a**	**1**, yield%
0,5	0%	0%
5	35%	20%
10	**100%**	**87%**
20	100%	85%

Recycling of alumina

The exploited alumina (100g) can be easily recycled after successive washing with 250 ml of methanol, and 500 ml of water. The reactivation can be achieved in accordance with the general procedure. Thus, 10 g of alumina has been successfully recycled five times enabling the transformation of 100mg x 6 (0,6 g) of **1a**.

Table S2. Recycling of alumina.

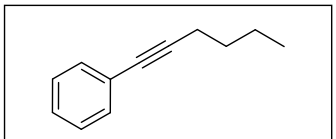
Cycle No	**1**, yield%
1	87%
2	82%
3	89%
4	77%
5	83%
6	81%

Synthesis of precursors.

1a and **19a** were purchased from SigmaAldrich®**, 1b** and **2a** were purchased from TCI®, **2b** was purchased from ABCR®.

Sonogashira reactions were carried out according to procedure described in (*46*).

Hex-1-yn-1-ylbenzene (3a).


Chemical Formula: $C_{12}H_{14}$
Molecular Weight: 158.2440

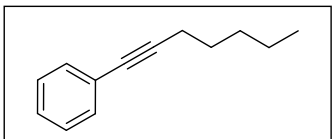
A mixture of 1-hexyne (0.34 mL, 3.0 mmol), $PdCl_2(PPh_3)_2$ (47.9 mg, 68.2 μmol), iodobenzene (0.40 mL, 3.6 mmol) in Et_3N (30 mL) was stirred at room temperature for 5 min under an argon atmosphere. And then, CuI (6.5 mg, 34 μmol) was added and stirred at the same temperature overnight. After the reaction mixture was concentrated and the residue was purified by chromatography on silica gel (hexane as eluent) to obtain hex-1-yn-1-ylbenzene as a colorless oil in 95% yield (450 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.40 (m, 2H), 7.32 – 7.25 (m, 3H), 2.42 (t, *J* = 7.1 Hz, 2H), 1.66 – 1.56 (m, 2H), 1.55 – 1.45 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 131.5, 128.1, 127.4, 124.1, 90.4, 80.5, 30.9, 22.0, 19.1, 13.6.

The spectroscopic data were consistent with previously reported(*47*).

Hept-1-yn-1-ylbenzene (4a).


Chemical Formula: $C_{13}H_{16}$
Molecular Weight: 172.2710

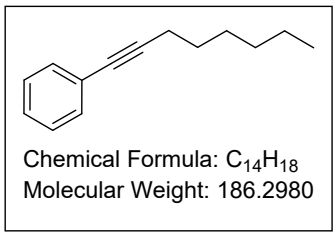
A mixture of 1-heptyne (0.39 mL, 3.0 mmol), $PdCl_2(PPh_3)_2$ (47.9 mg, 68.2 μmol), iodobenzene (0.40 mL, 3.6 mmol) in Et_3N (30 mL) was stirred at room temperature for 5 min under an argon atmosphere. And then, CuI (6.5 mg, 34 μmol) was added and stirred at the same temperature overnight. After the reaction mixture was concentrated and the residue was purified by chromatography on silica gel (hexane as eluent) to obtain hept-1-yn-1-ylbenzene as a yellow oil in 91% yield (470 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 – 7.36 (m, 2H), 7.34 – 7.23 (m, 3H), 2.41 (t, *J* = 7.1 Hz, 2H), 1.62 (p, *J* = 7.1 Hz, 2H), 1.50 – 1.41 (m, 2H), 1.37 (m, *J* = 14.6, 7.0 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 131.5, 128.2, 127.4, 124.1, 90.5, 80.5, 31.1, 28.5, 22.2, 19.4, 14.0.

The spectroscopic data were consistent with previously reported(*48*).

Oct-1-yn-1-ylbenzene (5a).



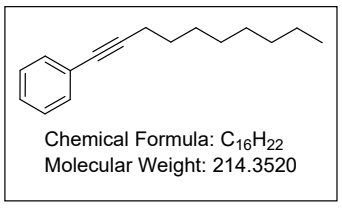
A mixture of 1-octyne (0.44 mL, 3.0 mmol), $PdCl_2(PPh_3)_2$ (47.9 mg, 68.2 μmol), iodobenzene (0.40 mL, 3.6 mmol) in Et_3N (30 mL) was stirred at room temperature for 5 min under an argon atmosphere. And then, CuI (6.5 mg, 34 μmol) was added and stirred at the same temperature overnight. After the reaction mixture was concentrated and the residue was purified by chromatography on silica gel (hexane as eluent) to obtain oct-1-yn-1-ylbenzene as a yellow oil in 84% yield (468 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.40 (m, 2H), 7.32 – 7.24 (m, 3H), 2.42 (t, *J* = 7.1 Hz, 2H), 1.66 – 1.59 (m, 2H), 1.53 – 1.45 (m, 2H), 1.39 – 1.31 (m, 4H), 0.95 – 0.90 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 131.5, 128.4, 127.4, 124.1, 90.4, 80.6, 31.4, 28.7, 28.6, 22.6, 19.4, 14.0.

The spectroscopic data were consistent with previously reported(*49*).

Dec-1-yn-1-ylbenzene (6a).



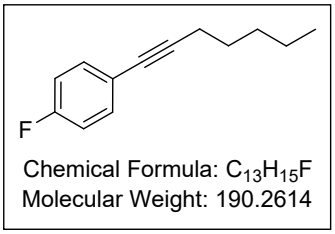
A mixture of 1-decyne (0.54 mL, 3.0 mmol), $PdCl_2(PPh_3)_2$ (47.9 mg, 68.2 μmol), iodobenzene (0.40 mL, 3.6 mmol) in Et_3N (30 mL) was stirred at room temperature for 5 min under an argon atmosphere. And then, CuI (6.5 mg, 34 μmol) was added and stirred at the same temperature overnight. After the reaction mixture was concentrated and the residue was purified by chromatography on silica gel (hexane as eluent) to obtain odec-1-yn-1-ylbenzene as a yellow oil in 78% yield (500 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 – 7.38 (m, 2H), 7.31 – 7.23 (m, 3H), 2.42 (t, *J* = 7.1 Hz, 2H), 1.62 (p, *J* = 7.2 Hz, 2H), 1.50 – 1.43 (m, 2H), 1.31 (dd, *J* = 15.1, 5.7 Hz, 10H), 0.91 (t, *J* = 6.7 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 131.5, 128.2, 127.4, 124.2, 90.5, 80.6, 31.9, 29.2, 29.1, 29.0, 28.8, 22.7, 19.4, 14.1.

The spectroscopic data were consistent with previously reported(*50*).

1-fluoro-4-(hex-1-yn-1-yl)benzene (7a).



Chemical Formula: $C_{13}H_{15}F$
Molecular Weight: 190.2614

A mixture of 1-hexyne (0.34 mL, 3.0 mmol), $PdCl_2(PPh_3)_2$ (47.9 mg, 68.2 μmol), 1-iodonaphtalene (790 mg, 3.6 mmol) in Et_3N (30 mL) was stirred at room temperature for 5 min under an argon atmosphere. And then, CuI (6.5 mg, 34 μmol) was added and stirred at the same temperature overnight. After the reaction mixture was concentrated and the residue was purified by chromatography on silica gel (hexane as eluent) to obtain 1-fluoro-4-(hex-1-yn-1-yl)benzene as a colorless oil in 90% yield (475 mg).

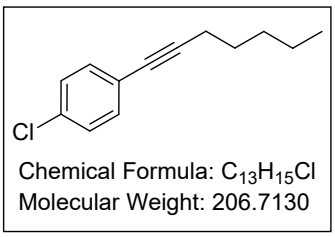
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.32 (m, 2H), 7.04 – 6.88 (m, 2H), 2.40 (t, *J* = 7.1 Hz, 2H), 1.63 – 1.55 (m, 2H), 1.54 – 1.46 (m, 2H), 0.96 (t, *J* = 7.3 Hz, 3H).

^{19}F NMR (470 MHz, $CDCl_3$) δ -112.52 (tt, *J* = 8.7, 5.4 Hz).

^{13}C NMR (126 MHz, $CDCl_3$) δ 162.0 (d, *J* = 248.0 Hz), 133.3 (d, *J* = 8.1 Hz), 120.2 (d, *J* = 3 Hz), 115.3 (d, *J* = 22.0 Hz), 90.0, 79.5, 30.8, 22.0, 19.0, 13.6.

The spectroscopic data were consistent with previously reported(*51*).

1-chloro-4-(hex-1-yn-1-yl)benzene (8a).



Chemical Formula: $C_{13}H_{15}Cl$
Molecular Weight: 206.7130

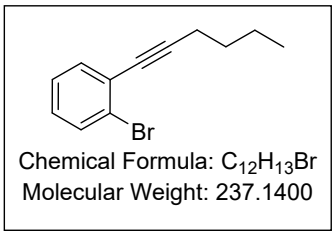
A mixture of 1-hexyne (0.34 mL, 3.0 mmol), $PdCl_2(PPh_3)_2$ (47.9 mg, 68.2 μmol), 1-iodonaphtalene (847 mg, 3.6 mmol) in Et_3N (30 mL) was stirred at room temperature for 5 min under an argon atmosphere. And then, CuI (6.5 mg, 34 μmol) was added and stirred at the same temperature overnight. After the reaction mixture was concentrated and the residue was purified by chromatography on silica gel (hexane as eluent) to obtain 1-chloro-4-(hex-1-yn-1-yl)benzene as a colorless oil in 94% yield (540mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (d, *J* = 8.5 Hz, 2H), 7.25 (d, *J* = 8.5 Hz, 2H), 2.40 (t, *J* = 7.1 Hz, 2H), 1.59 (p, *J* = 7.0 Hz, 2H), 1.48 (dq, *J* = 14.3, 7.2 Hz, 1H), 0.95 (t, *J* = 7.3 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 133.4, 132.7, 128.4, 122.6, 91.5, 79.5, 30.7, 22.0, 19.1, 13.6.

The spectroscopic data were consistent with previously reported(*52*).

1-bromo-2-(hex-1-yn-1-yl)benzene (9a).



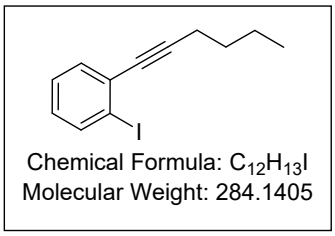
A mixture of 1-hexyne (0.34 mL, 3.0 mmol), $PdCl_2(PPh_3)_2$ (47.9 mg, 68.2 μmol), 2-bromoiodobenzene (1.02 g, 3.6 mmol) in Et_3N (30 mL) was stirred at room temperature for 5 min under an argon atmosphere. And then, CuI (6.5 mg, 34 μmol) was added and stirred at the same temperature overnight. After the reaction mixture was concentrated and the residue was purified by chromatography on silica gel (hexane as eluent) to obtain 1-bromo-2-(hex-1-yn-1-yl)benzene as a yellow oil in 86% yield (611 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 8.1, 0.9 Hz, 1H), 7.43 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.22 (td, *J* = 7.6, 1.1 Hz, 1H), 7.15 – 7.08 (m, 1H), 2.48 (t, *J* = 7.0 Hz, 2H), 1.69 – 1.60 (m, 2H), 1.60 – 1.49 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 133.3, 132.2, 128.6, 126.8, 126.1, 125.4, 95.6, 79.3, 30.6, 22.0, 19.2, 13.5.

The spectroscopic data were consistent with previously reported(*53*).

1-(hex-1-yn-1-yl)-2-iodobenzene (10a).



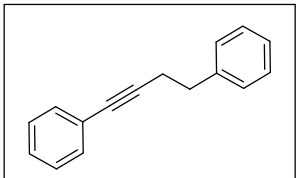
A mixture of 1-hexyne (0.34 mL, 3.0 mmol), $PdCl_2(PPh_3)_2$ (47.9 mg, 68.2 μmol), 1,2-diiodobenzene (1.17 g, 3.6 mmol) in Et_3N (30 mL) was stirred at room temperature for 5 min under an argon atmosphere. And then, CuI (6.5 mg, 34 μmol) was added and stirred at the same temperature overnight. After the reaction mixture was concentrated and the residue was purified by chromatography on silica gel (hexane as eluent) to obtain 1-(hex-1-yn-1-yl)-2-iodobenzene as a yellow oil in 56% yield (480 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.0 Hz, 1H), 7.40 (dd, *J* = 7.7, 1.6 Hz, 21H), 7.26 (t, *J* = 8.1 Hz, 1H), 6.98 – 6.89 (m, 1H), 2.48 (t, *J* = 7.0 Hz, 2H), 1.69 – 1.61 (m, 2H), 1.55 (dq, *J* = 16.1, 9.0, 8.1 Hz, 2H), 0.97 (t, *J* = 7.3 Hz, 4H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.5, 132.4, 130.5, 128.6, 127.6, 101.0, 94.8, 82.9, 30.6, 22.0, 19.2, 13.6.

The spectroscopic data were consistent with previously reported(*54*).

But-1-yne-1,4-diyldibenzene (11a).


Chemical Formula: $C_{16}H_{14}$
Molecular Weight: 206.2880

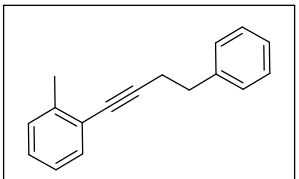
A mixture of but-3-yn-1-ylbenzene (390 mg, 3.0 mmol), $PdCl_2(PPh_3)_2$ (47.9 mg, 68.2 μmol), iodobenzene (0.40 mL, 3.6 mmol) in Et_3N (30 mL) was stirred at room temperature for 5 min under an argon atmosphere. And then, CuI (6.5 mg, 34 μmol) was added and stirred at the same temperature overnight. After the reaction mixture was concentrated and the residue was purified by chromatography on silica gel (hexane as eluent) to obtain but-1-yne-1,4-diyldibenzene as a colorless oil in 84% yield (520 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.39 (m, 2H), 7.38 – 7.33 (m, 2H), 7.33 – 7.29 (m, 5H), 7.29 – 7.24 (m, 1H), 2.96 (t, *J* = 7.5 Hz, 2H), 2.73 (t, *J* = 7.5 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 140.7, 131.5, 128.5, 128.4, 128.2, 127.6, 126.3, 123.8, 89.5, 81.3, 35.2, 21.7.

The spectroscopic data were consistent with previously reported(*55*).

1-methyl-2-(4-phenylbut-3-yn-1-yl)benzene (12a).

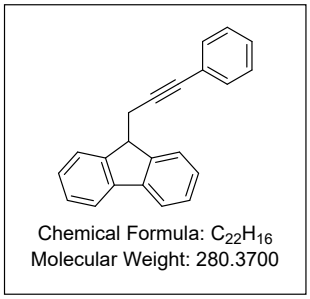

Chemical Formula: $C_{17}H_{16}$
Molecular Weight: 220.3150

A mixture of but-3-yn-1-ylbenzene (390 mg, 3.0 mmol), $PdCl_2(PPh_3)_2$ (47.9 mg, 68.2 μmol), 1-iodo-2-methylbenzene (776 mg, 3.6 mmol) in Et_3N (30 mL) was stirred at room temperature for 5 min under an argon atmosphere. And then, CuI (6.5 mg, 34 μmol) was added and stirred at the same temperature overnight. After the reaction mixture was concentrated and the residue was purified by chromatography on silica gel (hexane as eluent) to obtain 1-methyl-2-(4-phenylbut-3-yn-1-yl)benzene as a colorless oil in 80% yield (530 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.30 (m, 5H), 7.29 – 7.24 (m, 1H), 7.21 – 7.18 (m, 2H), 7.16 – 7.10 (m, 1H), 2.98 (t, *J* = 7.4 Hz, 2H), 2.79 (t, *J* = 7.4 Hz, 2H), 2.38 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 140.7, 140.0, 131.8, 129.3, 128.5, 128.3, 127.6, 126.3, 125.4, 123.6, 93.4, 80.2, 35.3, 21.7, 20.6.

The spectroscopic data were consistent with previously reported(*55*).


Chemical Formula: $C_{22}H_{16}$
Molecular Weight: 280.3700

9-(3-phenylprop-2-yn-1-yl)-9H-fluorene (13a).

13a was synthesized according to procedure described in (*56*).

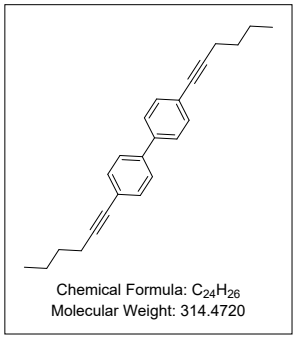
n-BuLi 2.5M in hexanes (1 ml, 2.5 mmol) was added dropwise over a solution of fluorene (400 mg, 2.4 mmol) in 20 ml of anhydrous THF at −80 °C in 100 mL screw-cap tube fitted with a septum under a nitrogen atmosphere. The mixture was stirred at −80 °C for 3 hours. Then, a solution of the 3-phenylpropargylchloride (360 mg, 2.4 mmol) in anhydrous THF was added dropwise and the mixture was allowed to warm to r.t. overnight. The reaction mixture was diluted with DCM and solvent was evaporated under reduced pressure. The crude residue was purified by column chromatography on silica gel with cyclohexane as eluent yielding 9-(3-phenylprop-2-yn-1-yl)-9H-fluorene as yellow solid in 37% yield (251 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.6 Hz, 4H), 7.48 – 7.41 (m, 4H), 7.35 (m, 5H), 4.18 (t, *J* = 7.3 Hz, 1H), 2.92 (d, *J* = 7.3 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 146.3, 140.9, 131.6, 128.3, 127.8, 127.5, 127.0, 124.7, 123.7, 119.9, 88.7, 81.2, 46.3, 24.5.

The spectroscopic data were consistent with previously reported(*56*).

4,4'-di(hex-1-yn-1-yl)-1,1'-biphenyl (14a).



A mixture of 1-hexyne (0.34 mL, 3.0 mmol), $PdCl_2(PPh_3)_2$ (47.9 mg, 68.2 μmol), 4,4'-di(hex-1-yn-1-yl)-1,1'-biphenyl (1.42 g, 3.6 mmol) in Et_3N (30 mL) was stirred at room temperature for 5 min under an argon atmosphere. And then, CuI (6.5 mg, 34 μmol) was added and stirred at the same temperature overnight. After the reaction mixture was concentrated and the residue was purified by chromatography on silica gel (hexane as eluent) to obtain 4,4'-di(hex-1-yn-1-yl)-1,1'-biphenyl as a colorless solid in 56% yield (630 mg).

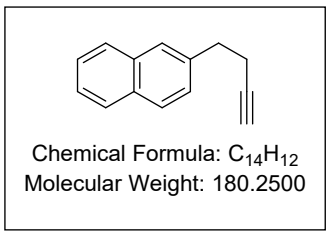
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.5 Hz, 4H), 7.46 (d, *J* = 8.5 Hz, 4H), 2.45 (t, *J* = 7.0 Hz, 4H), 1.74 – 1.55 (m, 4H), 1.58 – 1.40 (m, 4H), 0.98 (t, *J* = 7.3 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 139.4, 132.0, 126.6, 123.3, 91.3, 80.4, 30.8, 22.0, 19.2, 13.6.

HRMS (APPI; Toluene): Chemical Formula: $C_{24}H_{26}$, calc. 314.2030 found 314.2051.

15a-18a were synthesized according to procedure described in (*57*).

2-(but-3-yn-1-yl)naphthalene (15a).



To a solution of 1-triisopropylsilylprop-1-yne (1 g, 4.2 mmol) in THF (10 ml) was added *n*-BuLi (1.7 mL of 2.5 M in hexane, 4.2 mmol) at –78 °C dropwise over 5 min and stirred at this temperature for 2.5 h. Then, 2-(bromomethyl)naphthalene (890 mg, 4.1 mmol) in 5 mL of THF was added to the solution over 30 min at –78 °C. The cooling bath was removed, and the reaction temperature was allowed to raise to RT. After stirring the reaction at RT overnight, the solvent was evaporated under reduced pressure. The residue was purified by chromatography on silica gel (hexane as eluent) to obtain triisopropyl(4-(naphthalen-2-yl)but-1-yn-1-yl)silane as a colorless oil in 79% yield (1.09 g).

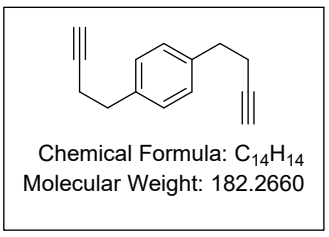
A 100 mL round bottom flask equipped with a magnetic stir bar and a condenser was charged with triisopropyl(4-(naphthalen-1-yl)but-1-yn-1-yl)silane (1 g,, 3.0 mmol) and TBAF (1.1 g, 4 mmol). After 10 ml of THF was added. The obtained mixture was stirred at room temperature overnight. After the completion of the reaction, the mixture was diluted with DCM (50 mL) and washed with H_2O (2x 50 mL). The organic layer was dried over $MgSO_4$. The solvent was evaporated yielding 2-(but-3-yn-1-yl)naphthalene as a colorless oil in quantitative yield (540 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 – 7.78 (m, 3H), 7.69 (s, 1H), 7.51 – 7.42 (m, 2H), 7.38 (dd, J = 8.4, 1.7 Hz, 1H), 3.04 (t, J = 7.5 Hz, 1H), 2.60 (td, J = 7.6, 2.6 Hz, 1H), 2.01 (t, J = 2.6 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.9, 133.5, 132.2, 128.0, 127.6, 127.5, 127.0, 126.6, 126.0, 125.4, 83.7, 69.0, 35.0, 20.5.

The spectroscopic data were consistent with previously reported(*58*).

1,4-di(but-3-yn-1-yl)benzene (16a).



To a solution of 1-triisopropylsilylprop-1-yne (1 g, 4.2 mmol) in THF (10 ml) was added *n*-BuLi (1.7 mL of 2.5 M in hexane, 4.2 mmol) at –78 °C dropwise over 5 min and stirred at this temperature for 2.5 h. Then, 1,4-bis(bromomethyl)benzene (526 mg, 2 mmol) in 10 mL of THF was added to the solution over 30 min at –78 °C. The cooling bath was removed, and the reaction temperature was allowed to raise to RT. After stirring the reaction at RT overnight, the solvent was evaporated under reduced pressure. The residue was purified by chromatography on silica gel (hexane as eluent) to obtain 1,4-bis(4-(triisopropylsilyl)but-3-yn-1-yl)benzene as a colorless oil in 66% yield (652 mg).

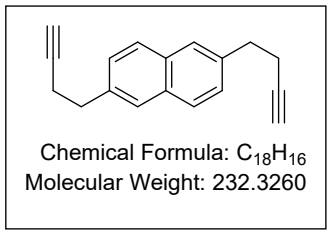
A 100 mL round bottom flask equipped with a magnetic stir bar and a condenser was charged with 1,4-bis(4-(triisopropylsilyl)but-3-yn-1-yl)benzene (650 mg,, 1.3 mmol) and TBAF (1.1 g, 4 mmol). After 10 ml of THF was added. The obtained mixture was stirred at room temperature overnight. After the completion of the reaction, the mixture was diluted with DCM (50 mL) and washed with H_2O (2x 50 mL). The organic layer was dried over $MgSO_4$. The solvent was evaporated yielding 1,4-di(but-3-yn-1-yl)benzene as a colorless oil in quantitative yield (240 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.16 (s, 4H), 2.83 (t, *J* = 7.6 Hz, 4H), 2.47 (td, *J* = 7.6, 2.6 Hz, 4H), 1.98 (t, *J* = 2.6 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.5, 128.4, 83.9, 68.8, 34.5, 20.5.

HRMS (m/z): $[M]^+$ calcd. for $C_{14}H_{14}$, 182.1091; found, 182.1099.

2,6-di(but-3-yn-1-yl)naphthalene (17a).



To a solution of 1-triisopropylsilylprop-1-yne (1 g, 4.2 mmol) in THF (10 ml) was added *n*-BuLi (1.7 mL of 2.5 M in hexane, 4.2 mmol) at –78 °C dropwise over 5 min and stirred at this temperature for 2.5 h. Then, 2,6-bis(bromomethyl)naphthalene (635 mg, 2 mmol) in 10 mL of THF was added to the solution over 30 min at –78 °C. The cooling bath was removed, and the reaction temperature was allowed to raise to RT. After stirring the reaction at RT overnight, the solvent was evaporated under reduced pressure. The residue was purified by chromatography on silica gel (hexane as eluent) to obtain 2,6-bis(4-(triisopropylsilyl)but-3-yn-1-yl)naphthalene as a colorless oil in 72% yield (783 mg).

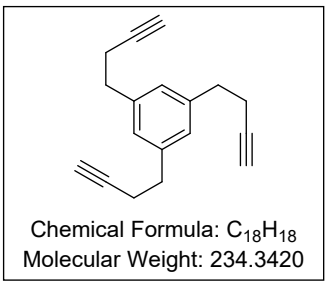
A 100 mL round bottom flask equipped with a magnetic stir bar and a condenser was charged with 2,6-bis(4-(triisopropylsilyl)but-3-yn-1-yl)naphthalene (780 mg, 1.45mmol) and TBAF (1.1 g, 4 mmol). After 10 ml of THF was added. The obtained mixture was stirred at room temperature overnight. After the completion of the reaction, the mixture was diluted with DCM (50 mL) and washed with H_2O (2x 50 mL). The organic layer was dried over $MgSO_4$. The solvent was evaporated yielding 2,6-di(but-3-yn-1-yl)naphthalene as a colorless oil in quantitative yield (330 mg).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.3 Hz, 2H), 7.63 (s, 2H), 7.34 (dd, *J* = 8.4, 1.3 Hz, 2H), 2.99 (t, *J* = 7.5 Hz, 4H), 2.56 (td, *J* = 7.5, 2.6 Hz, 4H), 2.00 (t, *J* = 2.6 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.4, 132.2, 127.6, 127.1, 126.3, 83.7, 69.0, 34.9, 20.4.

HRMS (m/z): $[M]^+$ calcd. for $C_{18}H_{16}$, 232.3255; found, 232.3270.

1,3,5-tri(but-3-yn-1-yl)benzene (18a).



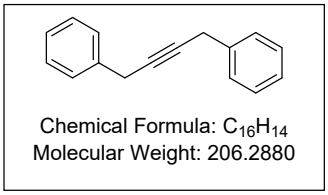
To a solution of 1-triisopropylsilylprop-1-yne (1 g, 4.2 mmol) in THF (10 ml) was added *n*-BuLi (1.7 mL of 2.5 M in hexane, 4.2 mmol) at –78 °C dropwise over 5 min and stirred at this temperature for 2.5 h. Then, 1,3,5-tris(bromomethyl)benzene (474 mg, 1.3 mmol) in 10 mL of THF was added to the solution over 30 min at –78 °C. The cooling bath was removed, and the reaction temperature was allowed to raise to RT. After stirring the reaction at RT overnight, the solvent was evaporated under reduced pressure. The residue was purified by chromatography on silica gel (hexane as eluent) to obtain 1,3,5-tris(4-(triisopropylsilyl)but-3-yn-1-yl)benzene as a colorless oil in 53% yield (485 mg).

A 100 mL round bottom flask equipped with a magnetic stir bar and a condenser was charged with 1,3,5-tris(4-(triisopropylsilyl)but-3-yn-1-yl)benzene (485 mg, 0.7 mmol) and TBAF (1.1 g, 4 mmol). After 10 ml of THF was added. The obtained mixture was stirred at room temperature overnight. After the completion of the reaction, the mixture was diluted with DCM (50 mL) and washed with H_2O (2x 50 mL). The organic layer was dried over $MgSO_4$. The solvent was evaporated yielding 1,3,5-tri(but-3-yn-1-yl)benzene as a colorless oil in quantitative yield (240 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96 (s, 3H), 2.83 (t, J = 7.6 Hz, 6H), 2.57 – 2.39 (m, 6H), 1.99 (t, J = 2.6 Hz, 6H).

HRMS (m/z): $[M]^+$ calcd. for $C_{18}H_{18}$, 234.1405; found, 234.1417.

1,4-diphenylbut-2-yne (19a).


Chemical Formula: $C_{16}H_{14}$
Molecular Weight: 206.2880

19a was synthesized according to modification of procedure described in (*59*).

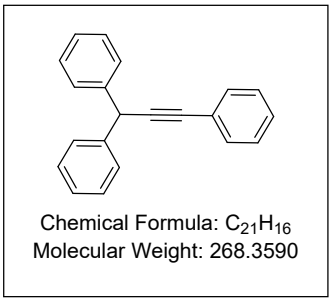
A 50 mL two-necked round bottom flask was charged with $PdCl_2(CH_3CN)_2$ (10 mg, 0.04 mmol) X-Phos (57 mg, 0.12 mmol), and Cs_2CO_3 (680 mg, 2.1 mmol. The flask was evacuated and back-filled with argon three times. The THF (10 ml) and benzyl bromide (340 mg, 2.0 mmol) were added. Benzylacetylene (300 mg, 2.60 mmol) was then added and the solution was heated to 60 °C and stirred at this temperature overnight. After cooling to r.t. the solvents were evaporated and the residue was purified by chromatography on silica gel (hexane as eluent) yielding 1,4-diphenylbut-2-yne as a colorless oil in 52% yield (214 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (dd, *J* = 5.2, 3.2 Hz, 4H), 7.40 – 7.34 (m, 4H), 7.31 – 7.25 (m, 2H), 3.70 (s, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.3, 128.4, 127.7, 126.4, 80.0, 25.2.

The spectroscopic data were consistent with previously reported(*60*).

Prop-2-yne-1,1,3-triyltribenzene (20a).


Chemical Formula: $C_{21}H_{16}$
Molecular Weight: 268.3590

20a was synthesized according to modification of procedure described in (*61*).

Diphenyl methanol (900 mg, 4.9 mmol) and phenylacetylene (5.9 mmol) were successively added to a round bottom flask, containing 1,2-dibromoethane (10 mL) and the stirred solution was treated with $Cu(OTf)_2$ (10 mg, 0.03 mmol). After heated the mixture at 120 ºC for 12 hours, the reaction was left to attain room temperature and concentrated under reduced pressure. The residue was purified by silica gel column chromatography, eluting with hexane yielding. prop-2-yne-1,1,3-triyltribenzene as yellow semisolid in 35% yield (460 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.61 (m, 6H), 7.52 – 7.35 (m, 6H), 5.39 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 141.7, 131.6, 128.5, 128.2, 127.9, 127.8, 126.8, 123.4, 90.2, 84.9, 43.7.

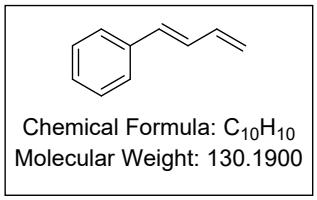
The spectroscopic data were consistent with previously reported(*62*).

Acetylene-diene rearrangement.

General procedure.

10 g of γ-Al_2O_3 was preactivated in glass ampule at 450°C under air conditions for 3 hours and then activated at 550°C under vacuum (10^{-2} mbar) for another 4 hours. Activated aluminium oxide was added to a Schlenk tube containing 100 mg of alkyne. All preparation steps were performed under argon atmosphere. The Schlenk tube was closed under vacuum and placed into water bath at 40°C or into oven at 60°C, 90°C or 190°C for 6 hours. After cooling to room temperature, the solid mixture was extracted with 70 ml of DCM. The organic solvent was evaporated under reduced pressure yielding the corresponding diene.

(E)-buta-1,3-dien-1-ylbenzene (1).

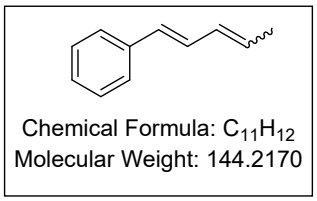


The compound was obtained according to the General Procedure at 40°C using but-3-yn-1-ylbenzene or but-1-yn-1-ylbenzene. Colorless oil. Yield 87 mg (87%) and 73 mg (73%) respectively.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (dd, *J* = 8.6, 0.9 Hz, 2H), 7.32 (t, *J* = 7.8 Hz, 2H), 7.23 (t, *J* = 7.3 Hz, 2H), 6.87 – 6.68 (m, 1H), 6.64 – 6.44 (m, 2H), 5.34 (d, *J* = 16.9 Hz, 1H), 5.18 (d, *J* = 10.8 Hz, 1H).

The spectroscopic data were consistent with previously reported(*63*).

Penta-1,3-dien-1-ylbenzene (2).

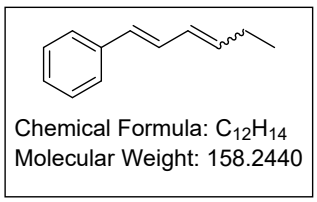


The compound was obtained according to the General Procedure at 40°C using pent-1-yn-1-ylbenzene or pent-4-yn-1-ylbenzene. Colorless oil. Yield 92 mg (92%) and 89 mg (89%) respectively.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.36 (m, 2H), 7.34 – 7.29 (m, 2H), 7.25 – 7.18 (m, 1H), 6.77 (dd, *J* = 15.7, 10.4 Hz, 1H), 6.45 (d, *J* = 15.7 Hz, 1H), 6.29 – 6.18 (m, 1H), 5.93 – 5.79 (m, 1H), 1.85 (dd, *J* = 6.8, 1.5 Hz, 3H).

The spectroscopic data were consistent with previously reported(*64*).

Hexa-1,3-dien-1-ylbenzene (3).

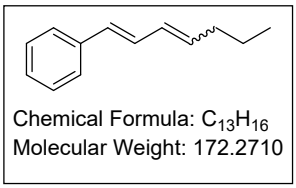


The compound was obtained according to the General Procedure 40°C using hex-1-yn-1-ylbenzene. Colorless oil. Yield 95 mg (95%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.9 Hz, 2H), 7.30 (t, *J* = 7.8 Hz, 2H), 7.23 – 7.17 (m, 1H), 6.76 (dd, *J* = 15.7, 10.4 Hz, 1H), 6.45 (d, *J* = 15.7 Hz, 1H), 6.26 – 6.17 (m, 1H), 5.92 – 5.84 (m, 1H), 2.27 – 2.08 (m, 2H), 1.06 (t, *J* = 7.5 Hz, 3H).

The spectroscopic data were consistent with previously reported(*31*).

Hepta-1,3-dien-1-yl)benzene (4).

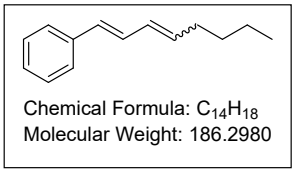


The compound was obtained according to the General Procedure at 40°C using hept-1-yn-1-ylbenzene. Colorless oil. Yield 93 mg (93%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.3 Hz, 2H), 7.32 (t, *J* = 7.7 Hz, 2H), 7.26 – 7.18 (m, 1H), 6.79 (dd, *J* = 15.7, 10.4 Hz, 1H), 6.47 (d, *J* = 15.7 Hz, 1H), 6.24 (dd, *J* = 15.5, 10.7 Hz, 1H), 5.86 (dt, *J* = 14.8, 7.1 Hz, 1H), 2.16 (q, *J* = 7.7 Hz, 2H), 1.56 – 1.40 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H).

The spectroscopic data were consistent with previously reported(*65*).

Octa-1,3-dien-1-ylbenzene (5).

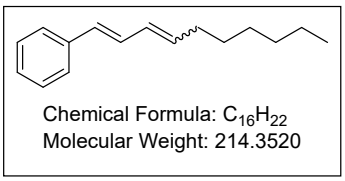


The compound was obtained according to the General Procedure at 40°C using octa-1-yn-1-ylbenzene. Colorless oil. Yield 88 mg (88%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.37 (m, 2H), 7.31 (t, *J* = 7.7 Hz, 2H), 7.24 – 7.18 (m, 1H), 6.78 (dd, *J* = 15.7, 10.4 Hz, 1H), 6.46 (d, *J* = 15.7 Hz, 1H), 6.23 (dd, *J* = 15.4, 10.1 Hz, 1H), 5.85 (dt, *J* = 14.7, 7.1 Hz, 1H), 2.17 (q, *J* = 7.2 Hz, 2H), 1.51 – 1.31 (m, 4H), 0.94 (t, *J* = 7.2 Hz, 3H).

The spectroscopic data were consistent with previously reported(*66*).

Deca-1,3-dien-1-ylbenzene (6).

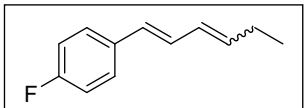


The compound was obtained according to the General Procedure at 40°C using deca-1-yn-1-ylbenzene. Colorless oil. Yield 87 mg (87%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.7 Hz, 2H), 7.22 (t, *J* = 7.3 Hz, 1H), 6.79 (dd, *J* = 15.7, 10.4 Hz, 1H), 6.48 (d, *J* = 15.7 Hz, 1H), 6.24 (dd, *J* = 15.0, 10.3 Hz, 1H), 5.87 (dt, *J* = 14.6, 7.0 Hz, 1H), 2.18 (d, *J* = 7.1 Hz, 2H), 1.45 – 1.24 (m, 8H), 0.94 (t, *J* = 6.9 Hz, 3H).

The spectroscopic data were consistent with previously reported(*67*).

1-fluoro-4-(hexa-1,3-dien-1-yl)benzene (7).



Chemical Formula: $C_{12}H_{13}F$
Molecular Weight: 176.2344

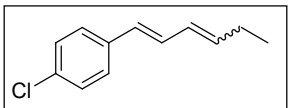
The compound was obtained according to the General Procedure at 40°C using 1-fluoro-4-(hex-1-yn-1-yl)benzene. Colorless oil. Yield 97 mg (97%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 8.7, 5.5 Hz, 2H), 6.99 (t, *J* = 8.7 Hz, 2H), 6.67 (dd, *J* = 15.7, 10.4 Hz, 1H), 6.41 (d, *J* = 15.7 Hz, 1H), 6.19 (dd, *J* = 15.4, 10.1 Hz, 1H), 5.93 – 5.81 (m, 1H), 2.17 (p, *J* = 7.0, 6.6 Hz, 2H), 1.06 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 162.0 (d, *J* = 246.5 Hz), 137.4 (d, *J* = 1.0 Hz), 133.9 (d, *J* = 3.4 Hz), 129.4, 129.3 (d, *J* = 2.4 Hz), 128.7 (d, *J* = 0.8 Hz), 127.5 (d, *J* = 7.9 Hz), 115.4 (d, *J* = 21.6 Hz), 25.8, 13.5.

HRMS (APPI; Toluene): Chemical Formula: $C_{12}H_{13}F$, calc. 176.0996 found 176.1009.

1-chloro-4-(hexa-1,3-dien-1-yl)benzene (8).



Chemical Formula: $C_{12}H_{13}Cl$
Molecular Weight: 192.6860

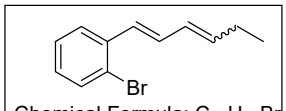
The compound was obtained according to the General Procedure at 40°C using 1-chloro-4-(hex-1-yn-1-yl)benzene. Colorless oil. Yield 74 mg (74%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.6 Hz, 2H), 7.26 (d, *J* = 8.7 Hz, 2H), 6.73 (dd, *J* = 15.7, 10.4 Hz, 1H), 6.39 (d, *J* = 15.7 Hz, 1H), 6.20 (dd, *J* = 15.1, 10.4 Hz, 1H), 5.97 – 5.83 (m, 1H), 2.18 (p, *J* = 7.1 Hz, 2H), 1.06 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.1, 136.2, 132.5, 130.1, 129.3, 128.7, 128.6, 127.2, 25.9, 13.5.

HRMS (APPI; Toluene): Chemical Formula: $C_{12}H_{13}Cl$, calc. 192.0701 found 192.0733.

Hexa-1,3-dien-1-yl-2-bromobenzene (9).



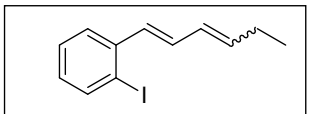
Chemical Formula: $C_{12}H_{13}Br$
Molecular Weight: 237.1400

The compound was obtained according to the General Procedure at 40°C using 1-(hex-1-yn-1-yl)-2-bromobenzene. Colorless oil. Yield 84 mg (84%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 – 7.50 (m, 2H), 7.29 – 7.23 (m, 1H), 7.09 – 7.03 (m, 1H), 6.80 (d, *J* = 15.6 Hz, 1H), 6.70 (dd, *J* = 15.6, 10.2 Hz, 1H), 6.35 – 6.25 (m, 1H), 5.97 – 5.87 (m, 1H), 2.27 – 2.11 (m, 2H), 1.07 (t, *J* = 7.5 Hz, 3H).

The spectroscopic data were consistent with previously reported(31).

Hexa-1,3-dien-1-yl-2-iodobenzene (10).

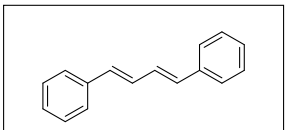

Chemical Formula: $C_{12}H_{13}I$
Molecular Weight: 284.1405

The compound was obtained according to the General Procedure at 40°C using 1-(hex-1-yn-1-yl)-2-iodobenzene. Yellow oil**.** Yield 82 mg (82%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.50 (d, *J* = 9.4 Hz, 1H), 7.32 – 7.24 (m, 2H), 6.89 (td, *J* = 7.7, 1.6 Hz, 1H), 6.68 – 6.58 (m, 2H), 6.35 – 6.25 (m, 1H), 5.93 (dt, *J* = 15.2, 6.6 Hz, 1H), 2.19 (p, *J* = 7.5 Hz, 2H), 1.07 (t, *J* = 7.5 Hz, 2H).

The spectroscopic data were consistent with previously reported(*31*).

(1E,3E)-1,4-diphenylbuta-1,3-diene (11).

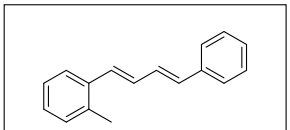

Chemical Formula: $C_{16}H_{14}$
Molecular Weight: 206.2880

The compound was obtained according to the General Procedure at 40°C using but-1-yne-1,4-diyldibenzene or 1,4-diphenylbut-2-yne. Colorless oil. Yield 91 mg (91%) or 88 mg (88%) respectively.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 – 7.45 (m, 4H), 7.36 (t, *J* = 7.7 Hz, 4H), 7.31 – 7.23 (m, 2H), 7.03 – 6.93 (m, 2H), 6.75 – 6.64 (m, 2H).

The spectroscopic data were consistent with previously reported(*68*).

1-methyl-2-((1E,3E)-4-phenylbuta-1,3-dien-1-yl)benzene (12).


Chemical Formula: $C_{17}H_{16}$
Molecular Weight: 220.3150

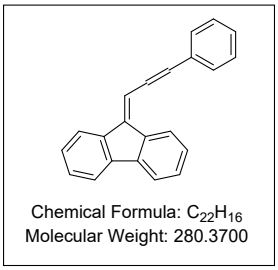
The compound was obtained according to the General Procedure using at 40°C 1-methyl-2-(4-phenylbut-3-yn-1-yl)benzene. Colorless oil. Yield 98 mg (98%).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 7.5 Hz, 1H), 7.52 – 7.44 (m, 2H), 7.40 – 7.33 (m, 2H), 7.30 – 7.16 (m, 4H), 7.03 (ddd, *J* = 15.5, 8.3, 1.5 Hz, 1H), 6.97 – 6.85 (m, 2H), 6.71 (d, *J* = 15.4 Hz, 1H), 2.43 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.4, 136.2, 135.6, 132.7, 130.5, 130.4, 130.3, 129.6, 128.6, 127.5, 127.5, 126.4, 126.1, 125.0, 19.9.

HRMS (APPI; Toluene): Chemical Formula: $C_{17}H_{16}$, calc. 220.1247 found 220.1266.

9-(3-phenylallylidene)-9H-fluorene (13)



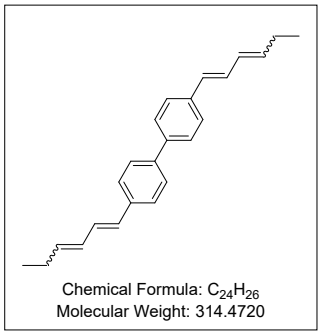
The compound was obtained according to the General Procedure at 190°C using 9-(3-phenylprop-2-yn-1-yl)-9H-fluorene. Yellow solid. Yield 80 mg (80%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 – 8.05 (m, 1H), 7.98 (dd, *J* = 15.2, 11.9 Hz, 1H), 7.79 – 7.72 (m, 3H), 7.61 (d, *J* = 7.3 Hz, 2H), 7.45 – 7.32 (m, 8H), 7.01 (d, *J* = 15.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.9, 139.6, 138.9, 138.7, 137.2, 137.0, 135.1, 128.8, 128.5, 127.9, 127.8, 127.1, 127.1, 126.9, 126.9, 125.0, 124.8, 120.1, 120.0, 119.6.

HRMS (APPI; Toluene): Chemical Formula: $C_{22}H_{16}$, calc. 280.1247 found 280.1266.

4,4'-di(hexa-1,3-dien-1-yl)-1,1'-biphenyl (14).



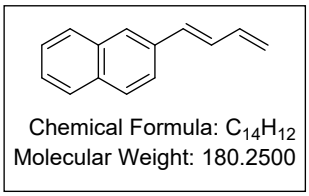
The compound was obtained according to the General Procedure at 90°C using 1,3,5-tri(but-3-yn-1-yl)benzene. Yellow solid. Yield 62 mg (62%).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 8.2 Hz, 4H), 7.47 – 7.39 (m, 4H), 6.80 (dd, *J* = 15.6, 10.4 Hz, 2H), 6.48 (d, *J* = 15.6 Hz, 2H), 6.23 (dd, *J* = 15.1, 10.5 Hz, 2H), 5.97 – 5.82 (m, 2H), 2.19 (p, *J* = 7.1 Hz, 4H), 1.07 (t, *J* = 7.5 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.5, 136.7, 132.0, 129.6, 129.6, 129.5, 126.9, 126.6, 25.9, 13.5.

HRMS (APPI; Toluene): Chemical Formula: $C_{24}H_{26}$, calc. 314.2030 found 314.2047.

(E)-2-(buta-1,3-dien-1-yl)naphthalene (15).

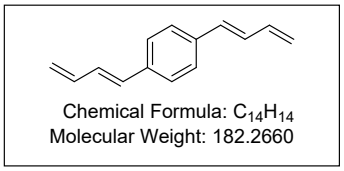


The compound was obtained according to the General Procedure at 40°C using 2-(but-3-yn-1-yl)naphthalene. Colorless oil . Yield 69 mg (69%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 16.5, 8.1 Hz, 4H), 7.63 (d, *J* = 8.7 Hz, 1H), 7.45 (p, *J* = 8.0, 7.3 Hz, 2H), 6.92 (dd, *J* = 15.7, 10.5 Hz, 1H), 6.73 (d, *J* = 15.7 Hz, 1H), 6.57 (dt, *J* = 16.9, 10.3 Hz, 1H), 5.39 (d, *J* = 16.6 Hz, 1H), 5.21 (d, *J* = 10.0 Hz, 1H).

The spectroscopic data were consistent with previously reported(*69*).

1,4-di((E)-buta-1,3-dien-1-yl)benzene (16).



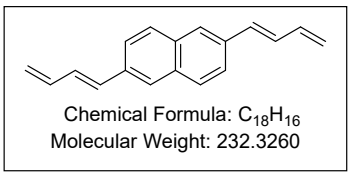
The compound was obtained according to the General Procedure at 90°C using 1,4-di(but-3-yn-1-yl)benzene. Colorless oil. Yield 67 mg (67%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (s, 4H), 6.79 (dd, *J* = 15.6, 10.5 Hz, 2H), 6.62 – 6.39 (m, 4H), 5.33 (d, *J* = 16.9 Hz, 2H), 5.17 (d, *J* = 10.1 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.2, 136.5, 132.5, 129.6, 126.7, 117.7.

HRMS (APPI; Toluene): Chemical Formula: $C_{14}H_{14}$, calc. 182.1091 found 182.1099.

2,6-di((E)-buta-1,3-dien-1-yl)naphthalene (17).



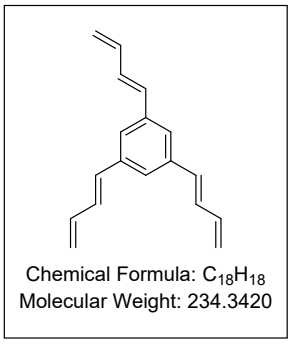
The compound was obtained according to the General Procedure at 90°C using 2,6-(but-3-yn-1-yl)naphthalene. Yellow oil. Yield 51 mg (51%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 – 7.69 (m, 4H), 7.60 (d, *J* = 9.8 Hz, 2H), 6.91 (dd, *J* = 15.6, 10.5 Hz, 2H), 6.71 (d, *J* = 15.7 Hz, 2H), 6.56 (dt, *J* = 16.9, 10.3 Hz, 2H), 5.38 (d, *J* = 16.9 Hz, 2H), 5.21 (d, *J* = 10.0 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.2, 134.7, 133.2, 132.9, 130.0, 128.3, 126.3, 124.0, 117.8.

HRMS (APPI; Toluene): Chemical Formula: $C_{18}H_{16}$, calc. 232.1247 found 232.1258.

1,3,5-tri((E)-buta-1,3-dien-1-yl)benzene (18).



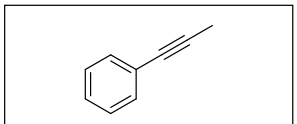
The compound was obtained according to the General Procedure at 90°C using 1,3,5-tri(but-3-yn-1-yl)benzene. Yellow oil. Yield 56 mg (56%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (s, 2H), 6.82 (dd, *J* = 15.7, 10.5 Hz, 3H), 6.59 – 6.44 (m, 6H), 5.36 (d, *J* = 16.9 Hz, 3H), 5.20 (d, *J* = 10.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.7, 137.1, 132.4, 130.2, 123.8, 118.0.

HRMS (APPI; Toluene): Chemical Formula: $C_{18}H_{18}$, calc. 234.1404 found 234.1415.

Prop-1-yn-1-ylbenzene (19).

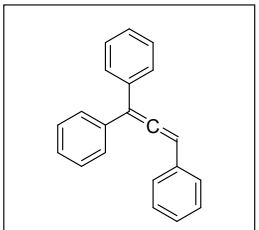

Chemical Formula: C_9H_8
Molecular Weight: 116.1630

The compound was obtained according to the General Procedure at 40°C using prop-2-yn-1-ylbenzene. Colorless liquid. Yield 92 mg (92%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.34 (m, 2H), 7.27 (dt, J = 4.5, 2.6 Hz, 3H), 2.05 (s, 3H).

The spectroscopic data were consistent with previously reported(*70*).

1,1,3-triphenylpropa-1,2-diene (20).


Chemical Formula: $C_{21}H_{16}$
Molecular Weight: 268.3590

The compound was obtained according to the General Procedure at 40°C using prop-2-yne-1,1,3-triyltribenzene. Yellow oil. Yield 90 mg (90%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 – 7.49 (m, 6H), 7.47 – 7.35 (m, 8H), 6.80 (s, 1H).

The spectroscopic data were consistent with previously reported(*71*).

Spectral appendix (^{1}H, ^{19}F, ^{13}C NMR).

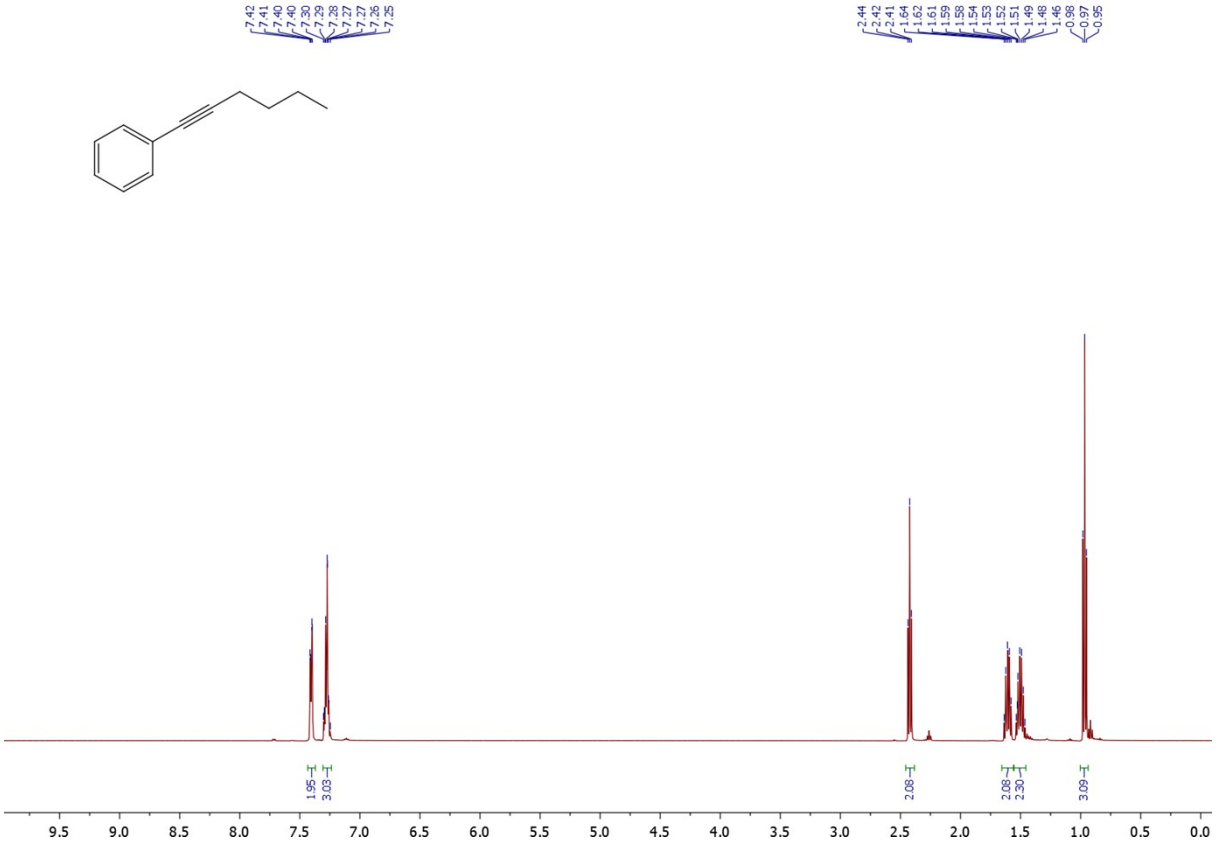


Figure S1. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of hex-1-yn-1-ylbenzene (**3a**).

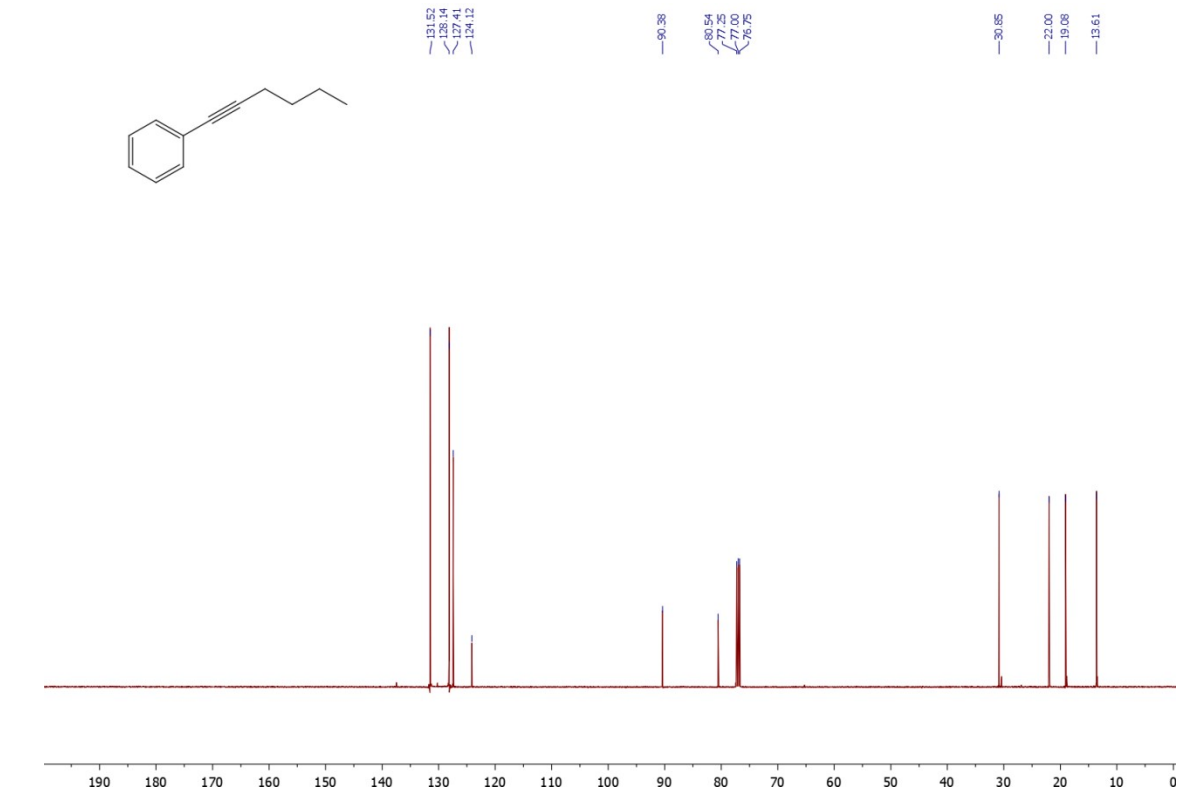


Figure S2. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of hex-1-yn-1-ylbenzene (**3a**).

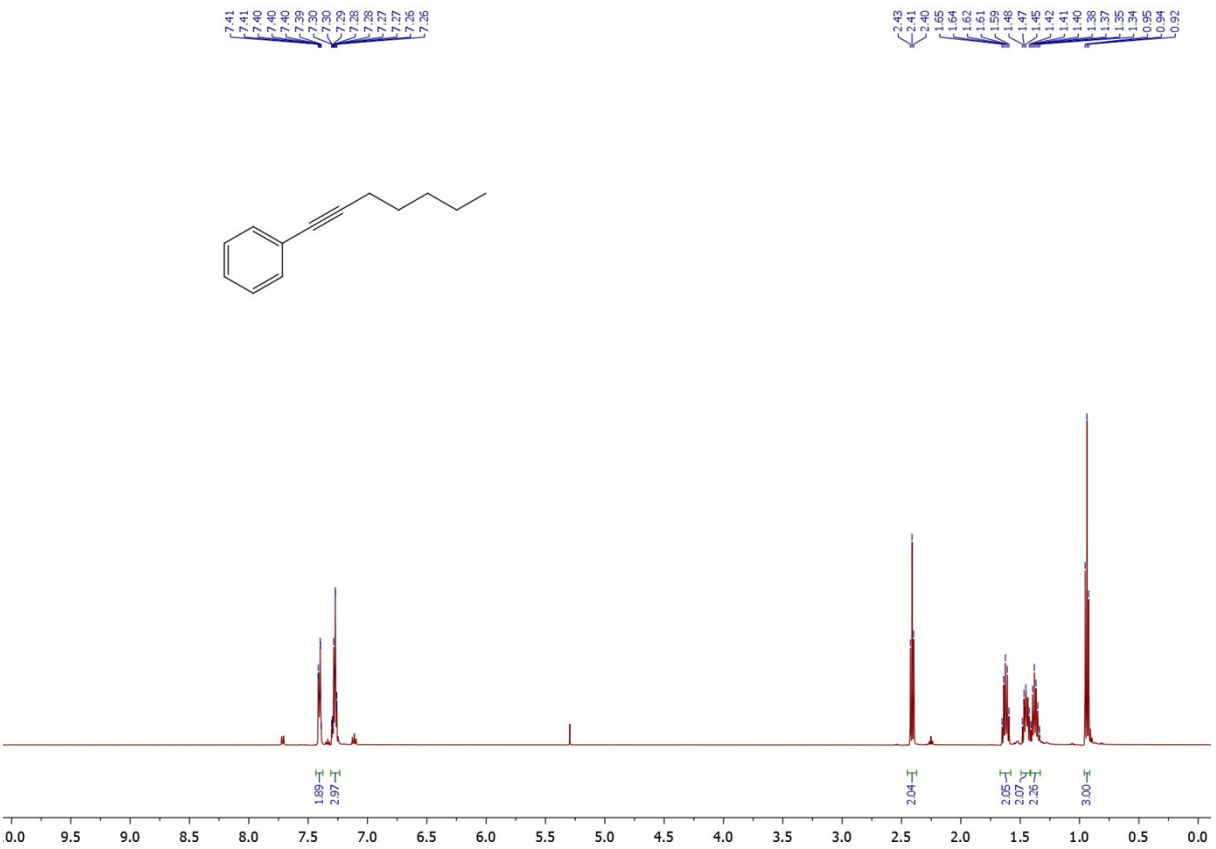


Figure S3. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of hept-1-yn-1-ylbenzene (**4a**).

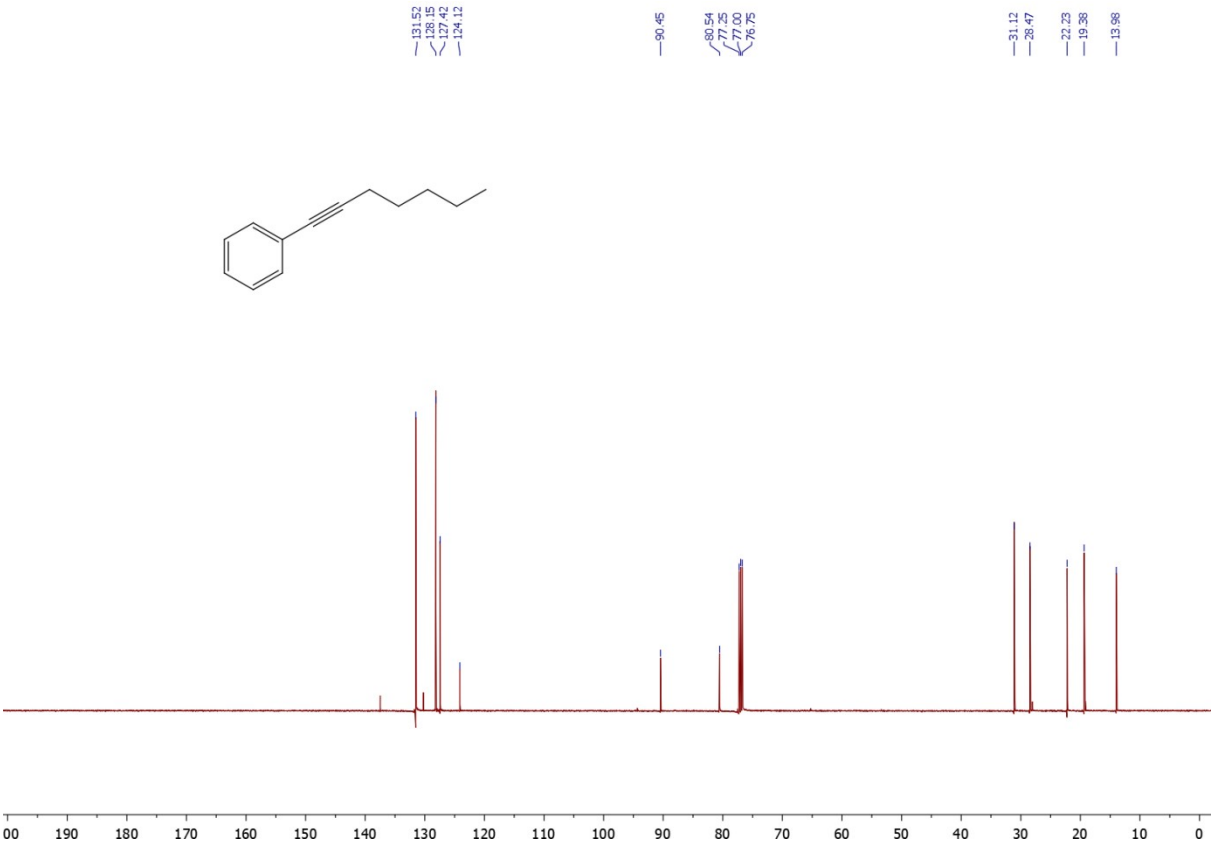


Figure S4. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of hex-1-yn-1-ylbenzene (**4a**).

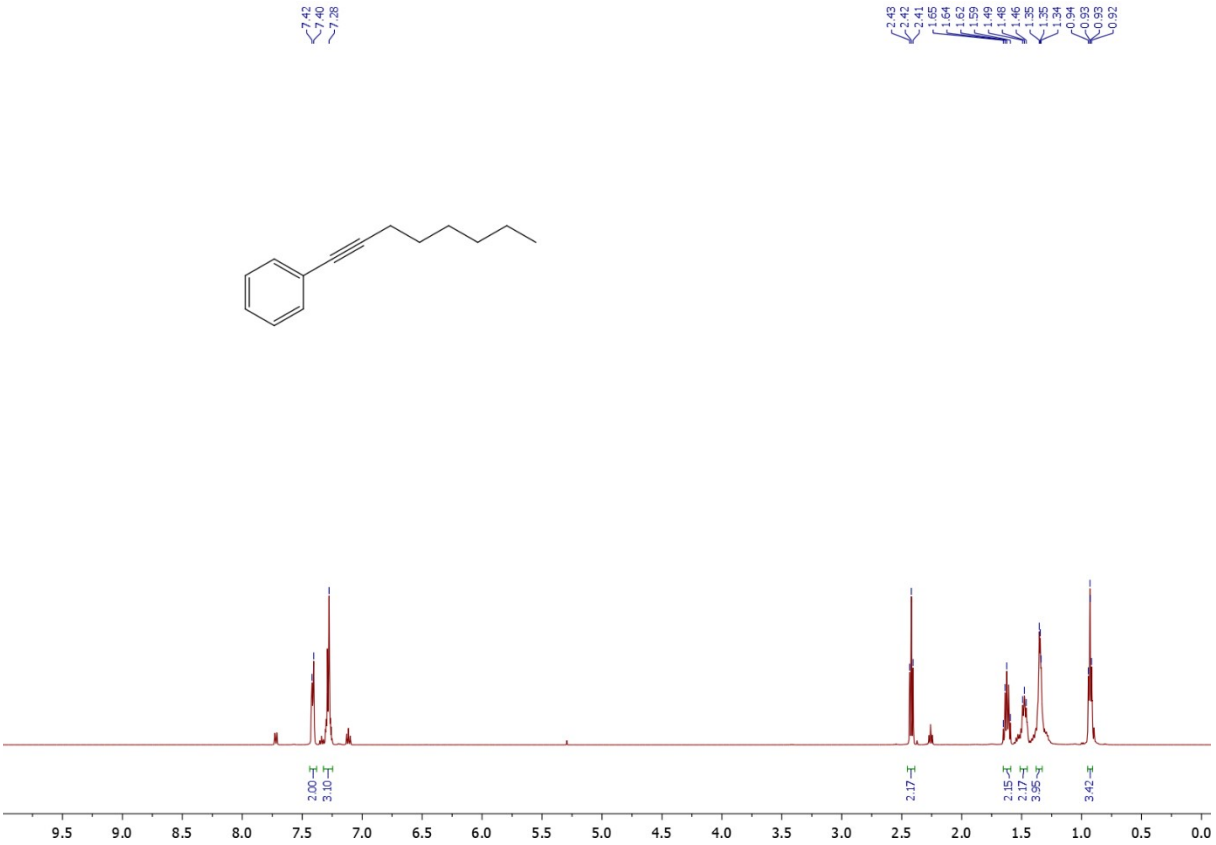


Figure S5. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of oct-1-yn-1-ylbenzene (**5a**).

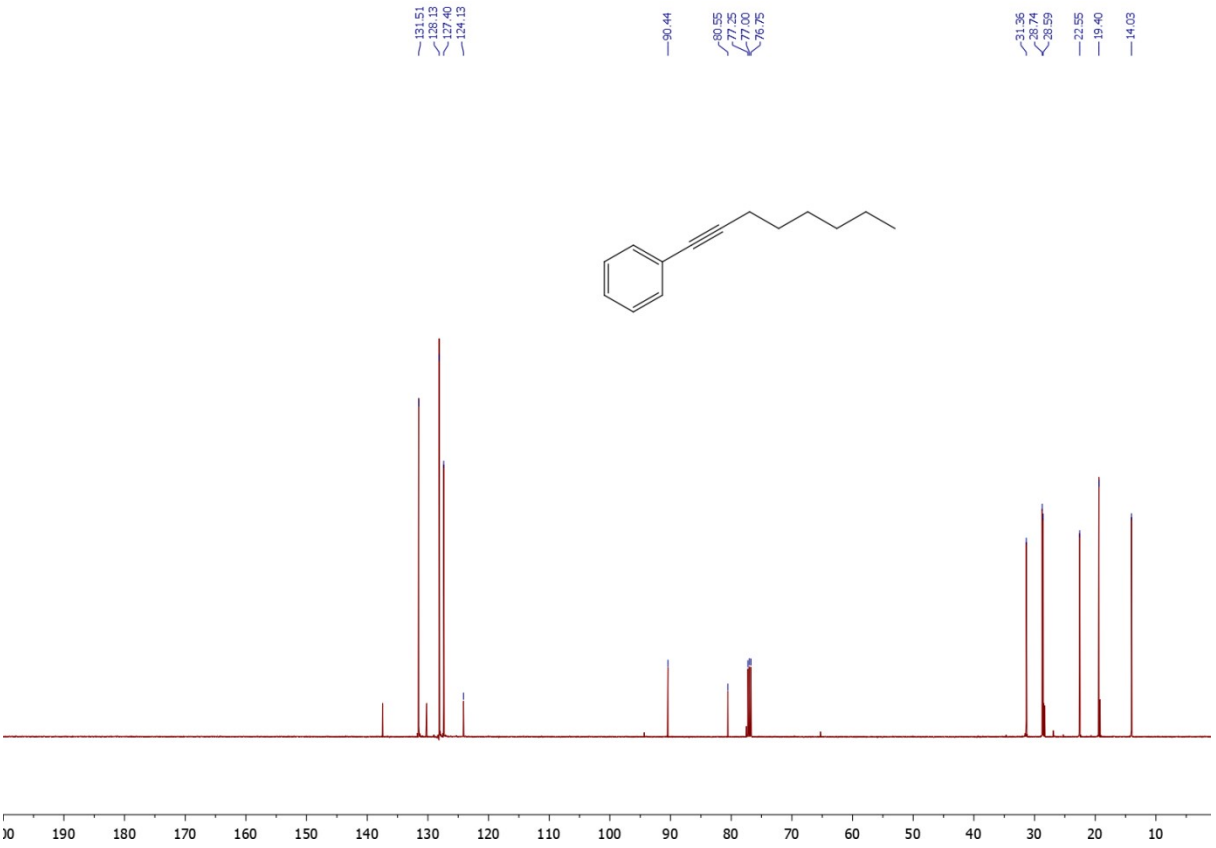


Figure S6. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of oct-1-yn-1-ylbenzene (**5a**).

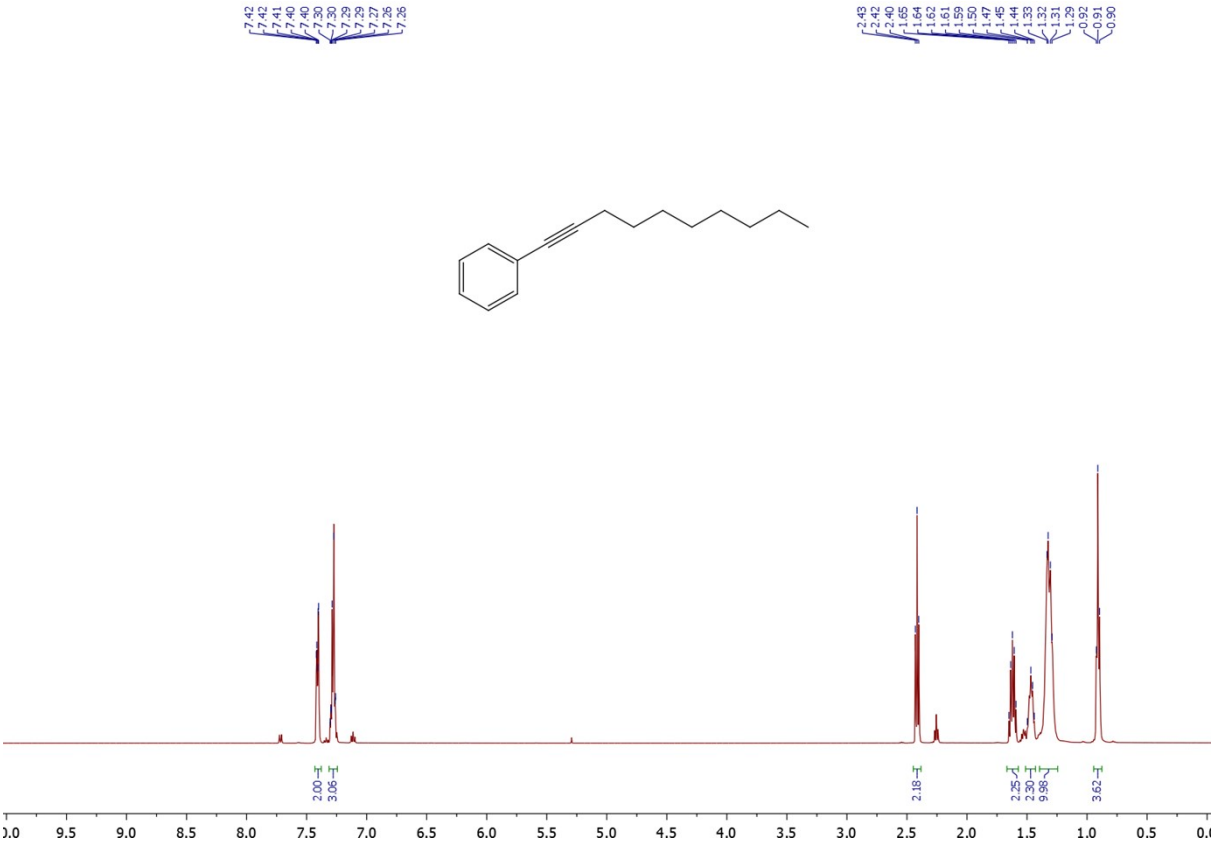


Figure S7. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of dec-1-yn-1-ylbenzene (**6a**).

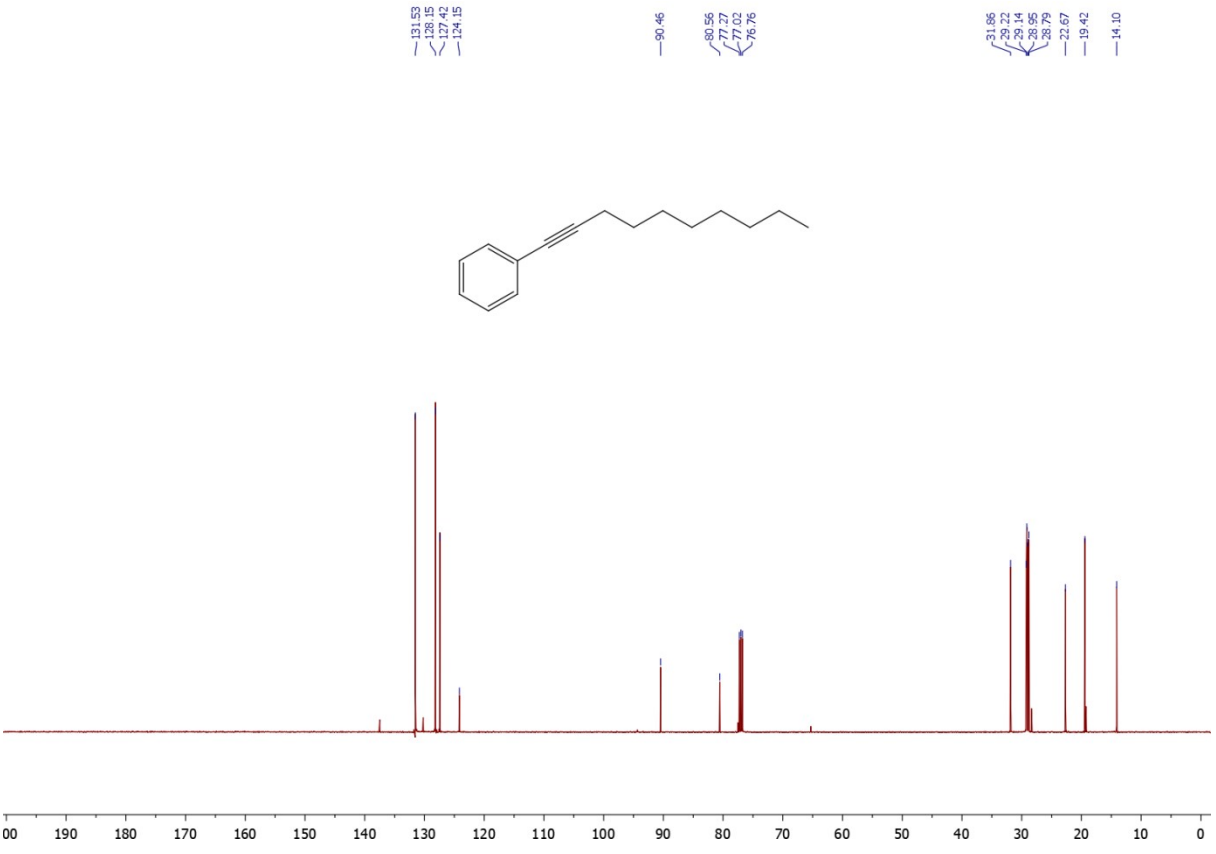


Figure S8. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of dec-1-yn-1-ylbenzene (**6a**).

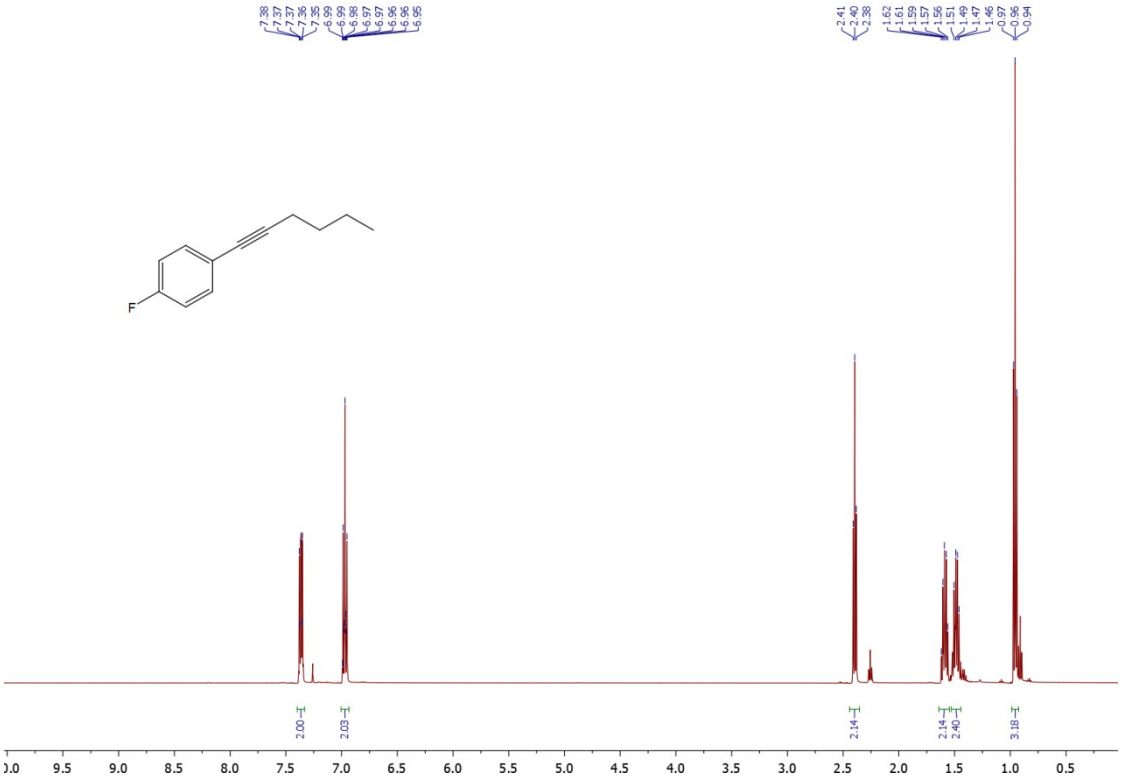


Figure S9. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1-fluoro-4-(hex-1-yn-1-yl)benzene (**7a**).

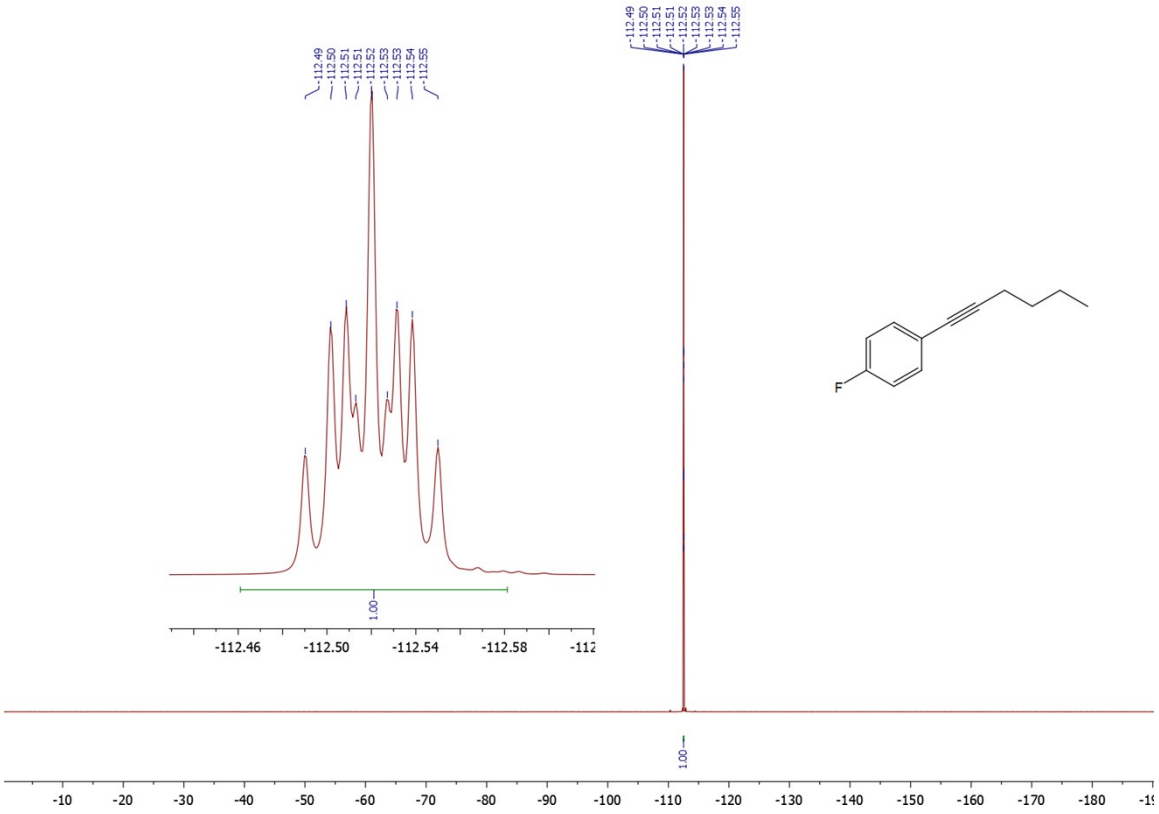


Figure S10. ^{19}F NMR (470 MHz, $CDCl_3$, 293 K) spectrum of 1-fluoro-4-(hex-1-yn-1-yl)benzene (**7a**).

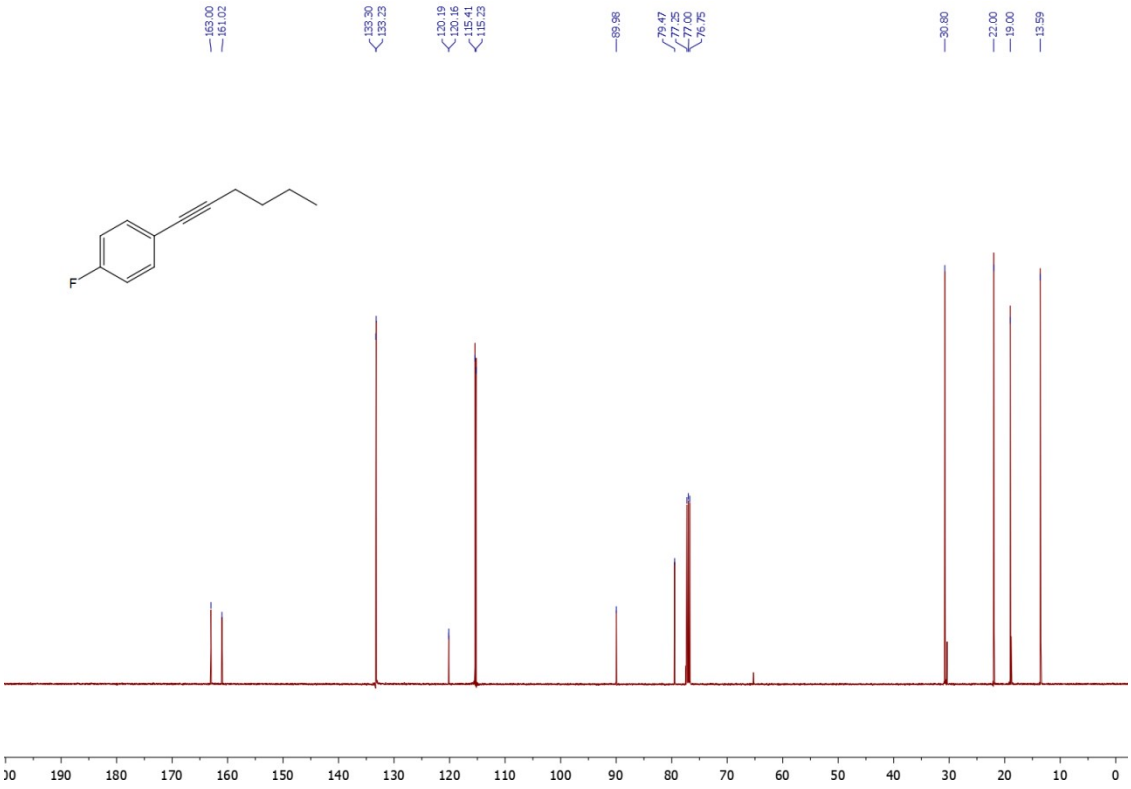


Figure S11. ^{13}C NMR (470 MHz, $CDCl_3$, 293 K) spectrum of 1-fluoro-4-(hex-1-yn-1-yl)benzene (**7a**).

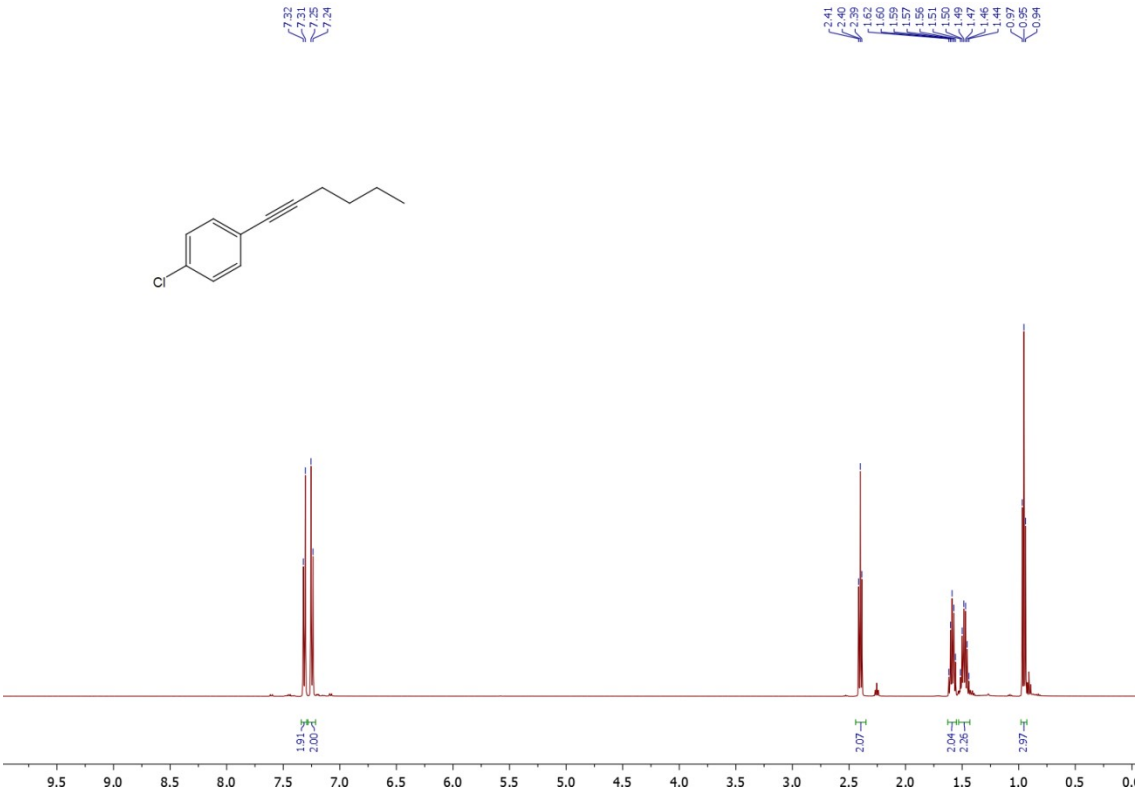


Figure S12. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1-chloro-4-(hex-1-yn-1-yl)benzene (**8a**).

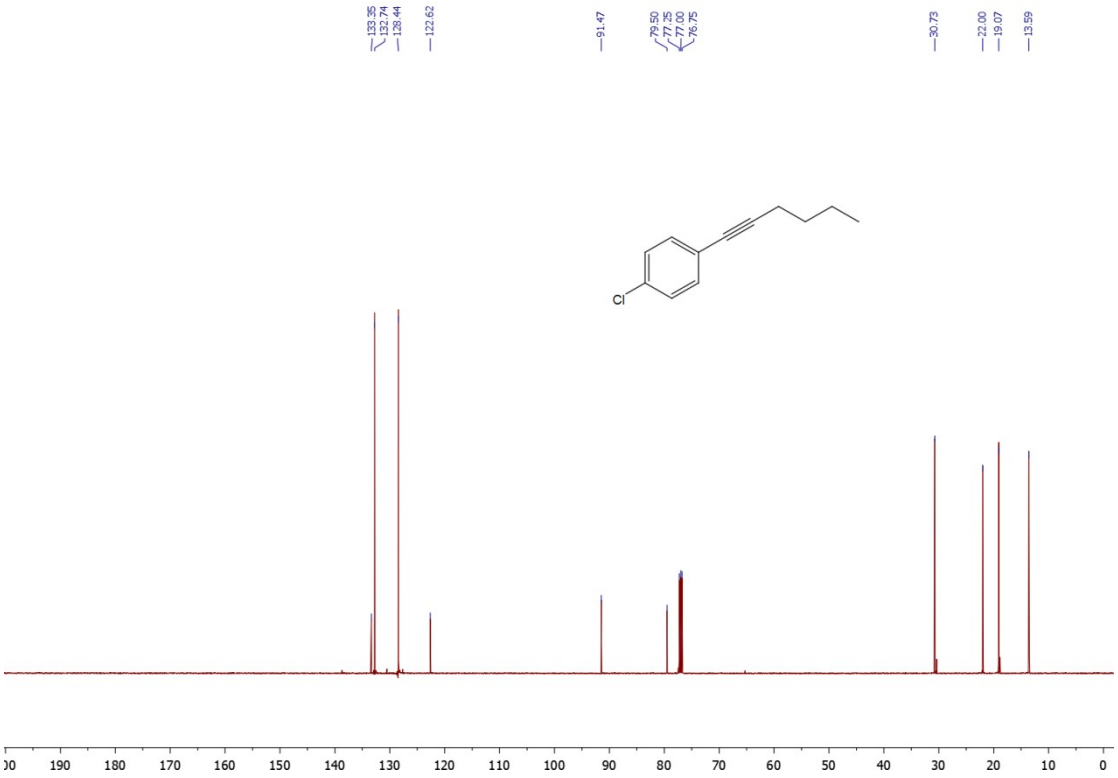


Figure S13. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 1-chloro-4-(hex-1-yn-1-yl)benzene (**8a**).

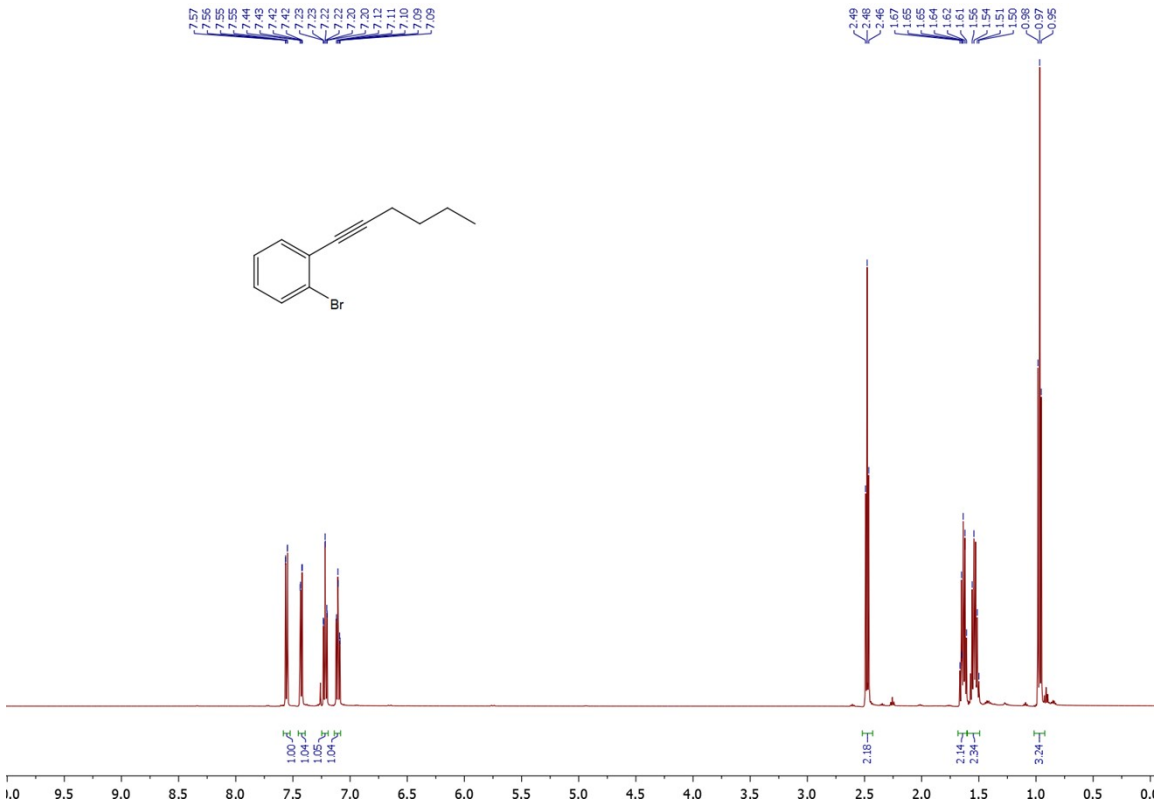


Figure S14. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1-bromo-2-(hex-1-yn-1-yl)benzene (**9a**).

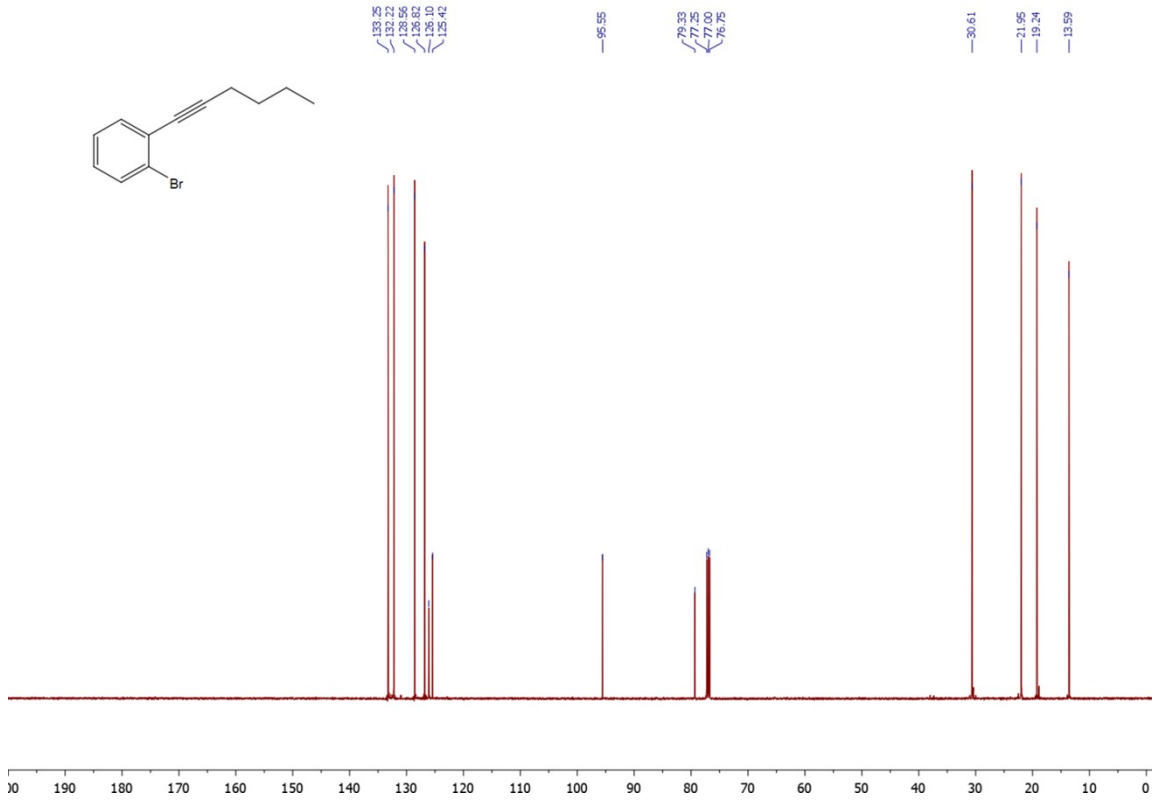


Figure S15. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 1-bromo-2-(hex-1-yn-1-yl)benzene (**9a**).

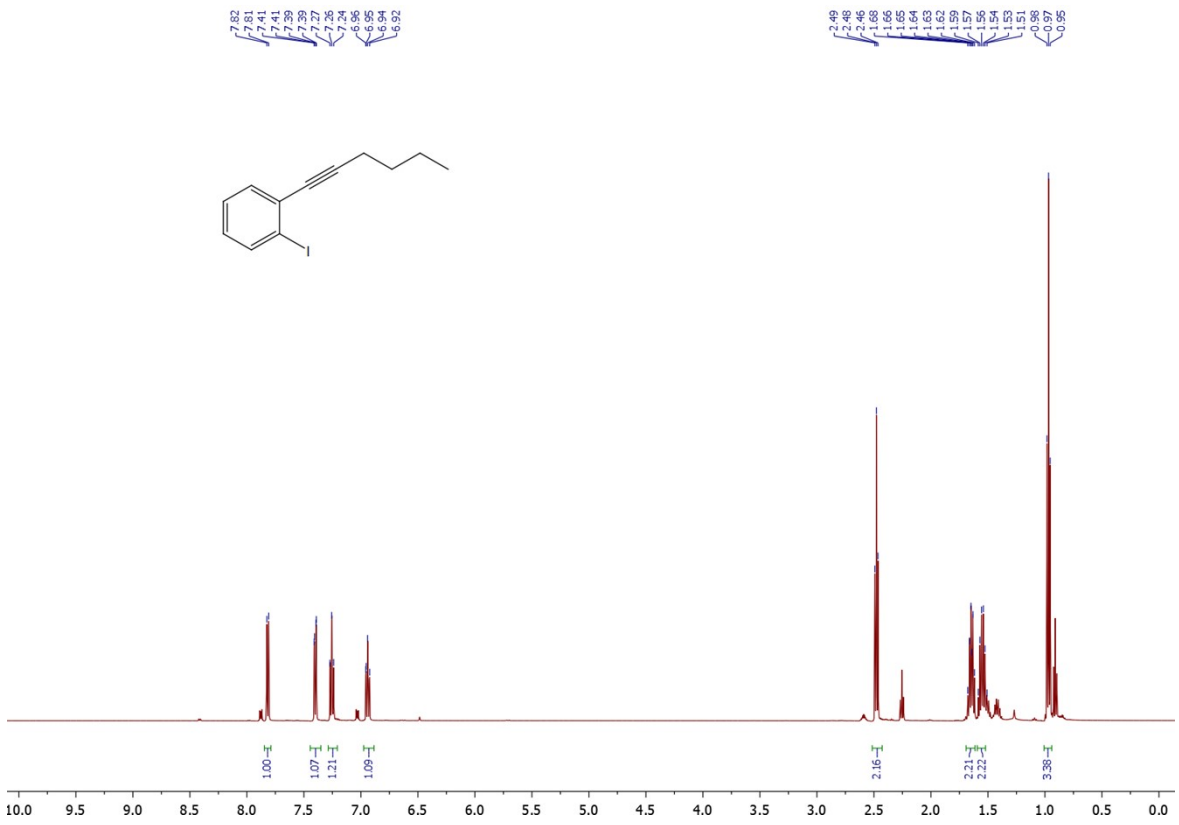


Figure S16. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1-(hex-1-yn-1-yl)-2-iodobenzene (**10a**).

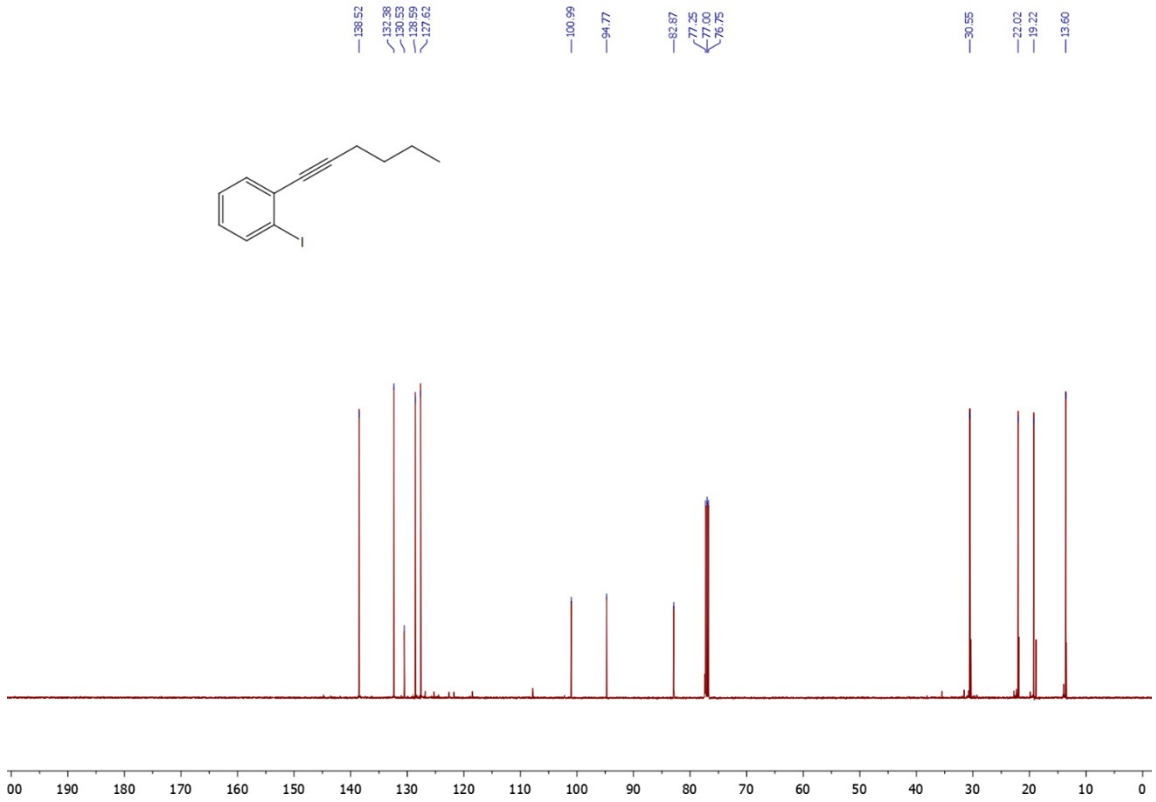


Figure S17. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 1-(hex-1-yn-1-yl)-2-iodobenzene (**10a**).

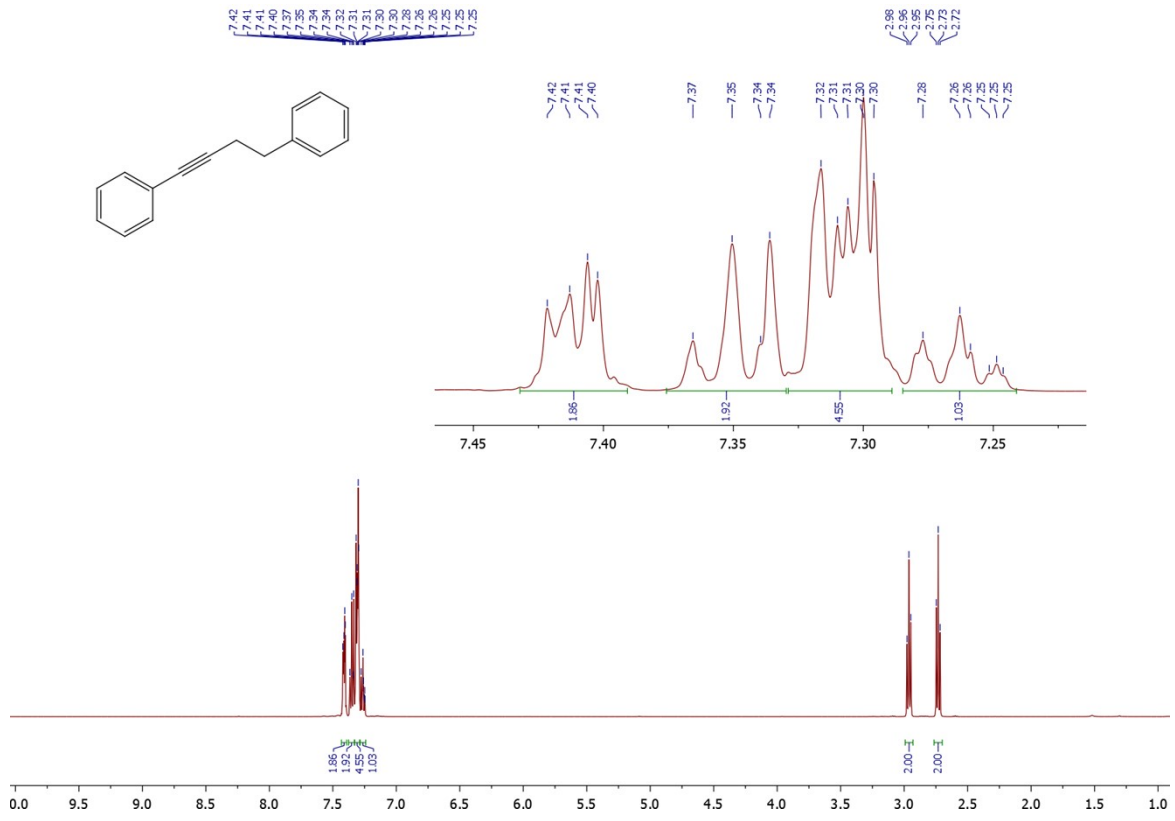


Figure S18. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of but-1-yne-1,4-diyldibenzene (**11a**).

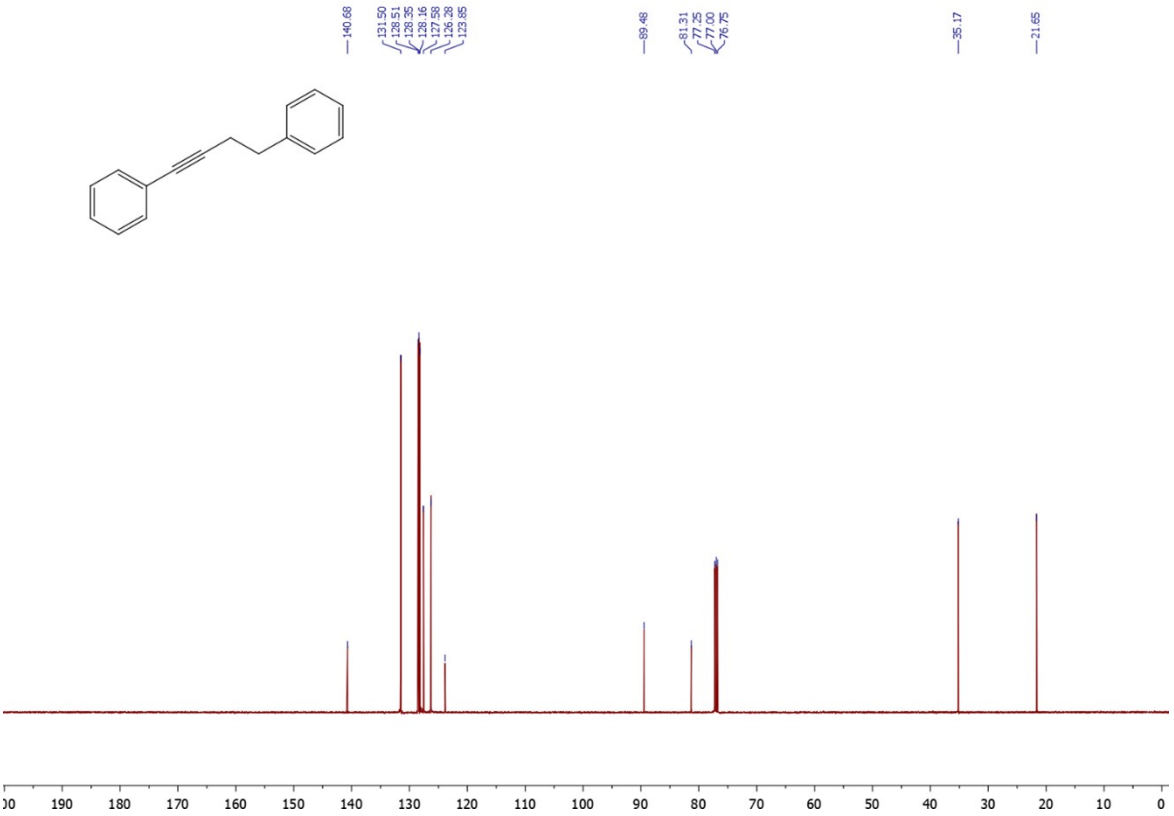


Figure S19. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of but-1-yne-1,4-diyldibenzene (**11a**).

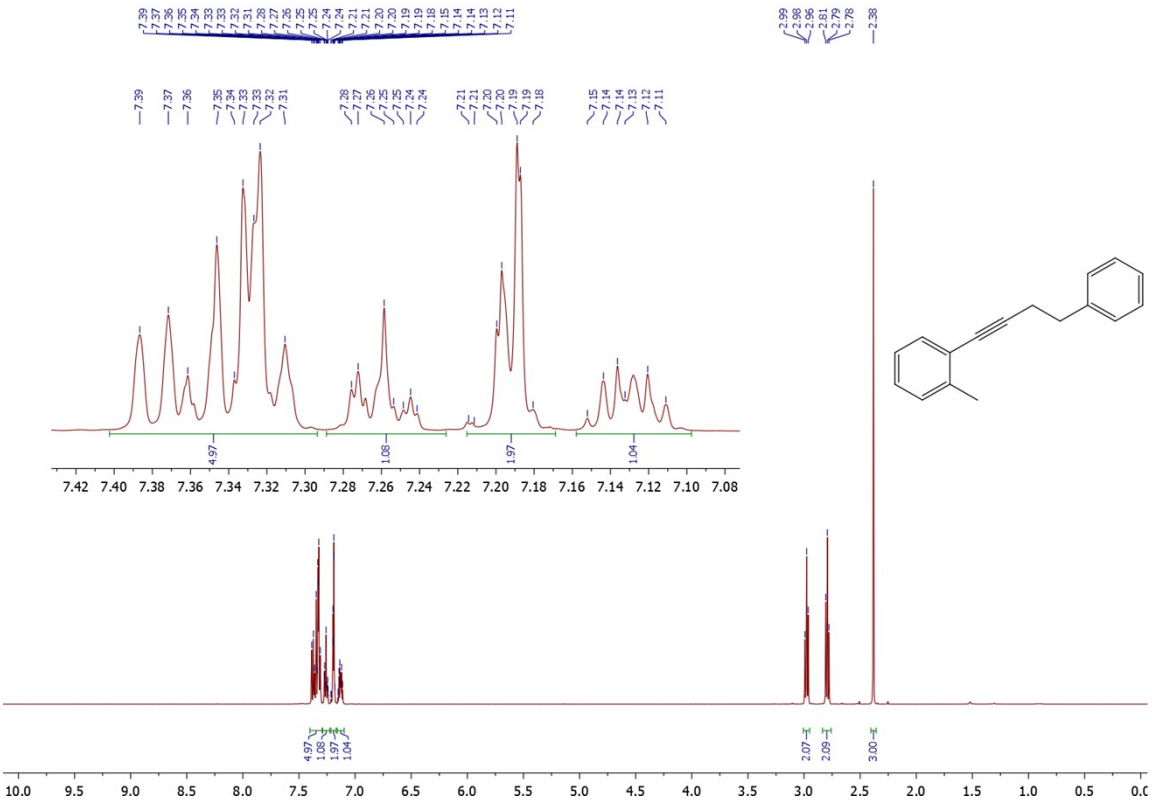


Figure S20. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1-methyl-2-(4-phenylbut-3-yn-1-yl)benzene (**12a**).

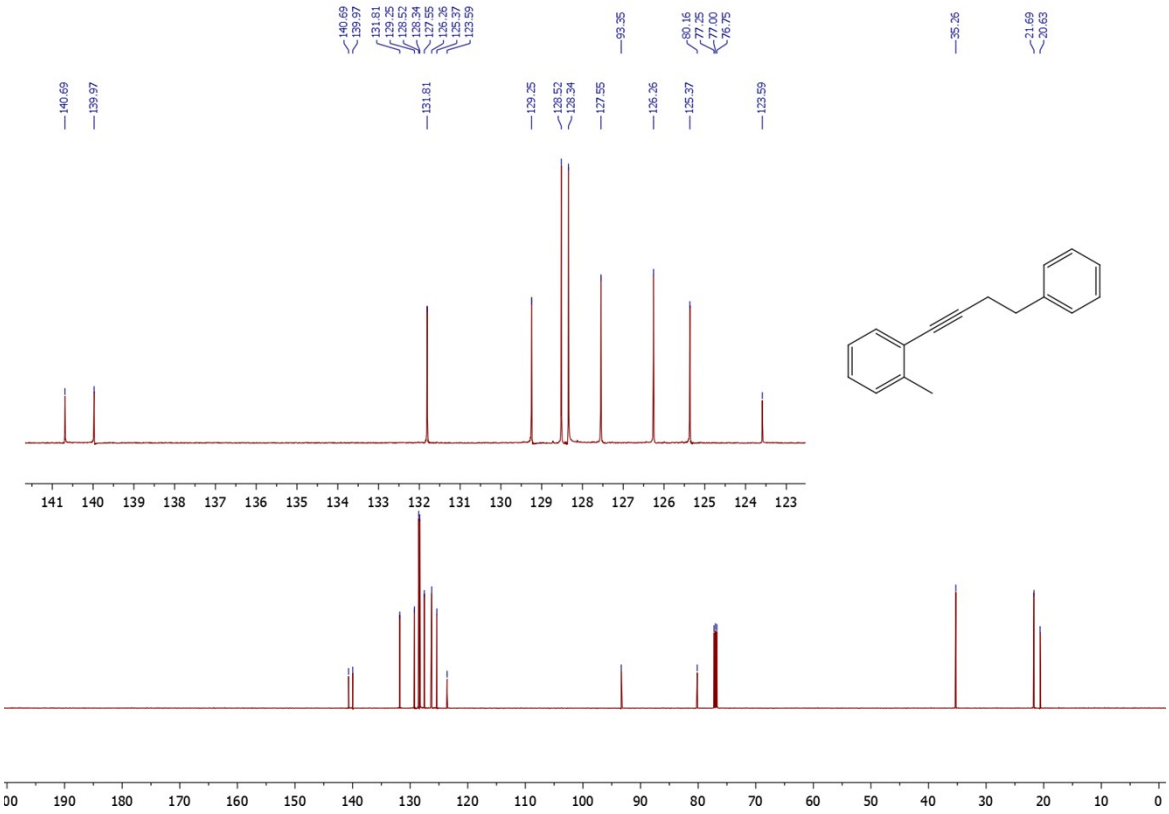


Figure S21. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 1-methyl-2-(4-phenylbut-3-yn-1-yl)benzene (**12a**).

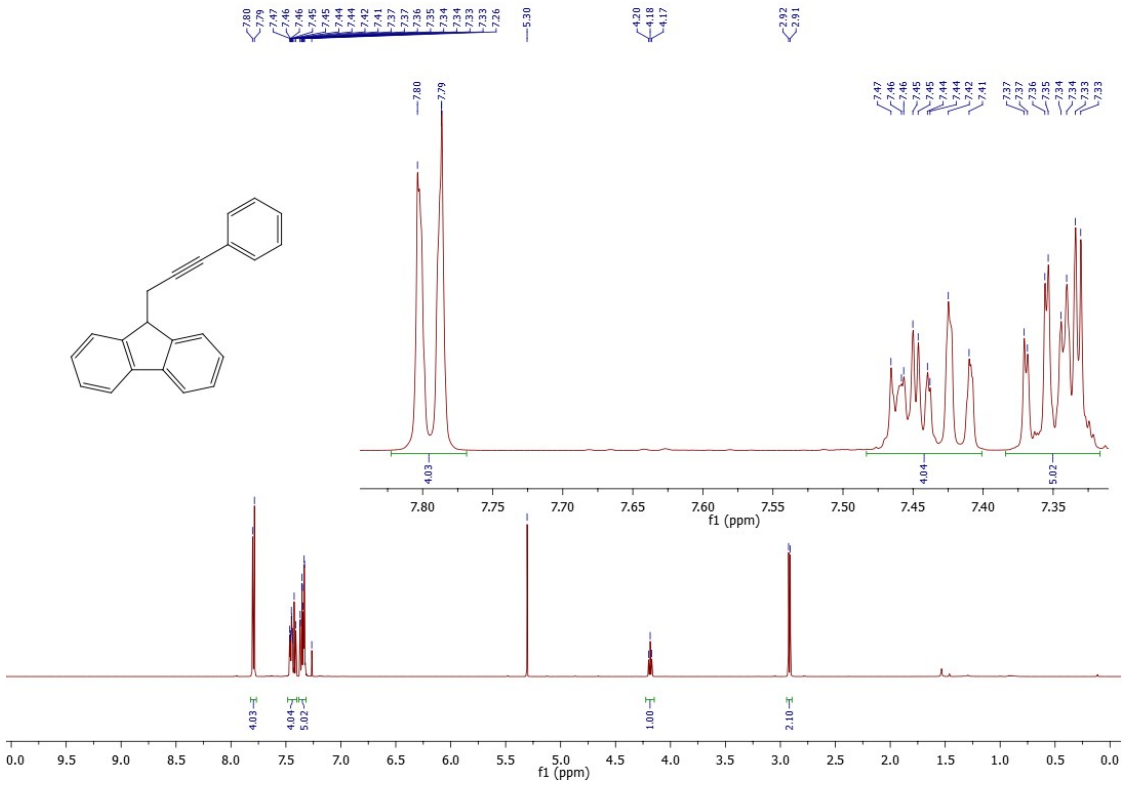


Figure S22. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of 9-(3-phenylprop-2-yn-1-yl)-9H-fluorene (**13a**).

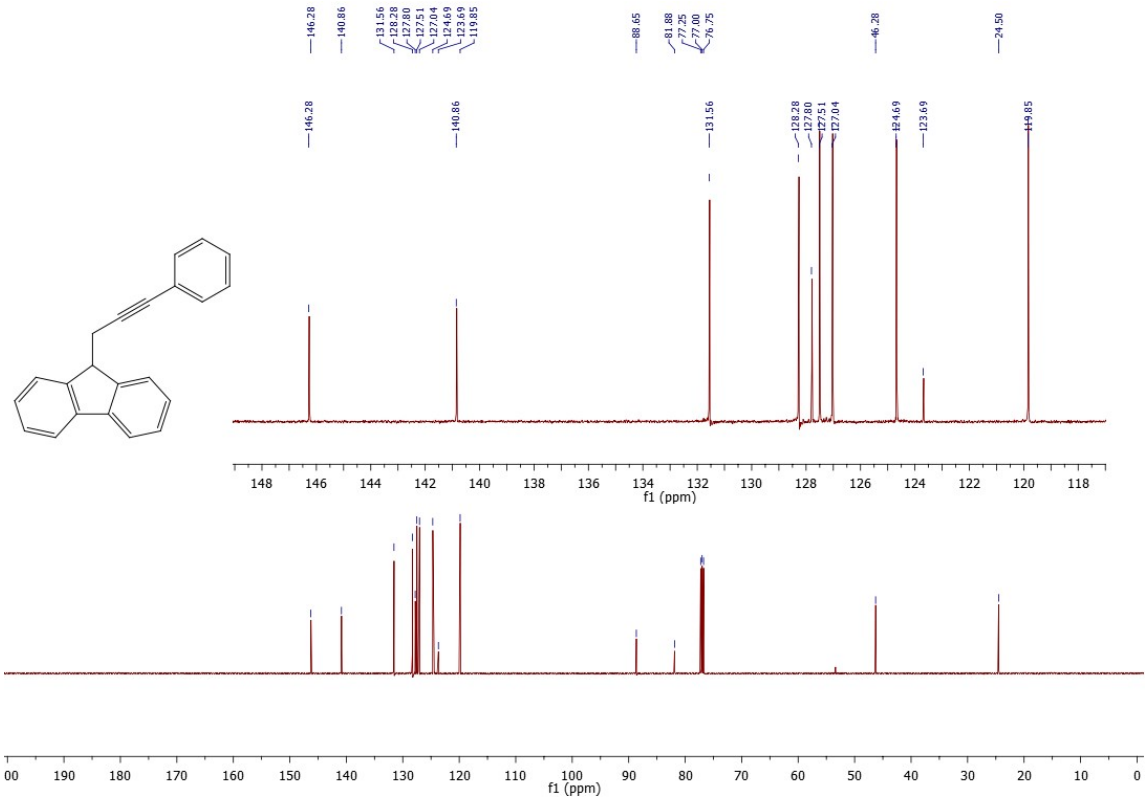


Figure S23. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of 9-(3-phenylprop-2-yn-1-yl)-9H-fluorene (**13a**).

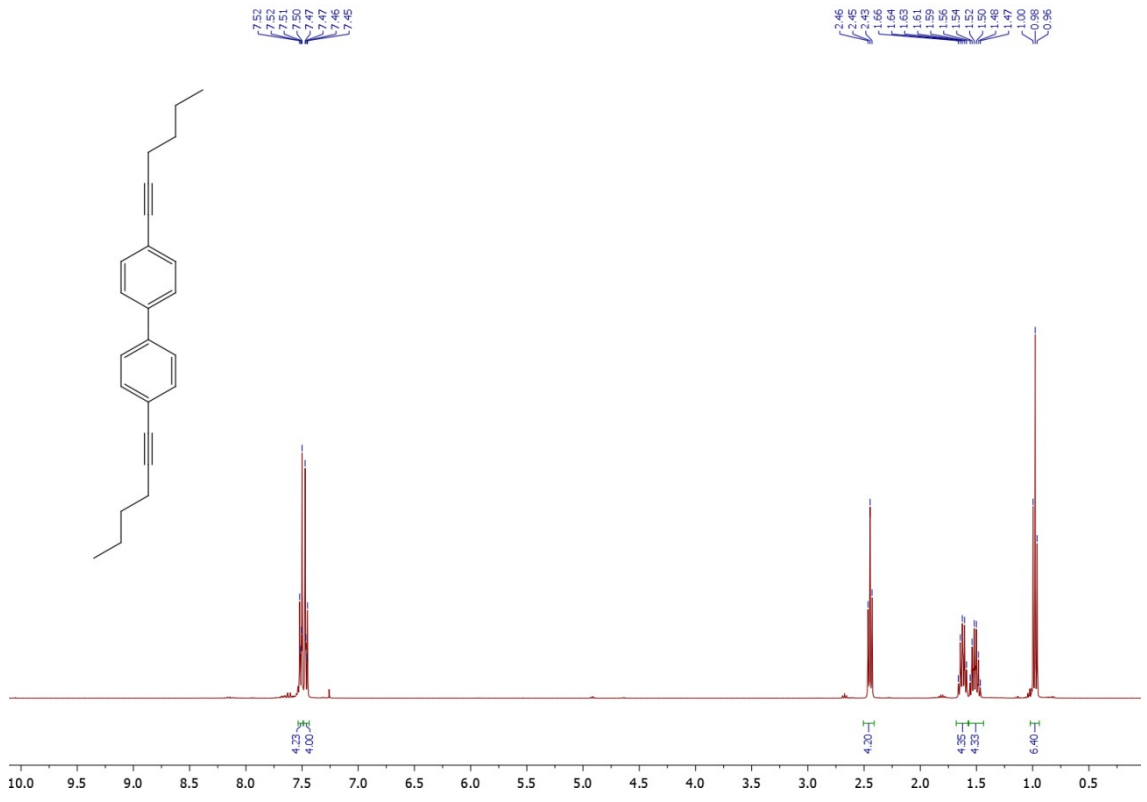


Figure S24. ^{1}H NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 4,4'-di(hex-1-yn-1-yl)-1,1'-biphenyl (**14a**).

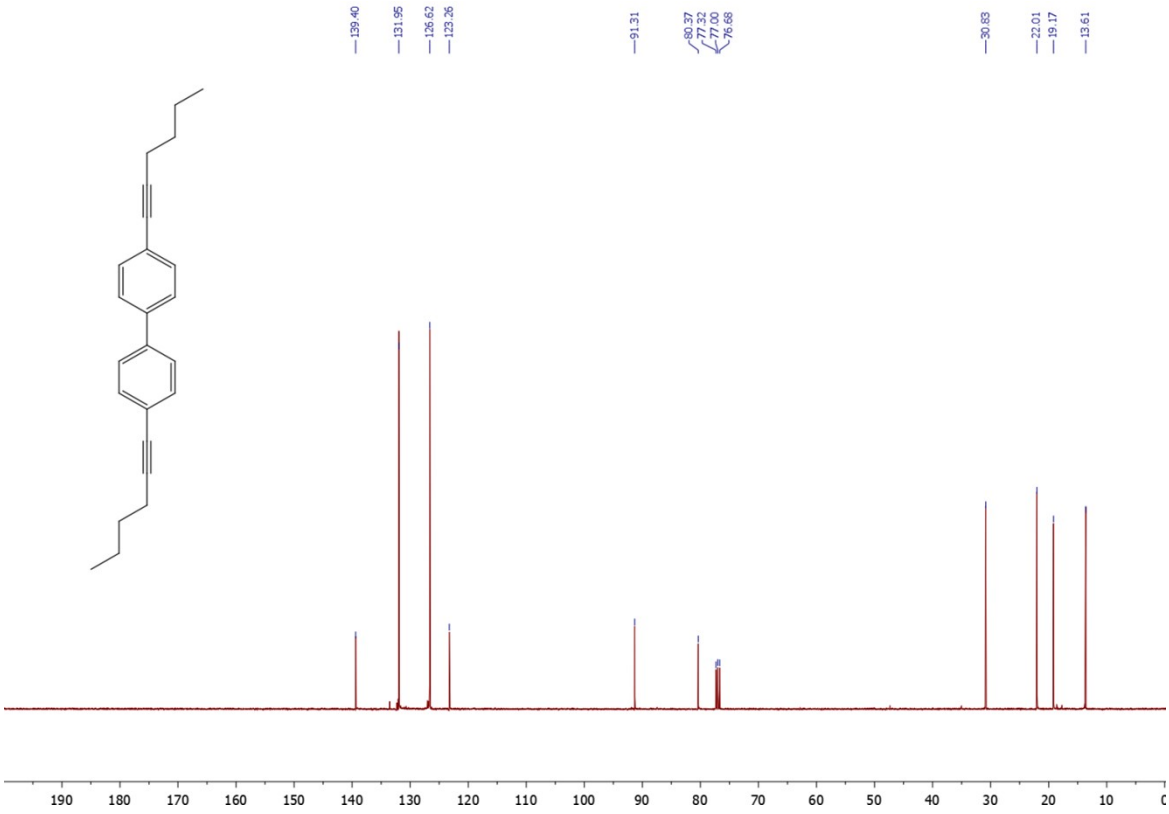


Figure S25. ^{13}C NMR (101 MHz, $CDCl_3$, 293 K) spectrum of 4,4'-di(hex-1-yn-1-yl)-1,1'-biphenyl (**14a**).

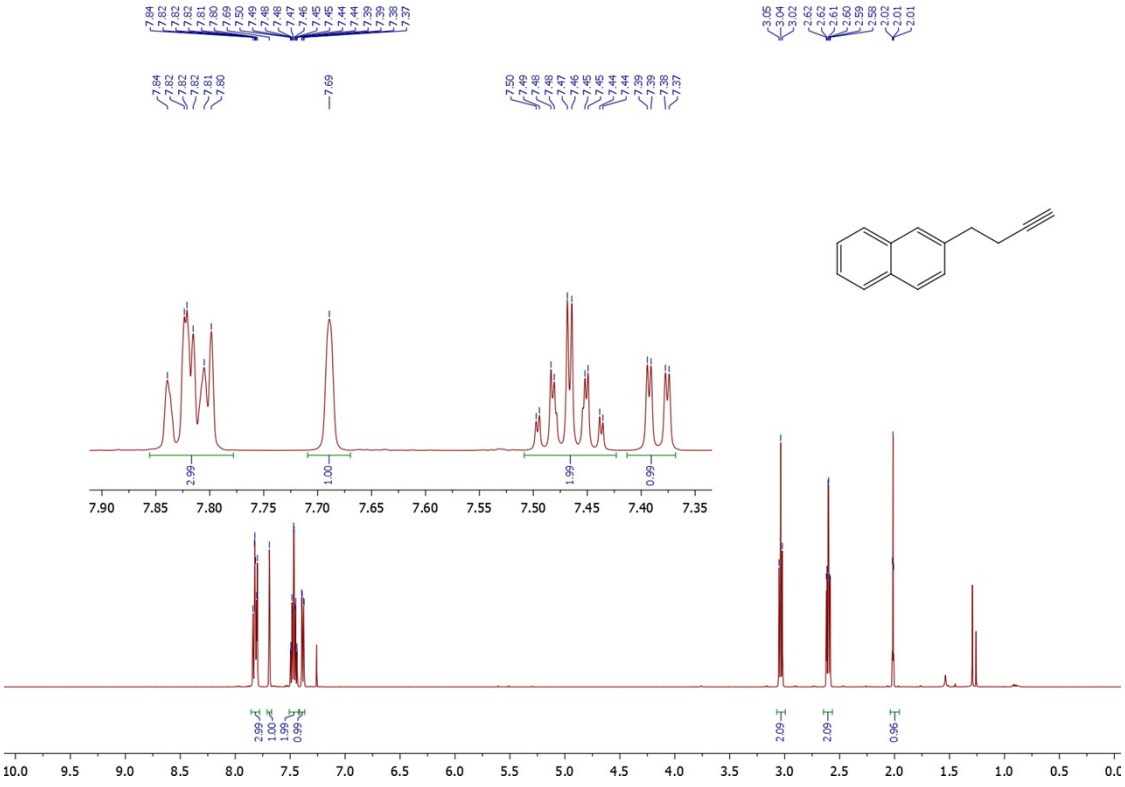


Figure S26. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 2-(but-3-yn-1-yl)naphthalene (**15a**).

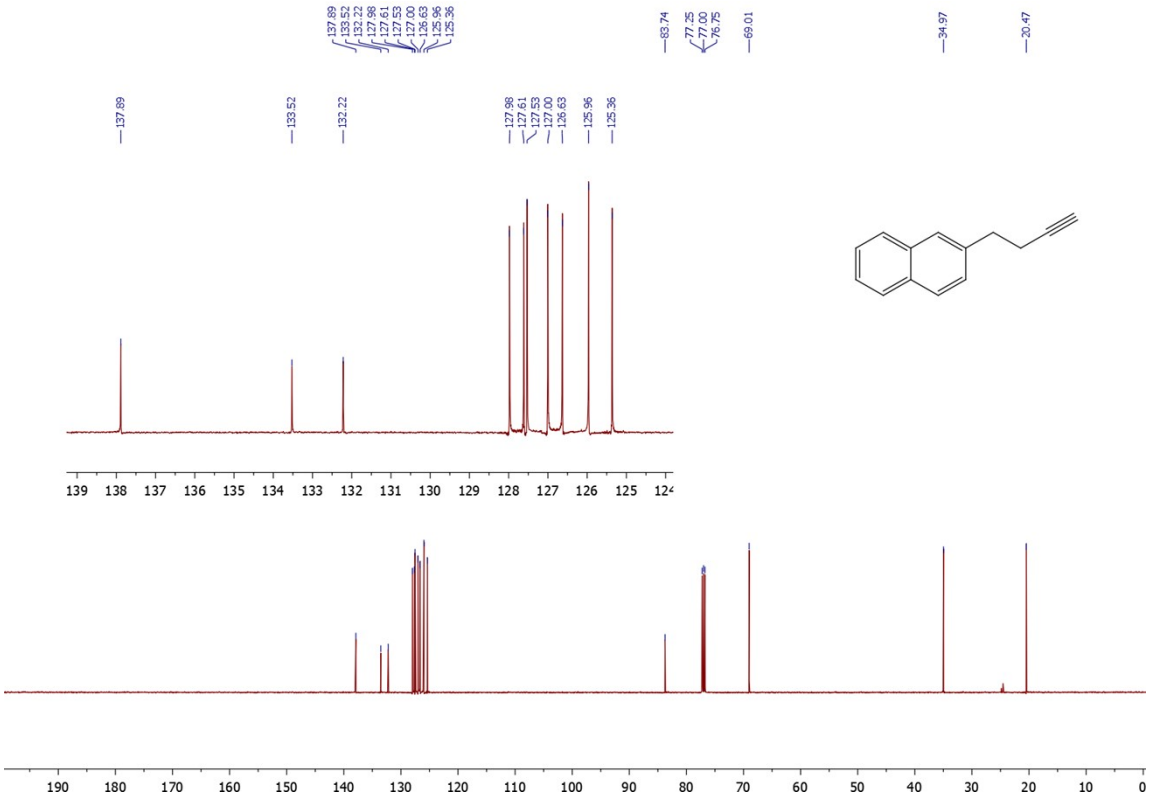


Figure S27. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 2-(but-3-yn-1-yl)naphthalene (**15a**).

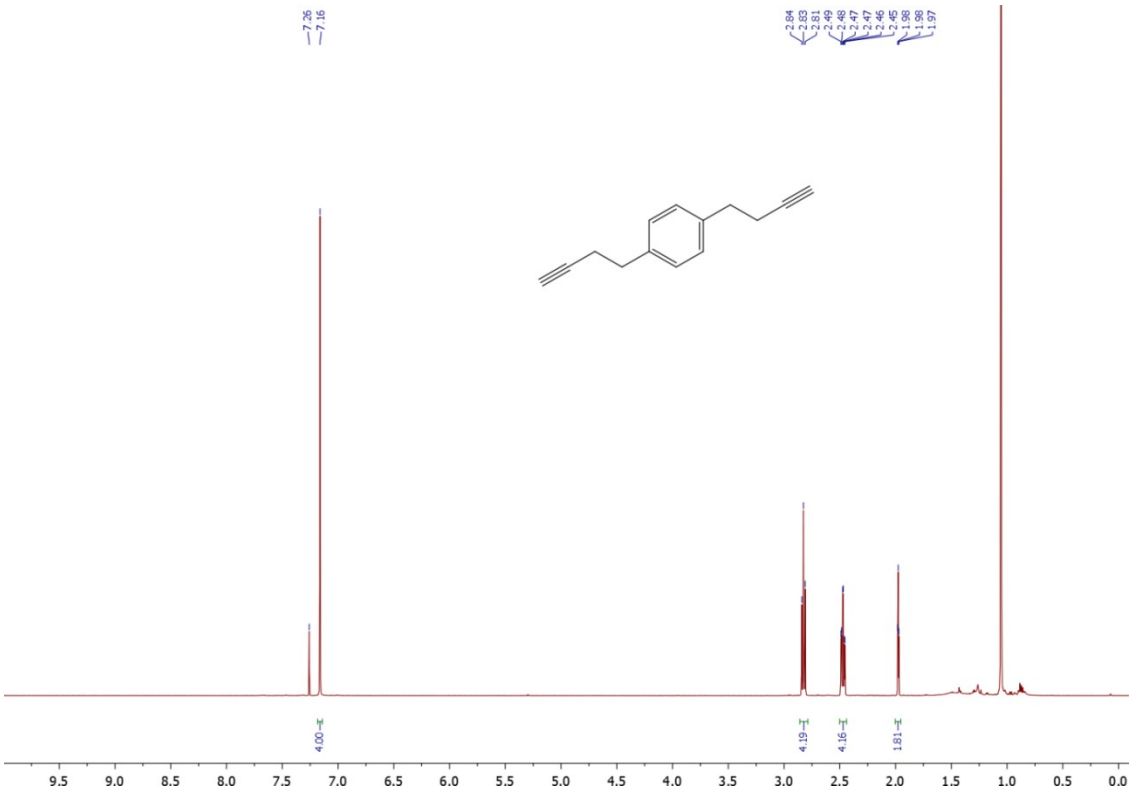


Figure S28. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1,4-di(but-3-yn-1-yl)benzene (**16a**).

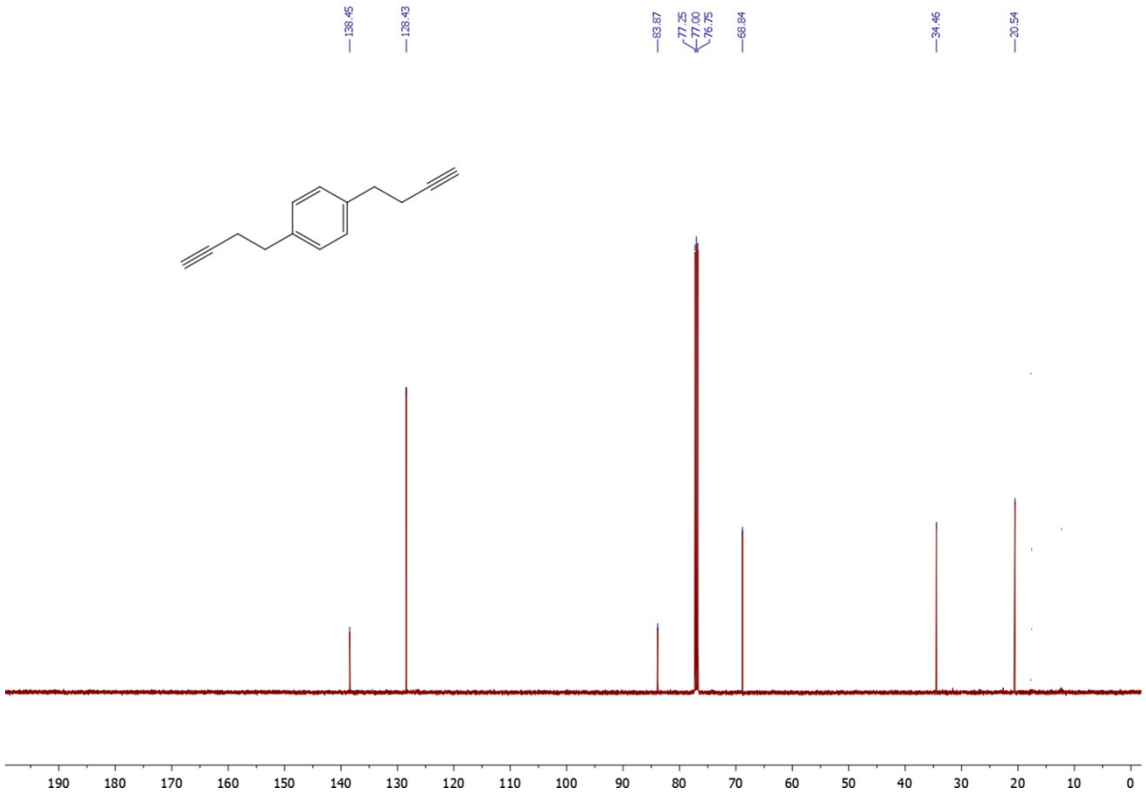


Figure S29. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 1,4-di(but-3-yn-1-yl)benzene (**16a**).

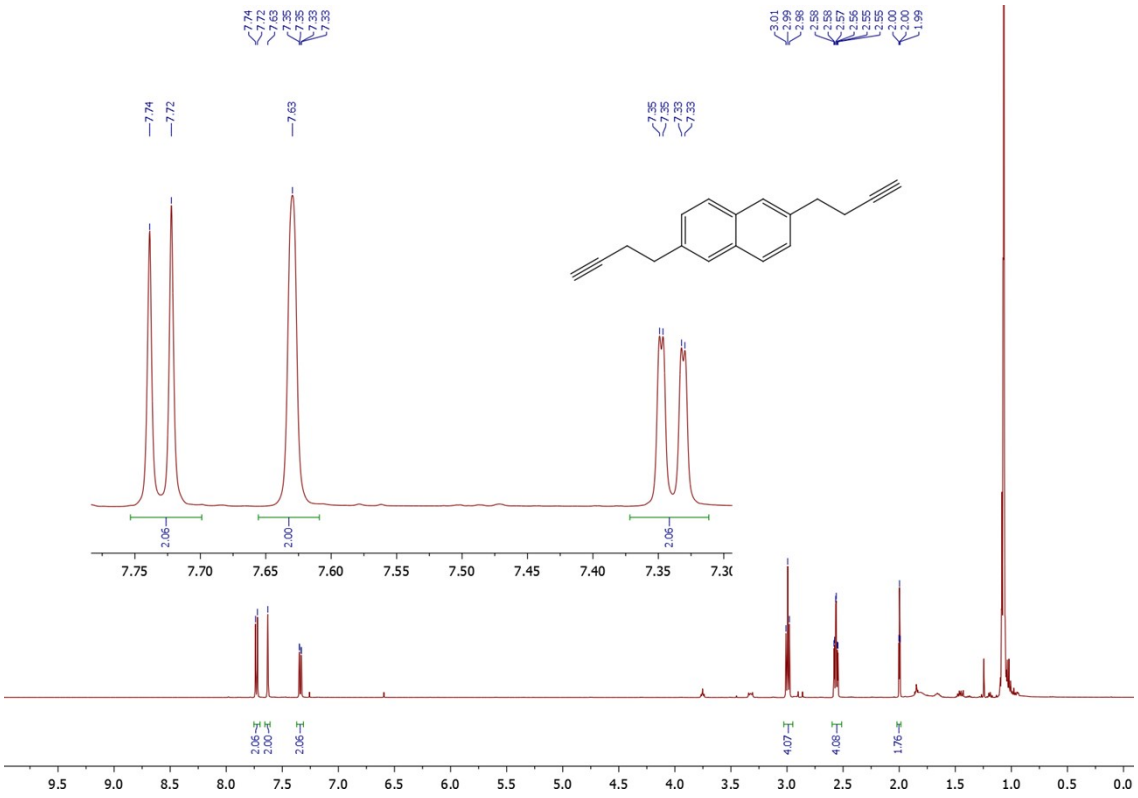


Figure S30. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 2,6-di(but-3-yn-1-yl)naphthalene (**17a**).

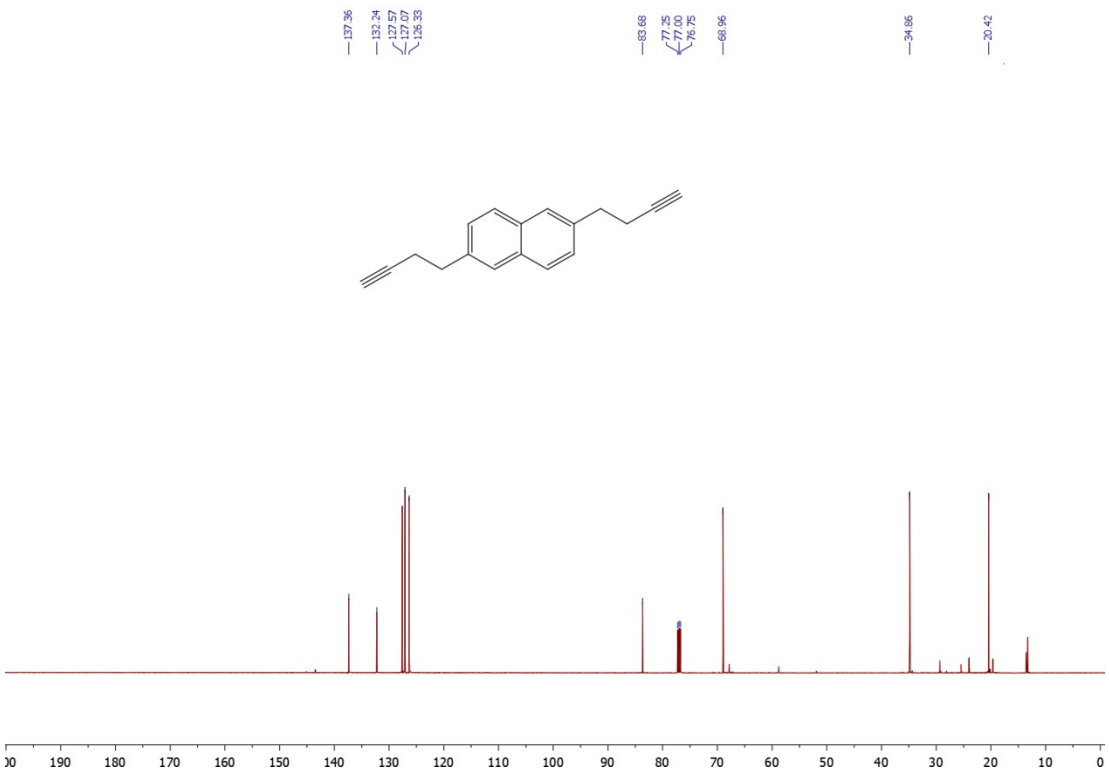


Figure S31. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 2,6-di(but-3-yn-1-yl)naphthalene (**17a**)..

Figure S32. ^{1}H NMR (400 MHz, $CDCl_3$, 293 K) spectrum of 1,3,5-tri(but-3-yn-1-yl)benzene (**18a**).

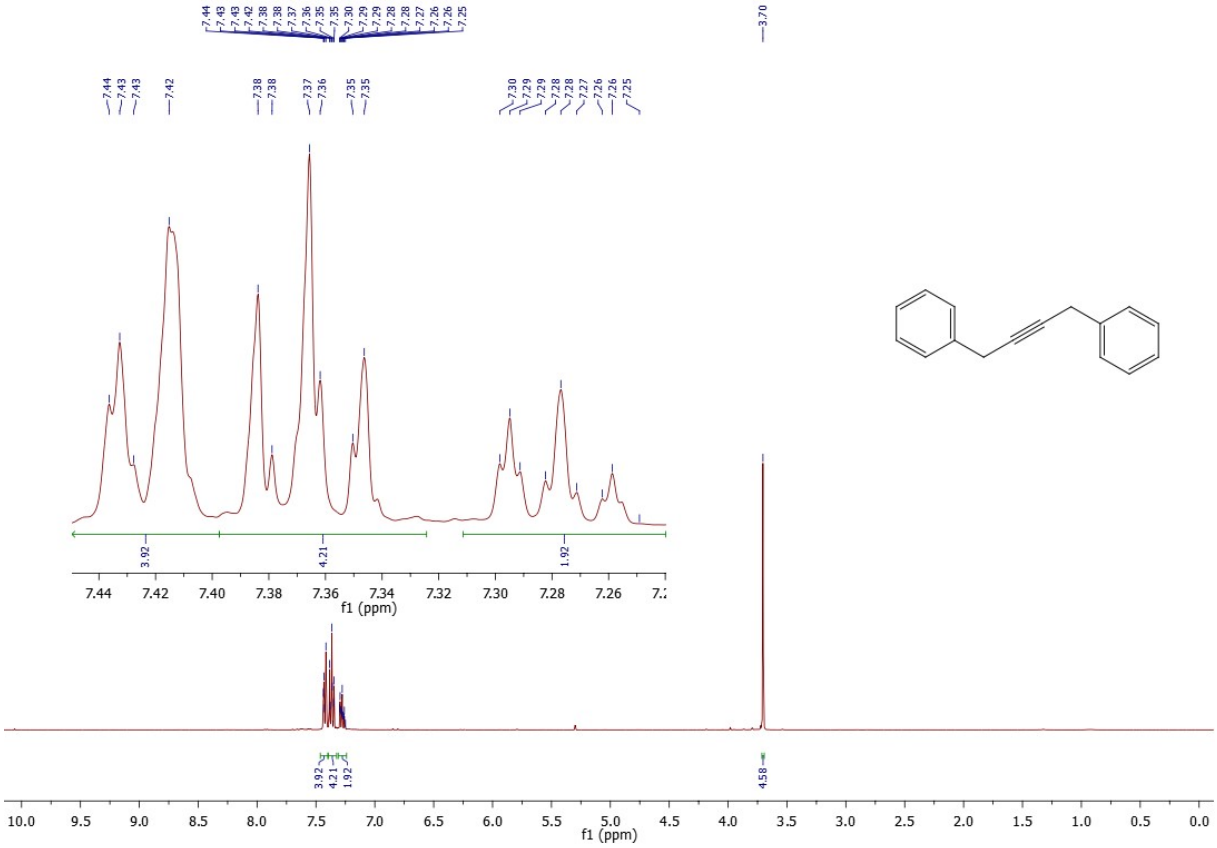


Figure S33. ^{1}H NMR (400 MHz, $CDCl_3$, 293 K) spectrum of 1,4-diphenylbut-2-yne (**11b**).

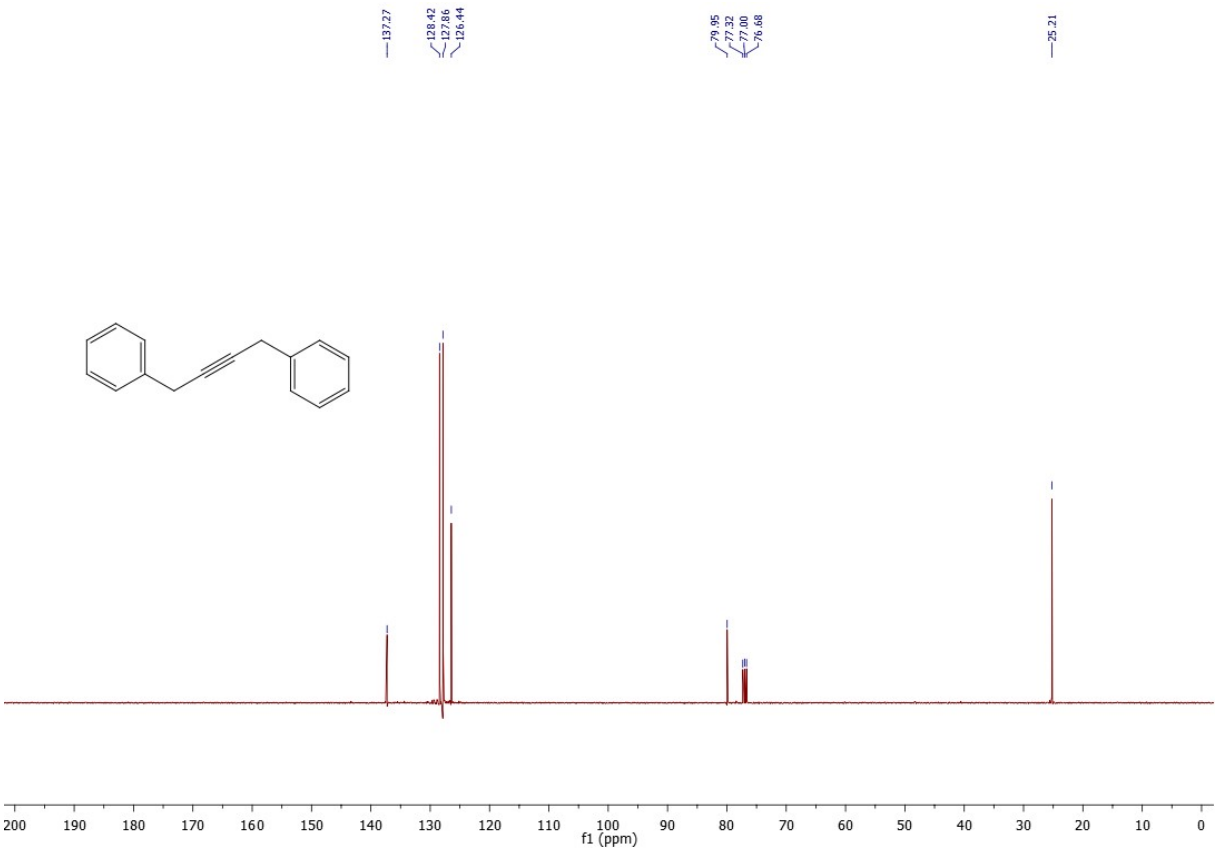


Figure S34. ^{13}C NMR (101 MHz, $CDCl_3$, 293 K) spectrum of 1,4-diphenylbut-2-yne (**11b**).

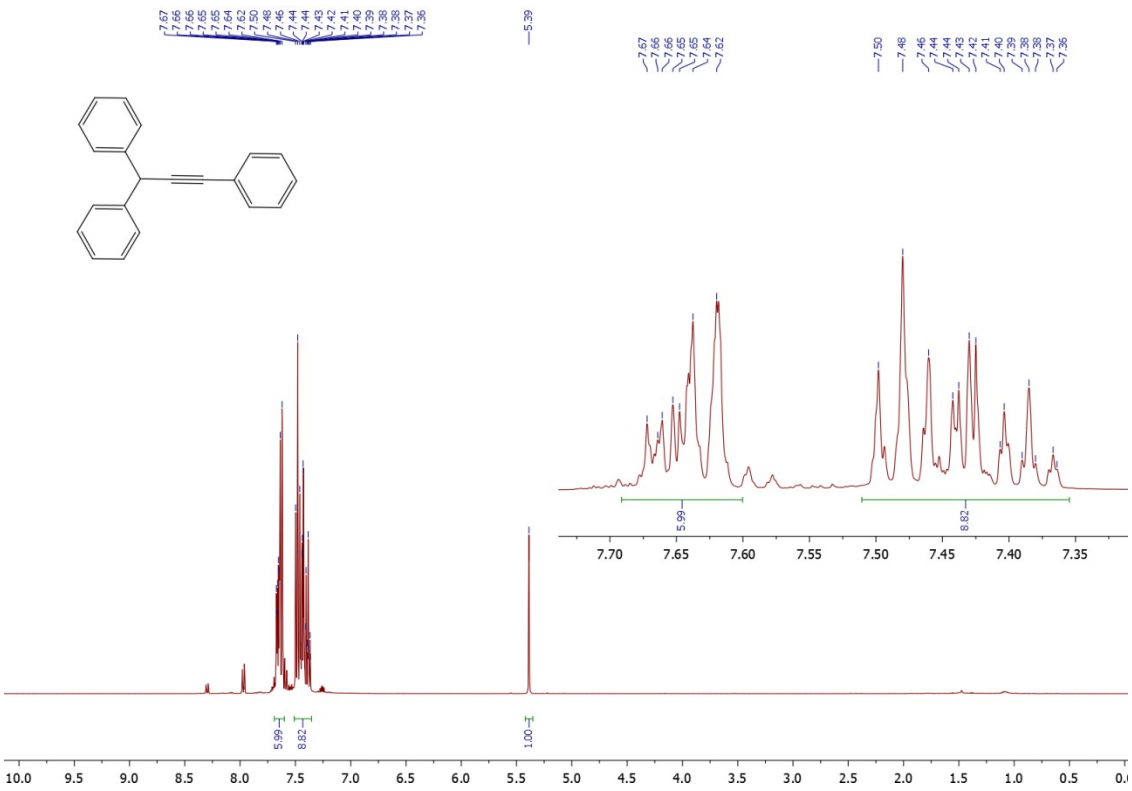


Figure S35. ^{1}H NMR (400 MHz, $CDCl_3$, 293 K) spectrum of prop-2-yne-1,1,3-triyltribenzene (**20a**).

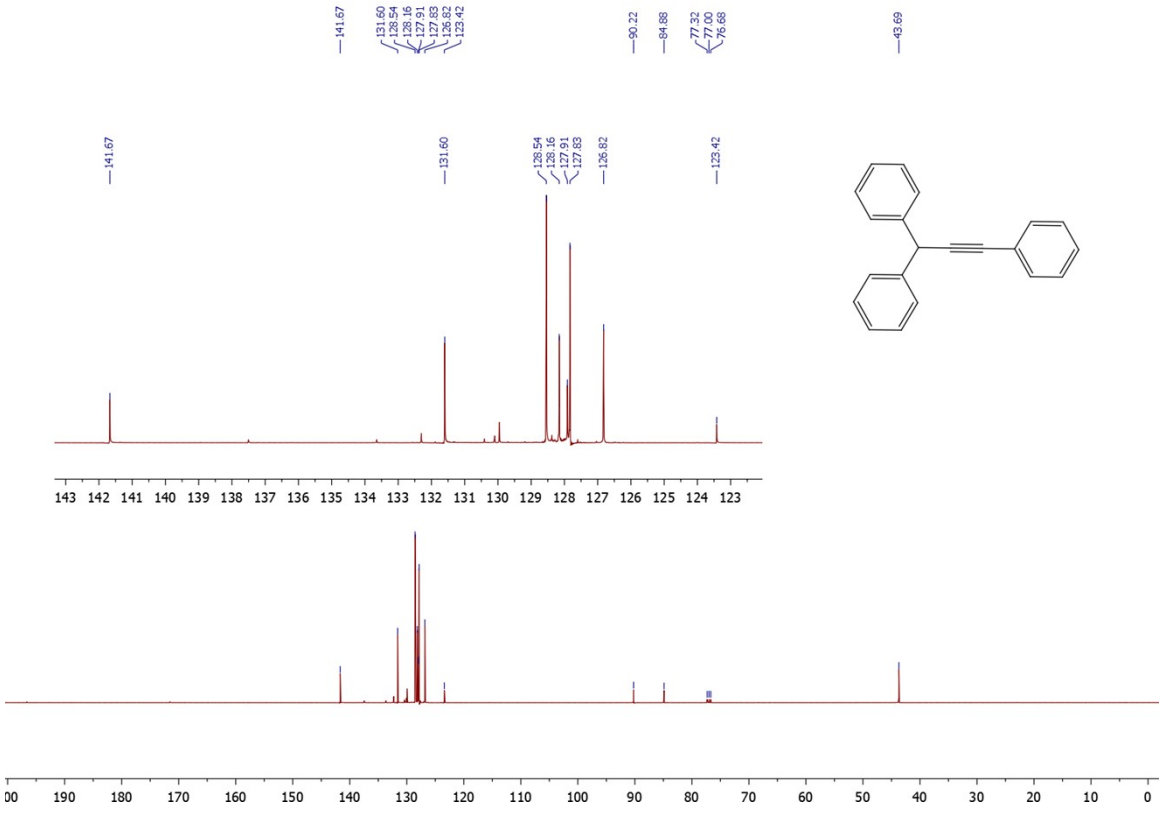


Figure S36. ^{13}C NMR (400 MHz, $CDCl_3$, 293 K) spectrum of prop-2-yne-1,1,3-triyltribenzene (**20a**).

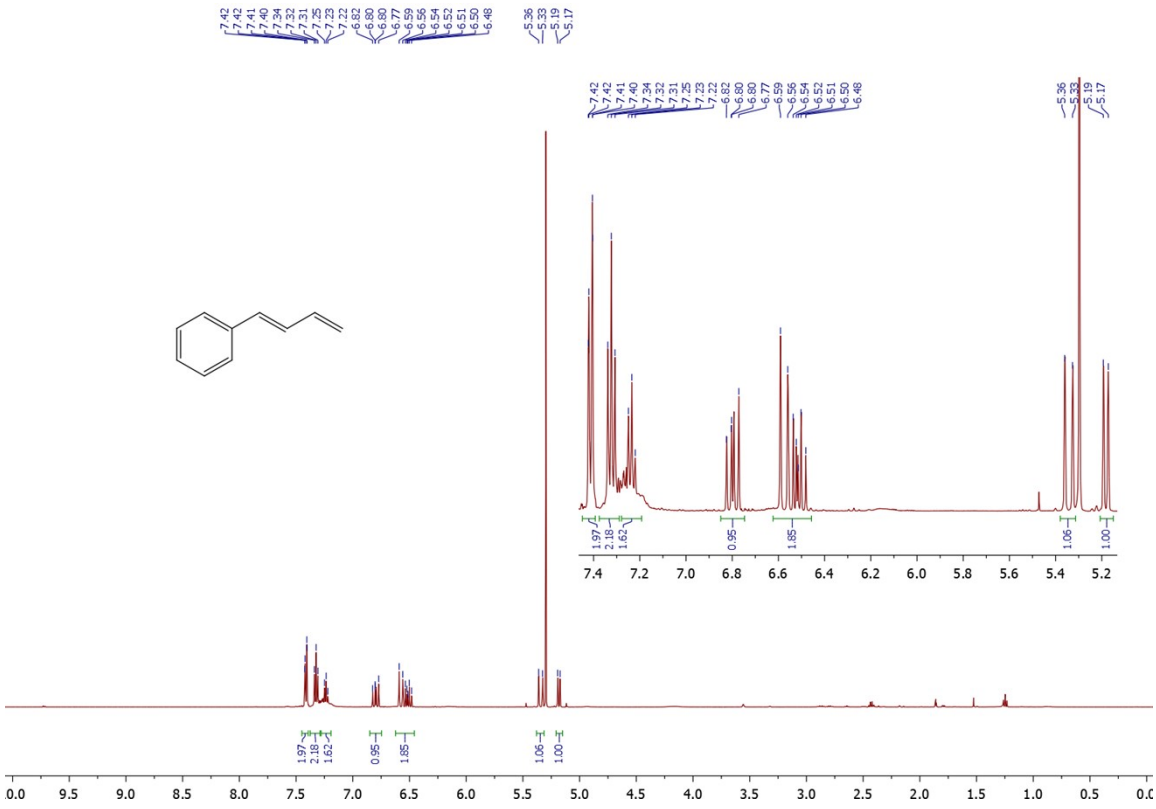


Figure S37. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of (E)-buta-1,3-dien-1-ylbenzene (**1**).

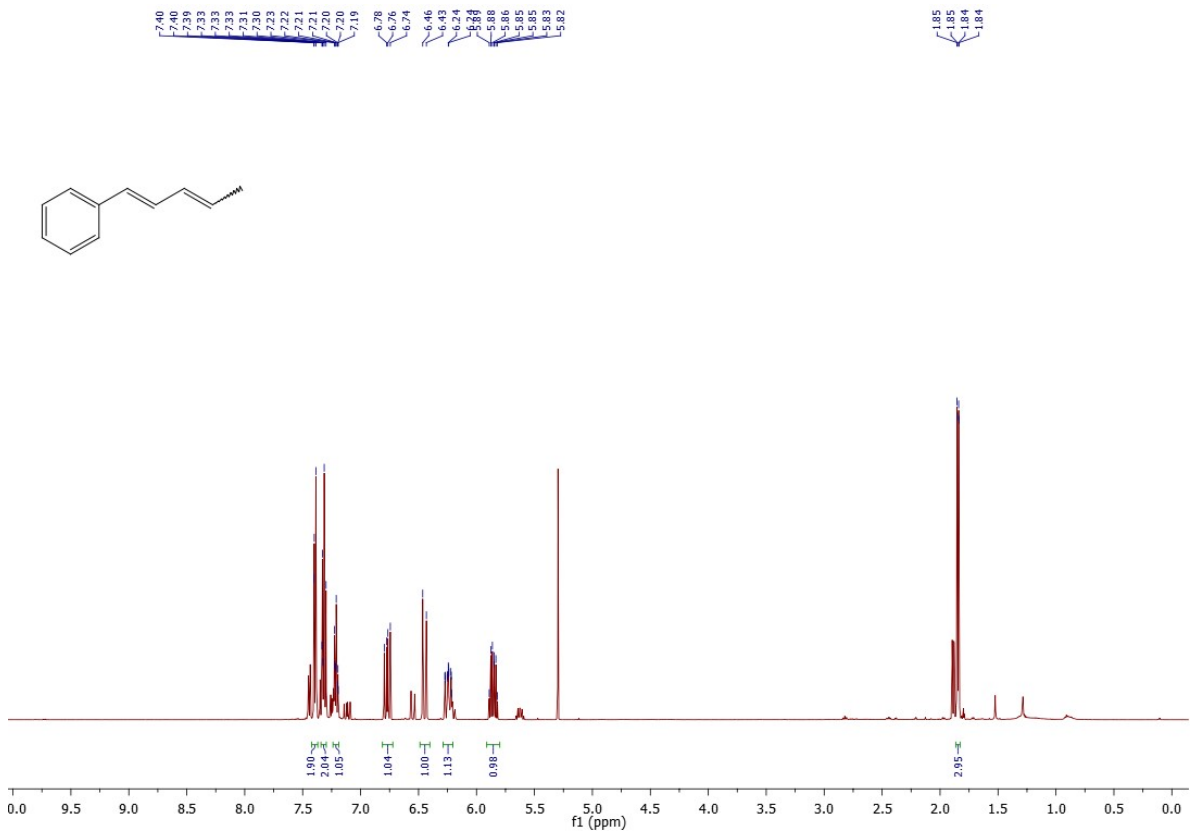


Figure S38. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of penta-1,3-dien-1-ylbenzene (**2**).

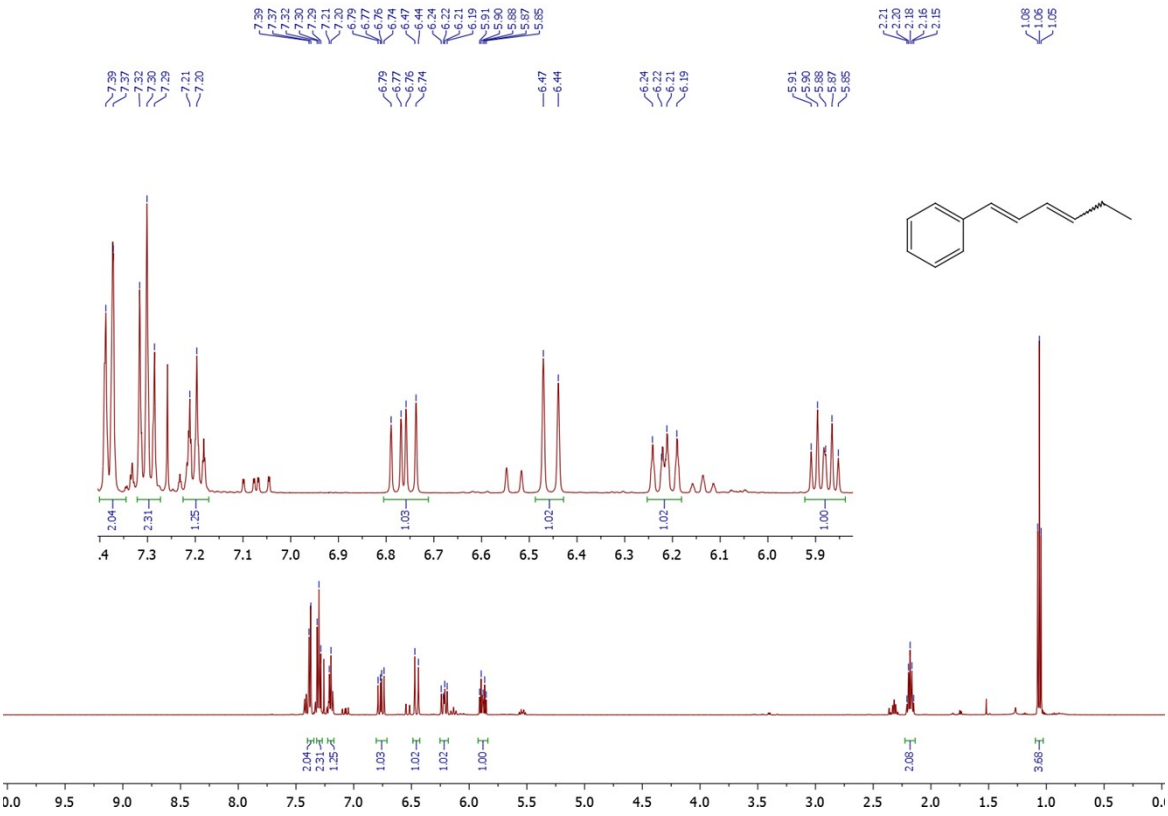


Figure S39. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of hexa-1,3-dien-1-ylbenzene (**3**).

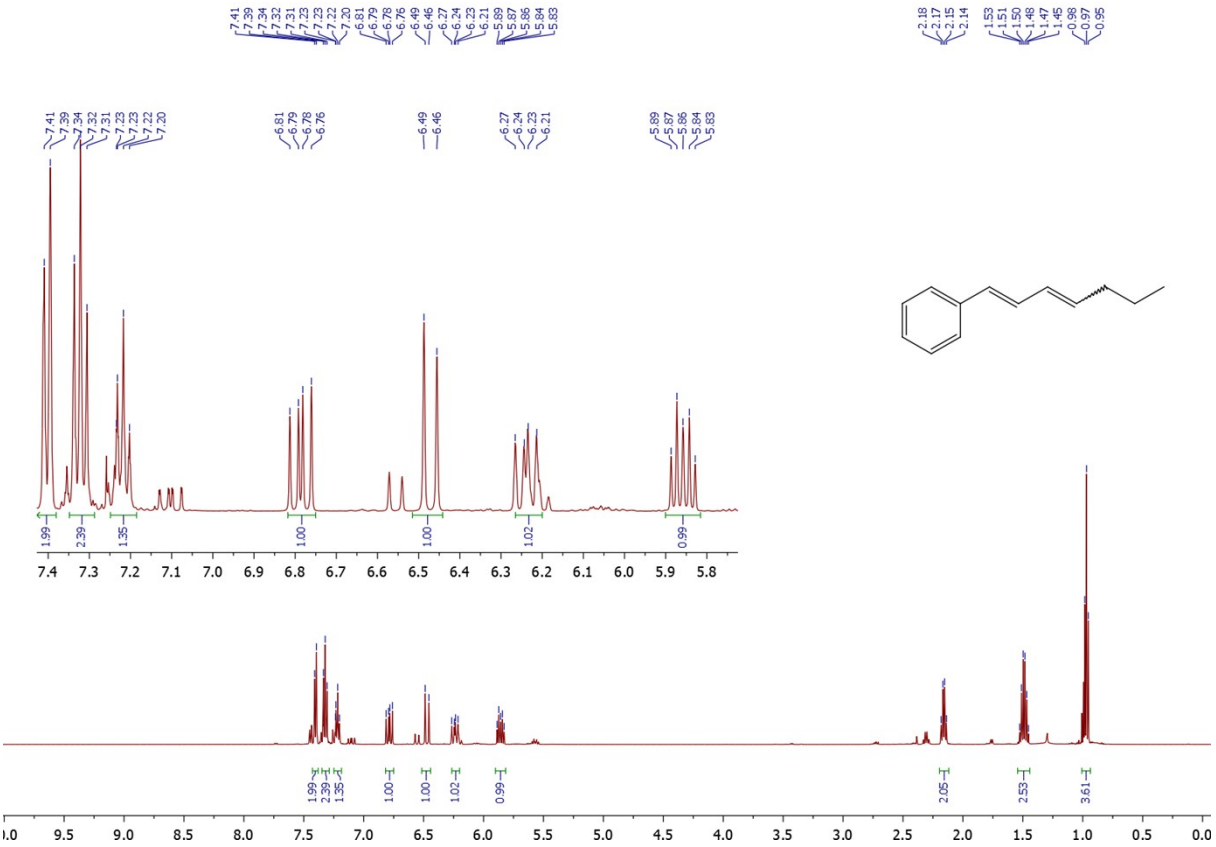


Figure S40. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of hepta-1,3-dien-1-ylbenzene (**4**).

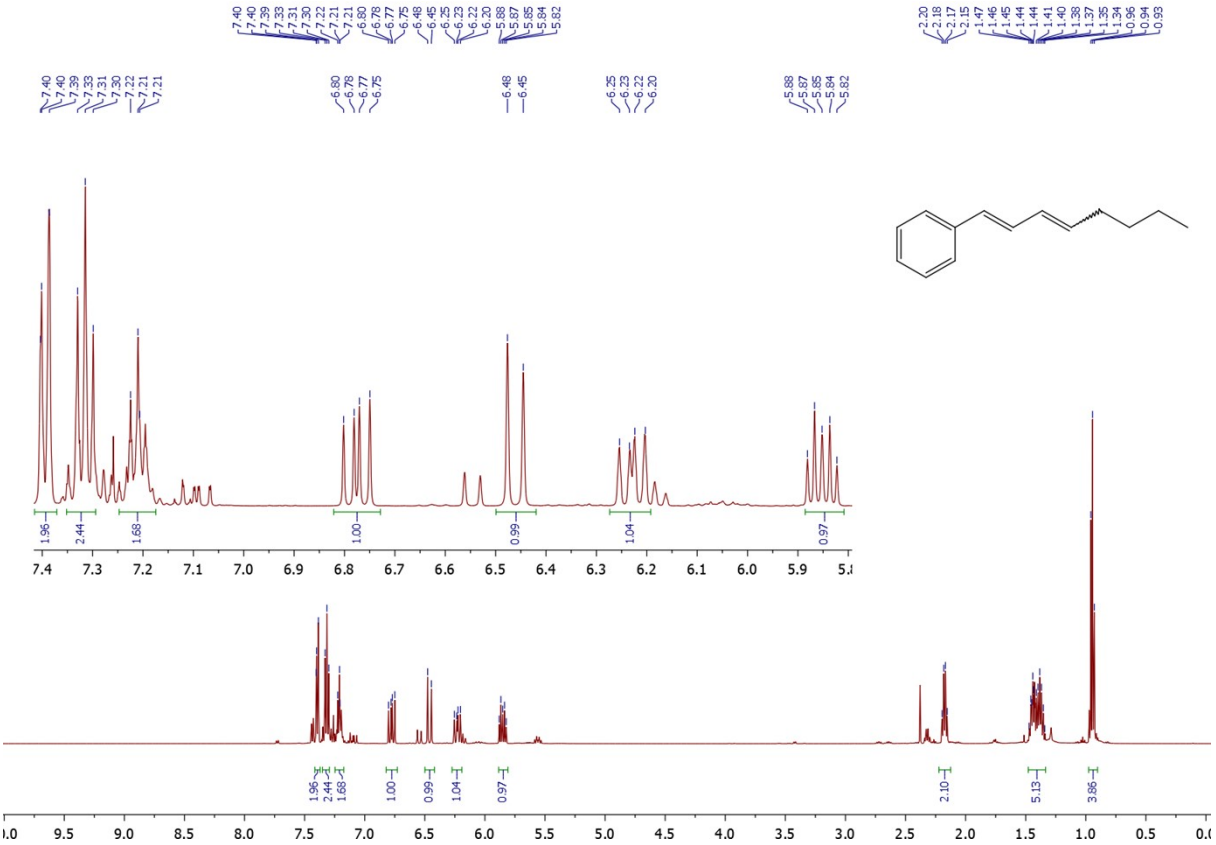


Figure S41. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of octa-1,3-dien-1-ylbenzene (**5**).

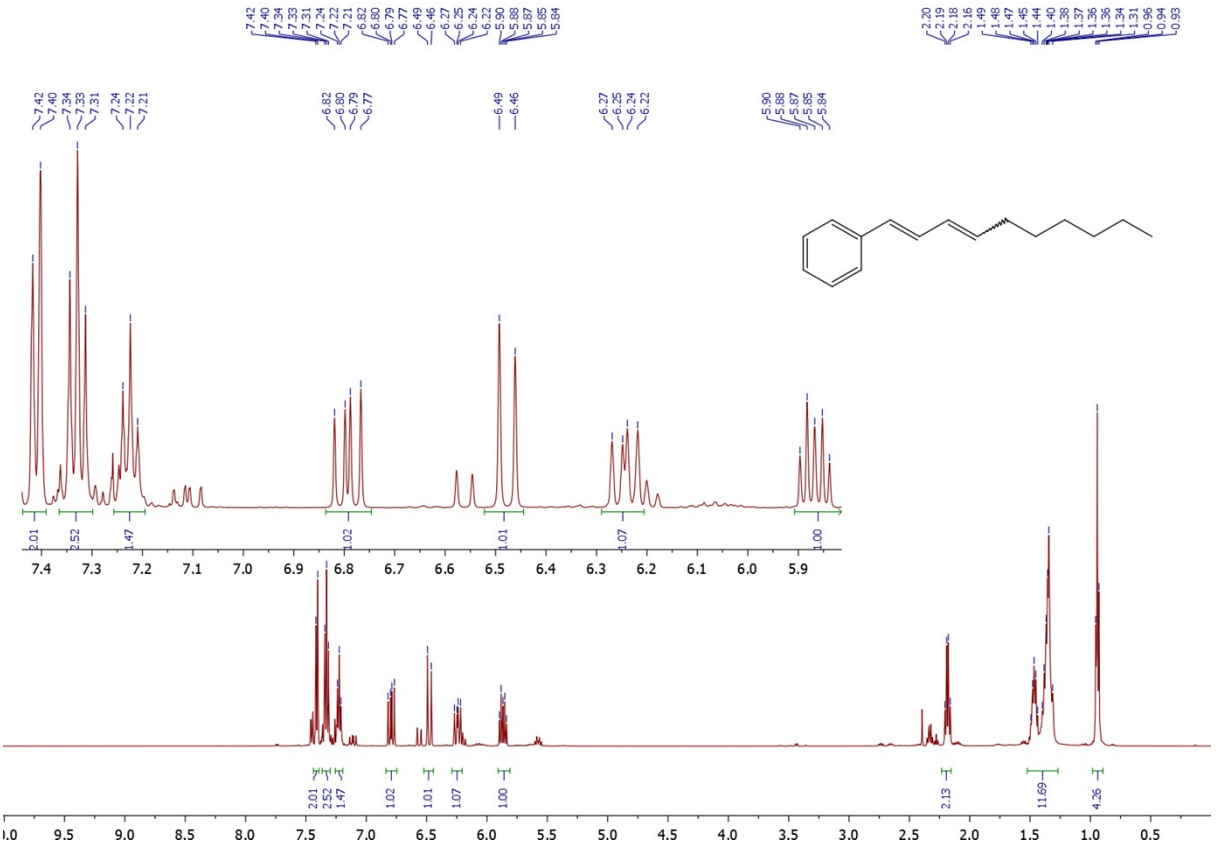


Figure S42. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of deca-1,3-dien-1-ylbenzene (**6**).

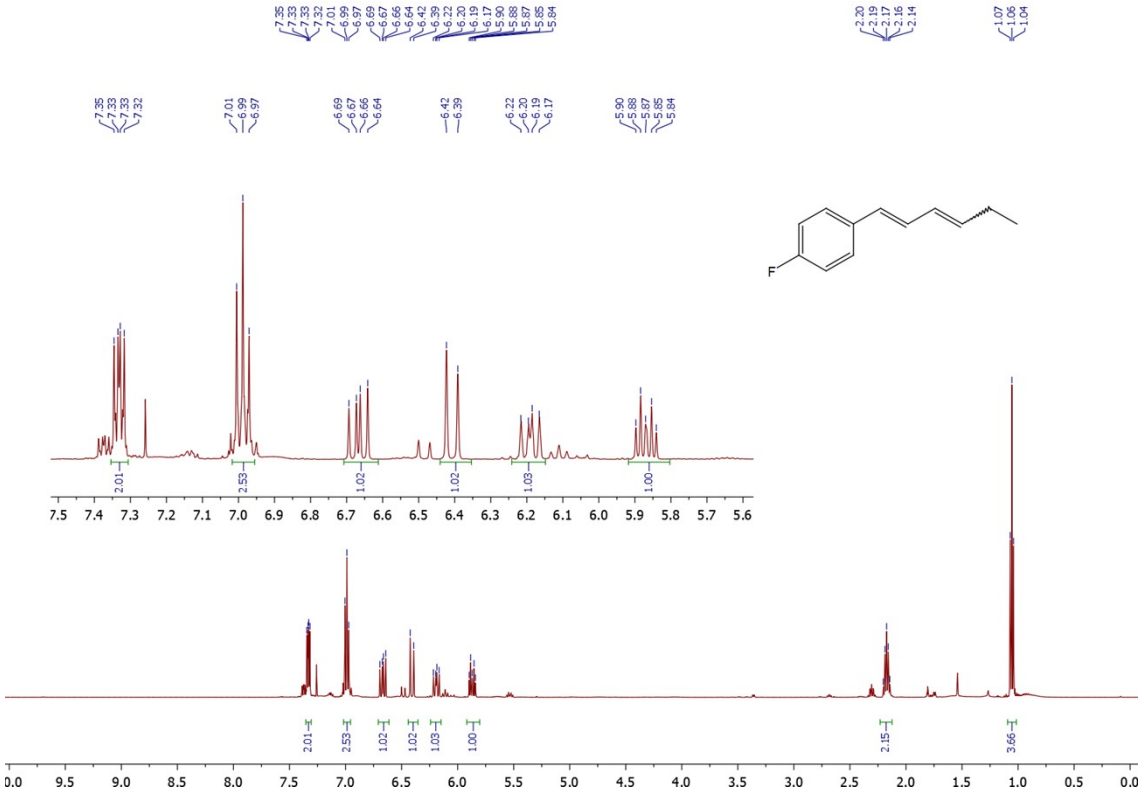


Figure S43. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1-fluoro-4-(hexa-1,3-dien-1-yl)benzene (**7**).

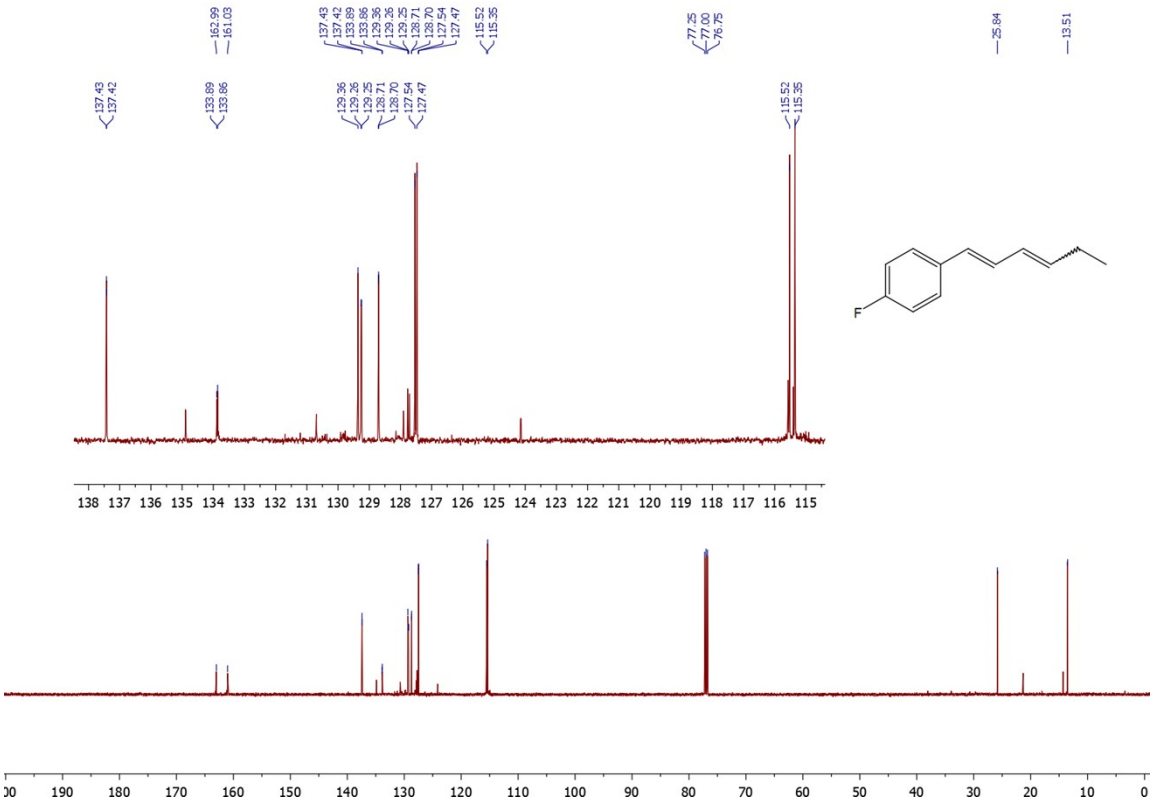


Figure S44. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 1-fluoro-4-(hexa-1,3-dien-1-yl)benzene (**7**).

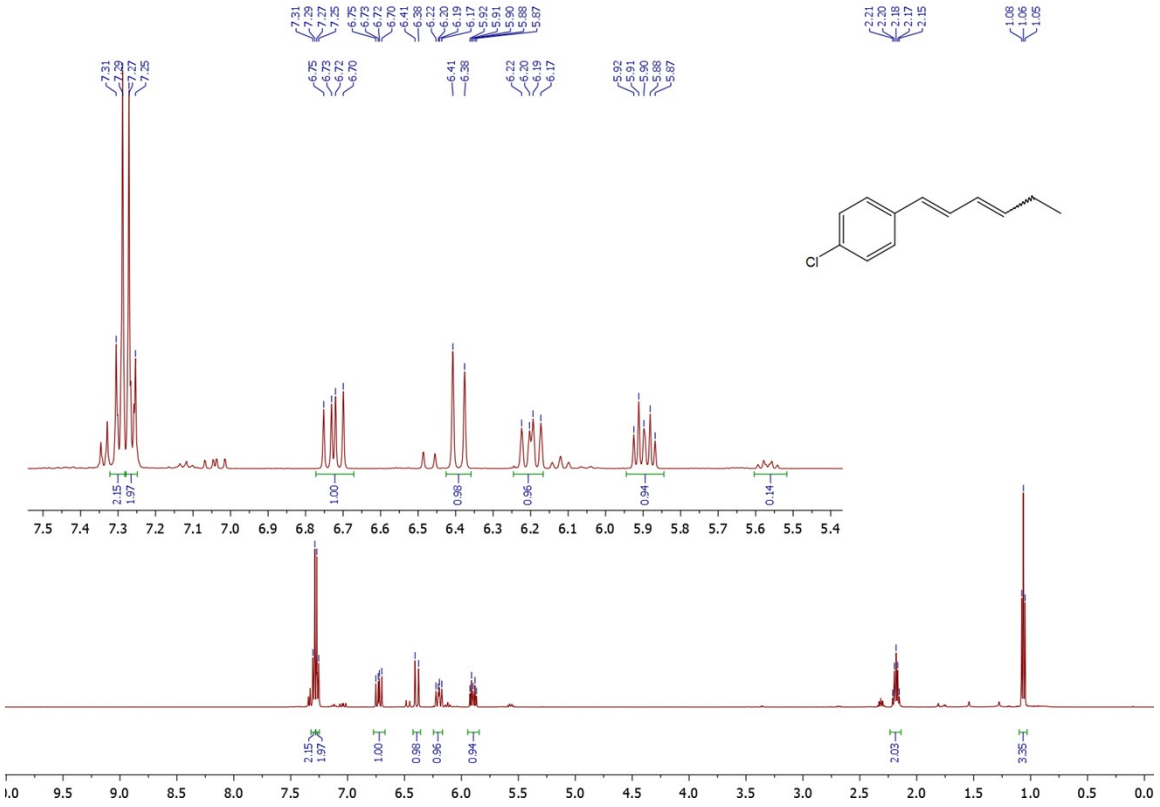


Figure S45. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1-chloro-4-(hexa-1,3-dien-1-yl)benzene (**8**).

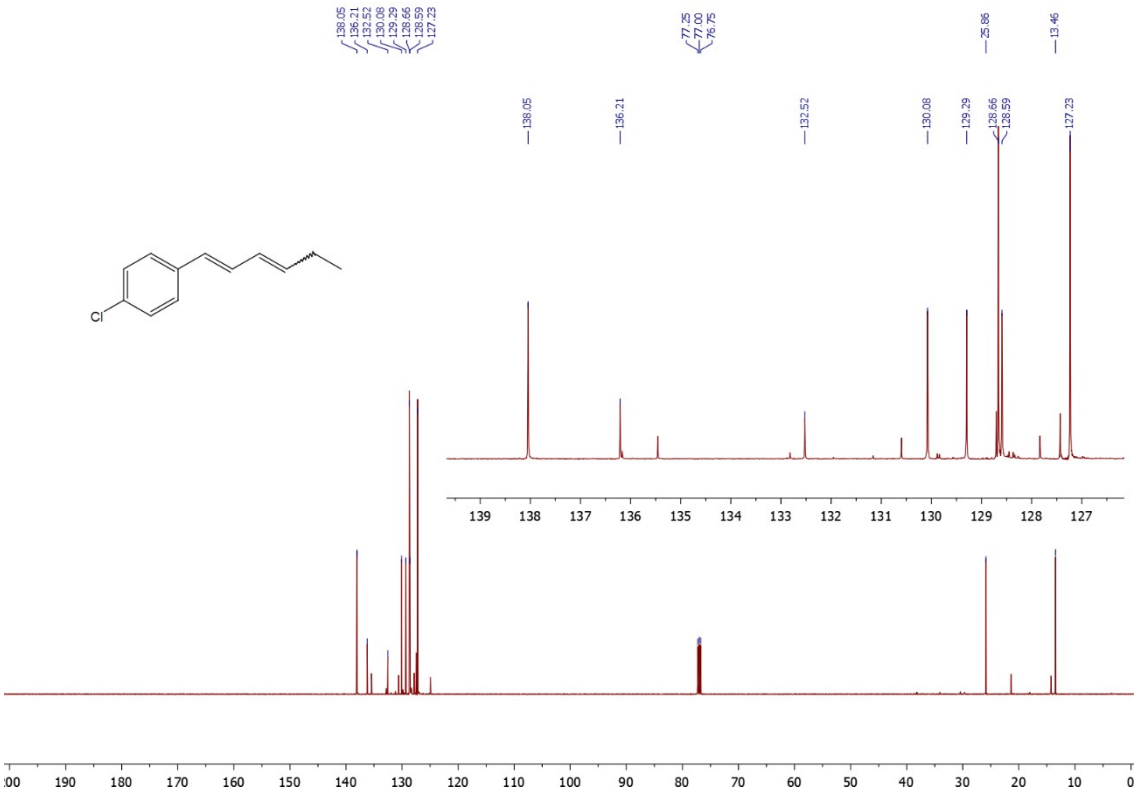


Figure S46. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 1-chloro-4-(hexa-1,3-dien-1-yl)benzene (**8**).

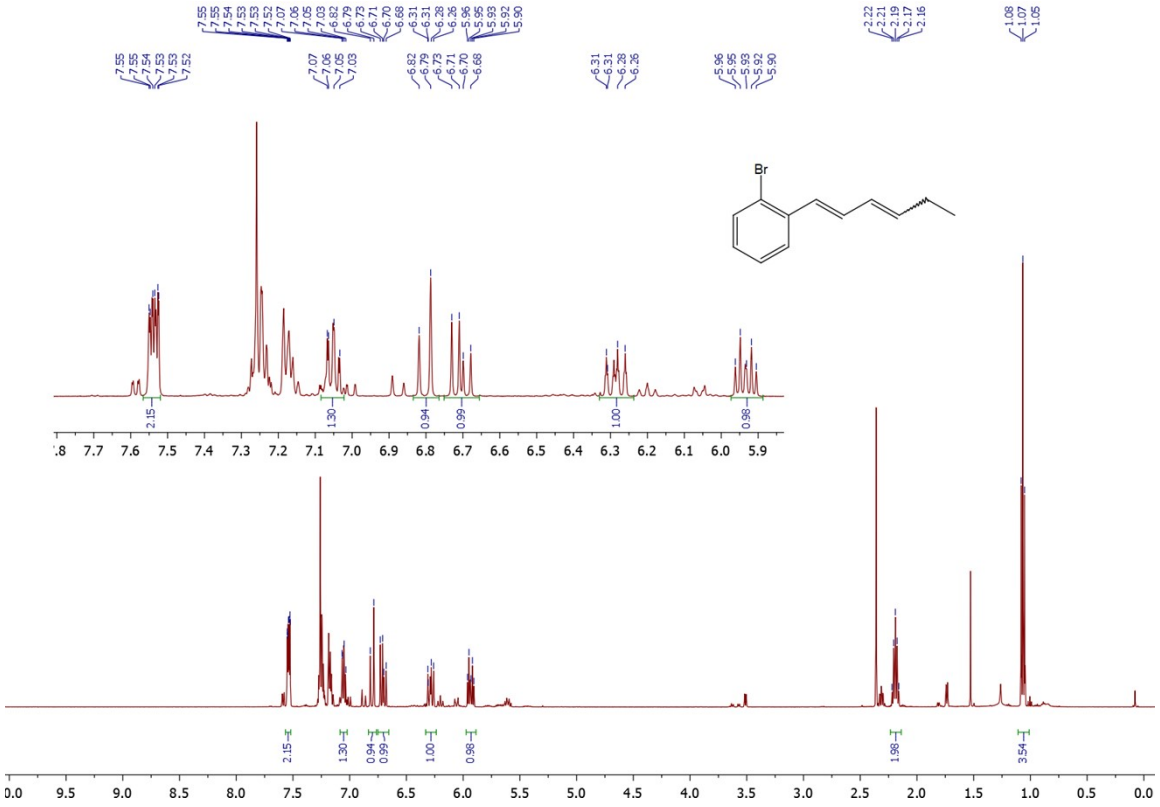


Figure S47. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of hexa-1,3-dien-1-yl-2-iodobenzene (**9**).

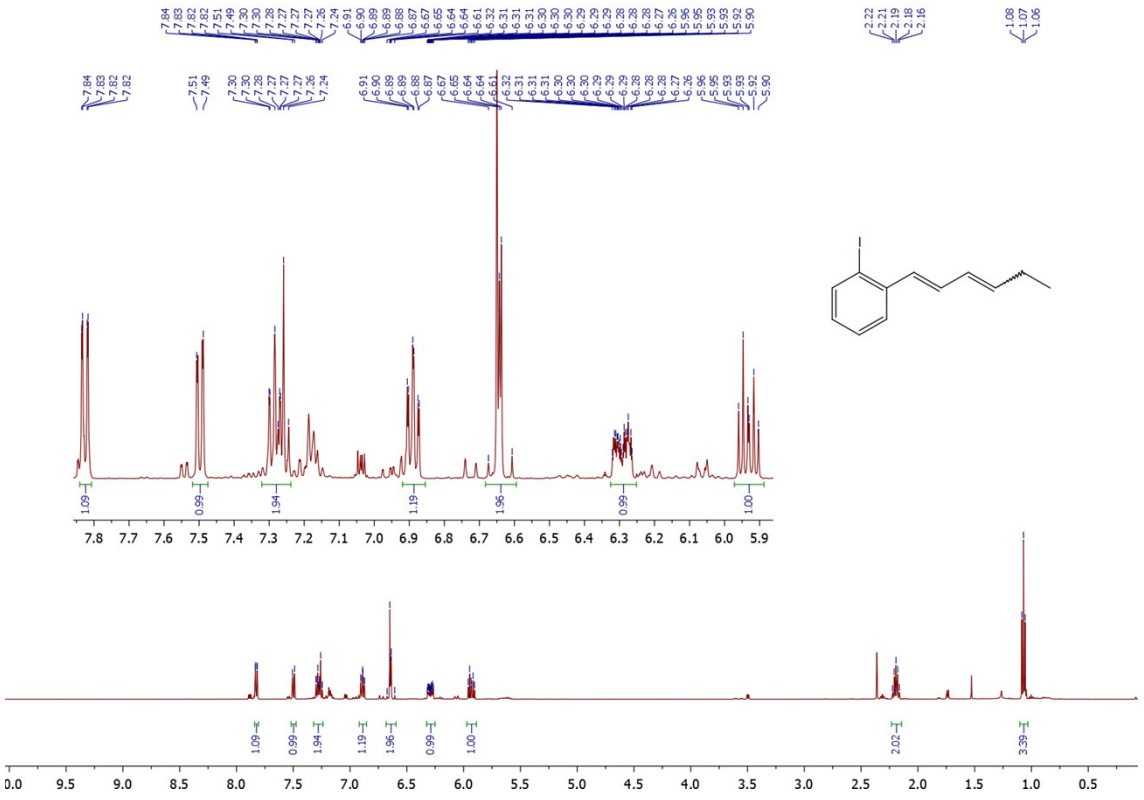


Figure S48. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of hexa-1,3-dien-1-yl-2-iodobenzene (**10**).

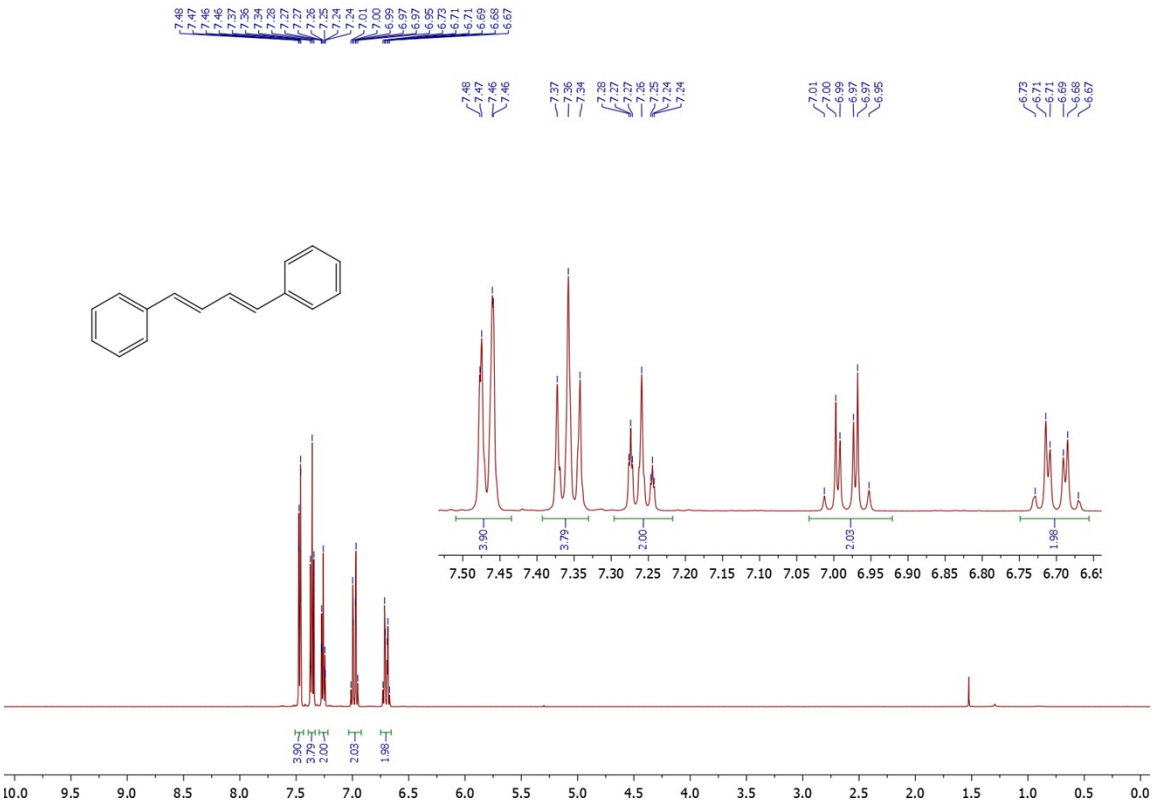


Figure S49. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of (1E,3E)-1,4-diphenylbuta-1,3-diene (**11**).

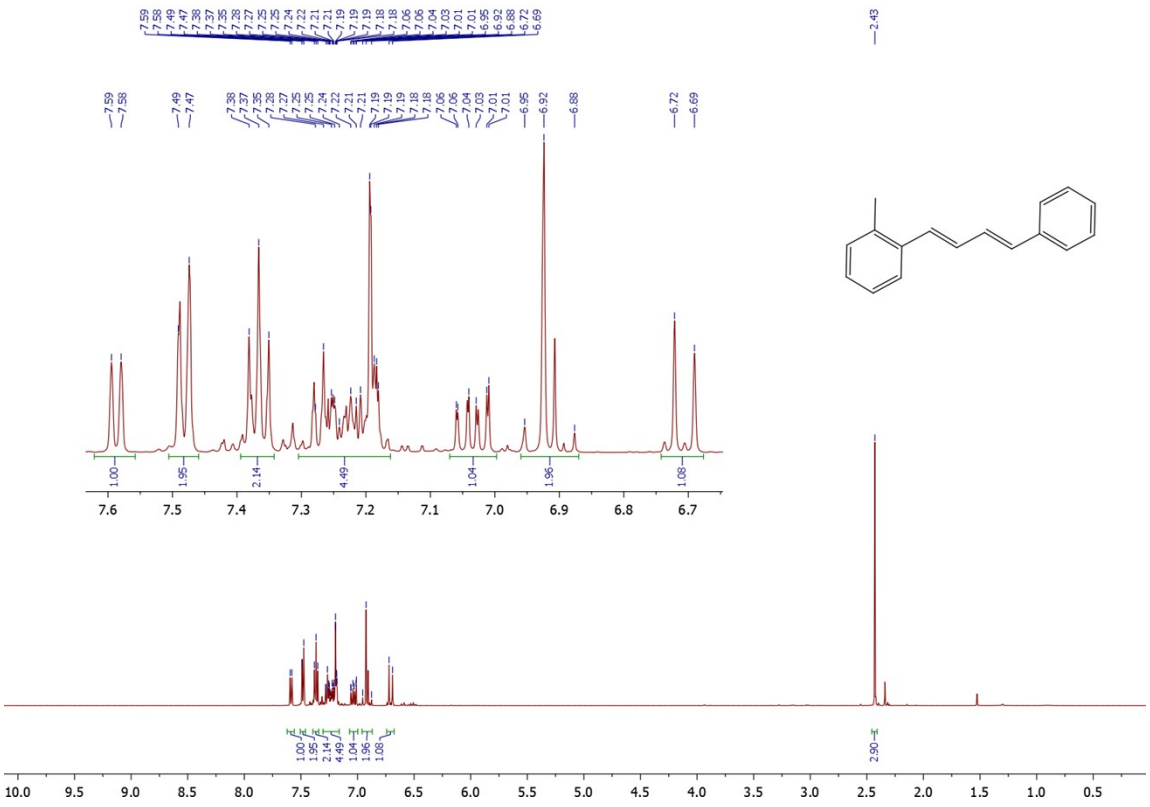


Figure S50. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1-methyl-2-((1E,3E)-4-phenylbuta-1,3-dien-1-yl)benzene (**12**).

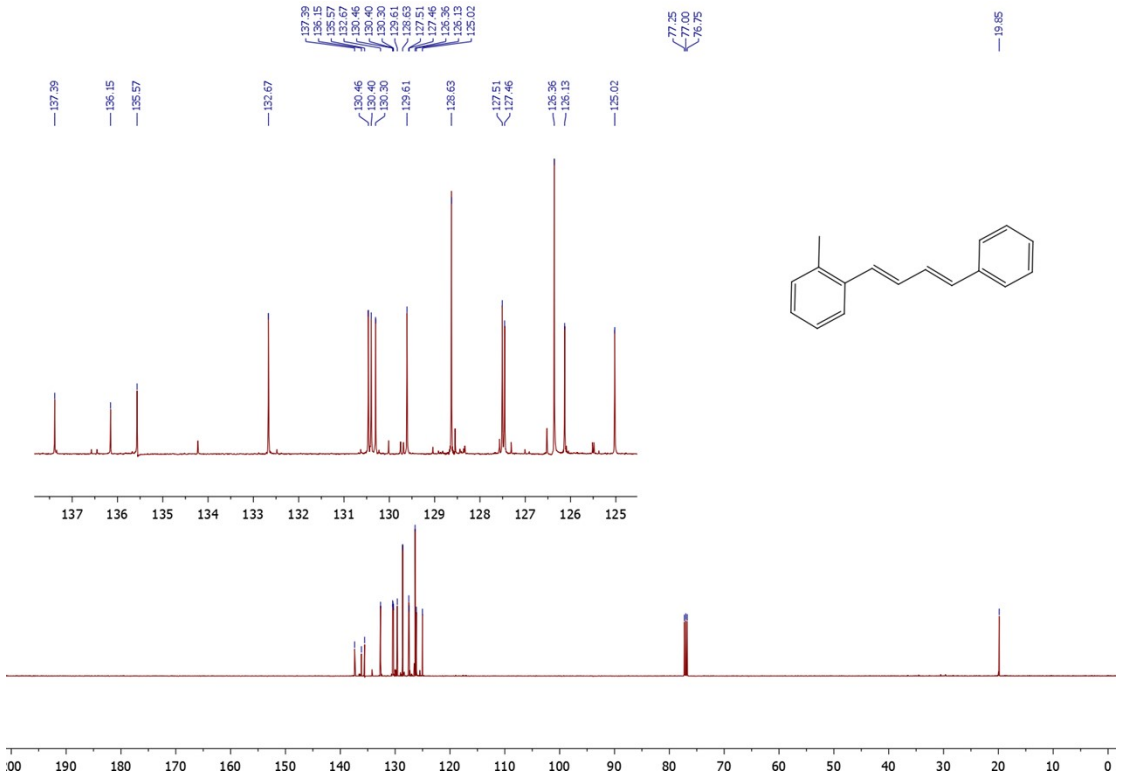


Figure S51. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 1-methyl-2-((1E,3E)-4-phenylbuta-1,3-dien-1-yl)benzene (**12**).

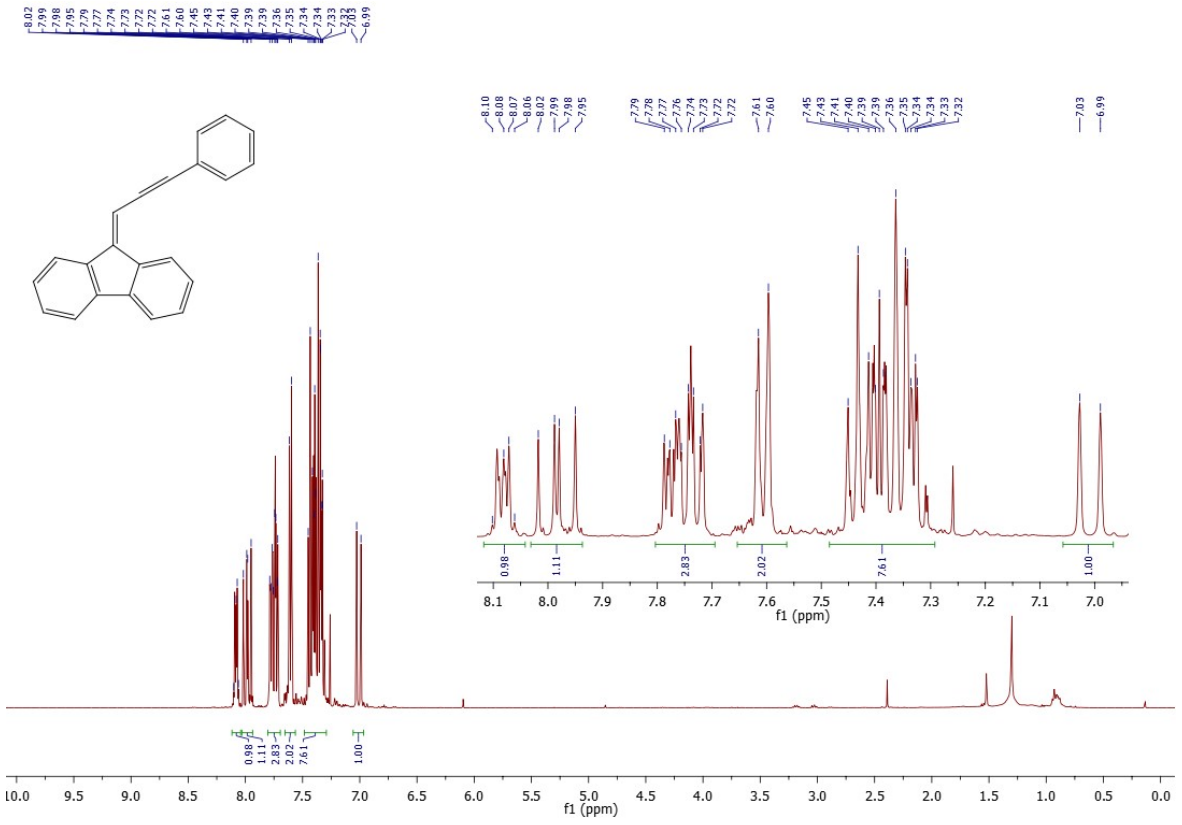


Figure S52. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 9-(3-phenylallylidene)-9H-fluorene (**13**).

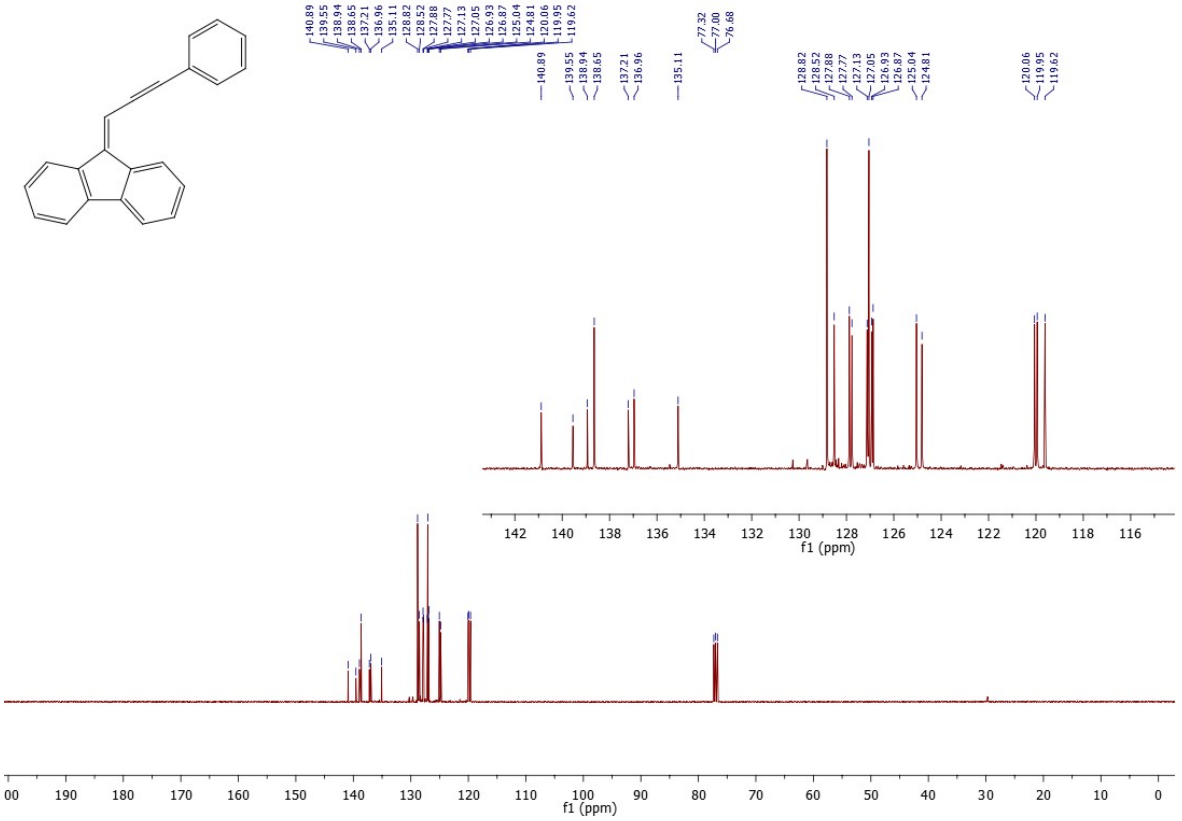


Figure S53. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 9-(3-phenylallylidene)-9H-fluorene (**13**).

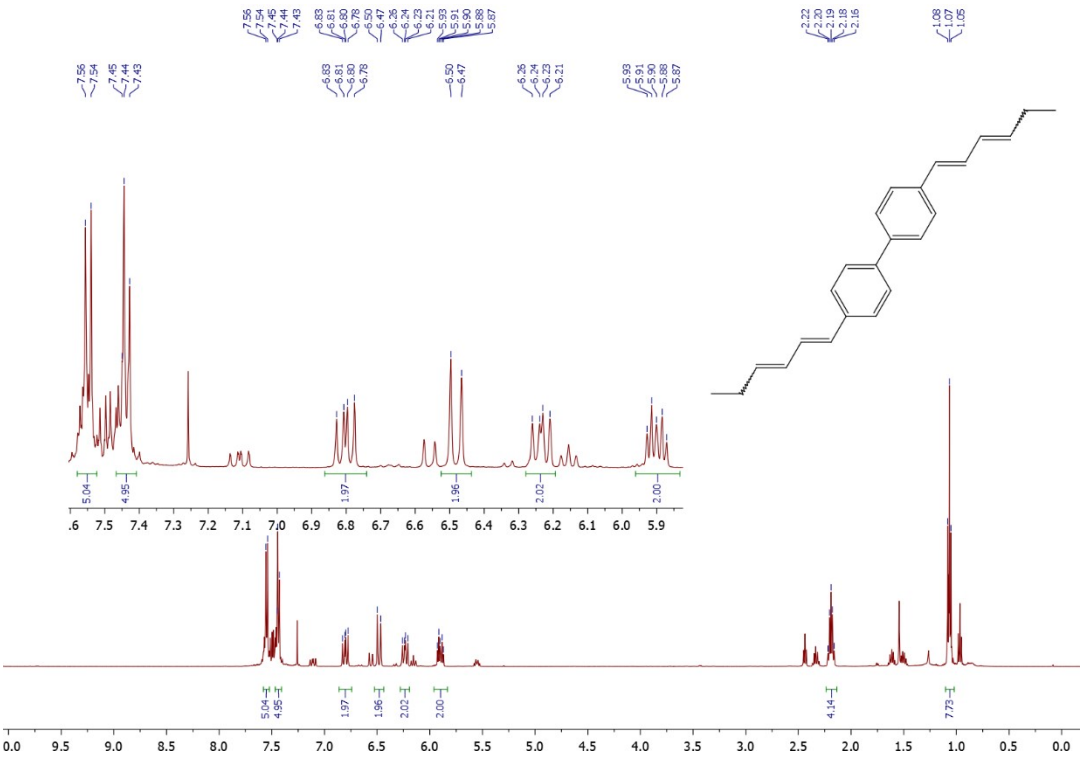


Figure S54. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 4,4'-di(hexa-1,3-dien-1-yl)-1,1'-biphenyl (**14**).

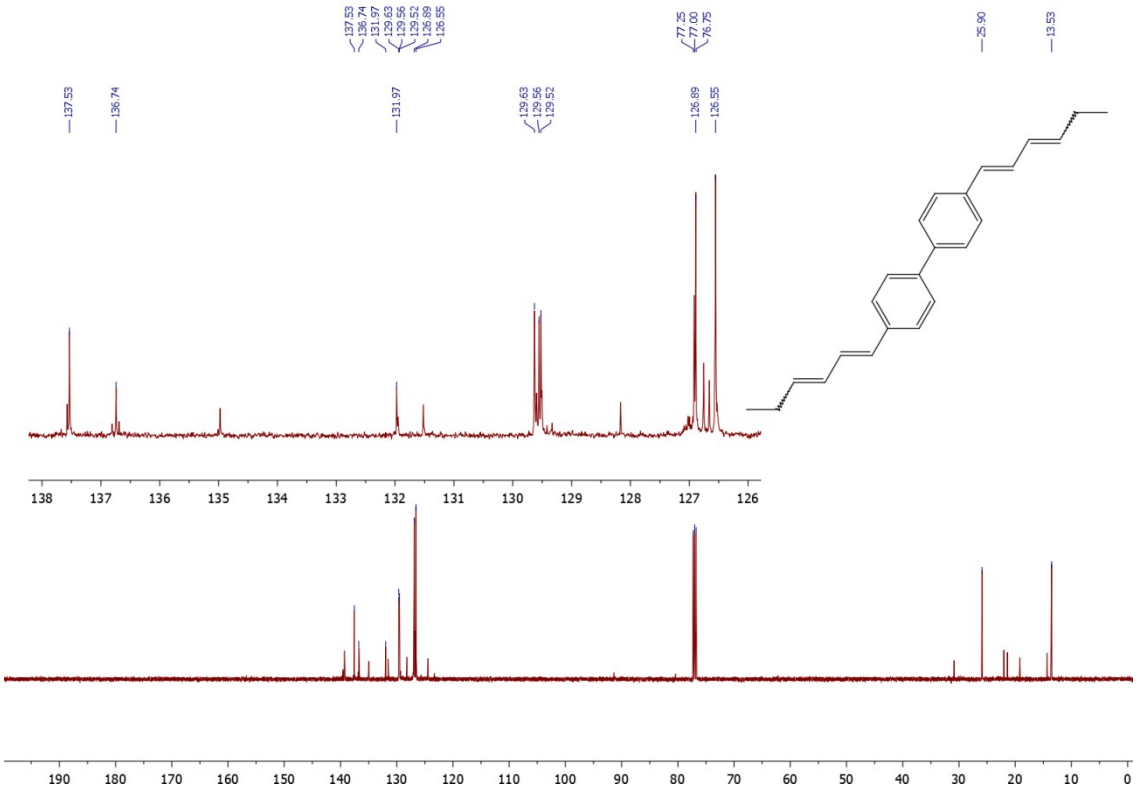


Figure S55. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 4,4'-di(hexa-1,3-dien-1-yl)-1,1'-biphenyl (**14**).

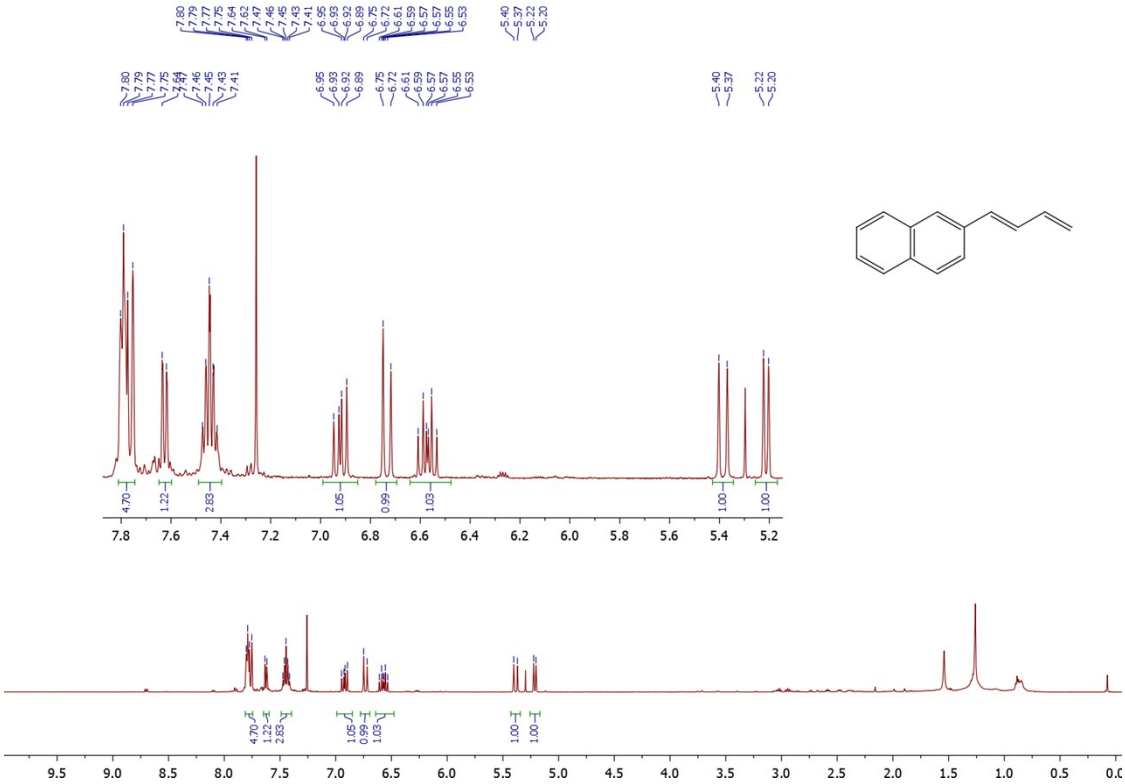


Figure S56. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of (E)-2-(buta-1,3-dien-1-yl)naphthalene (**15**).

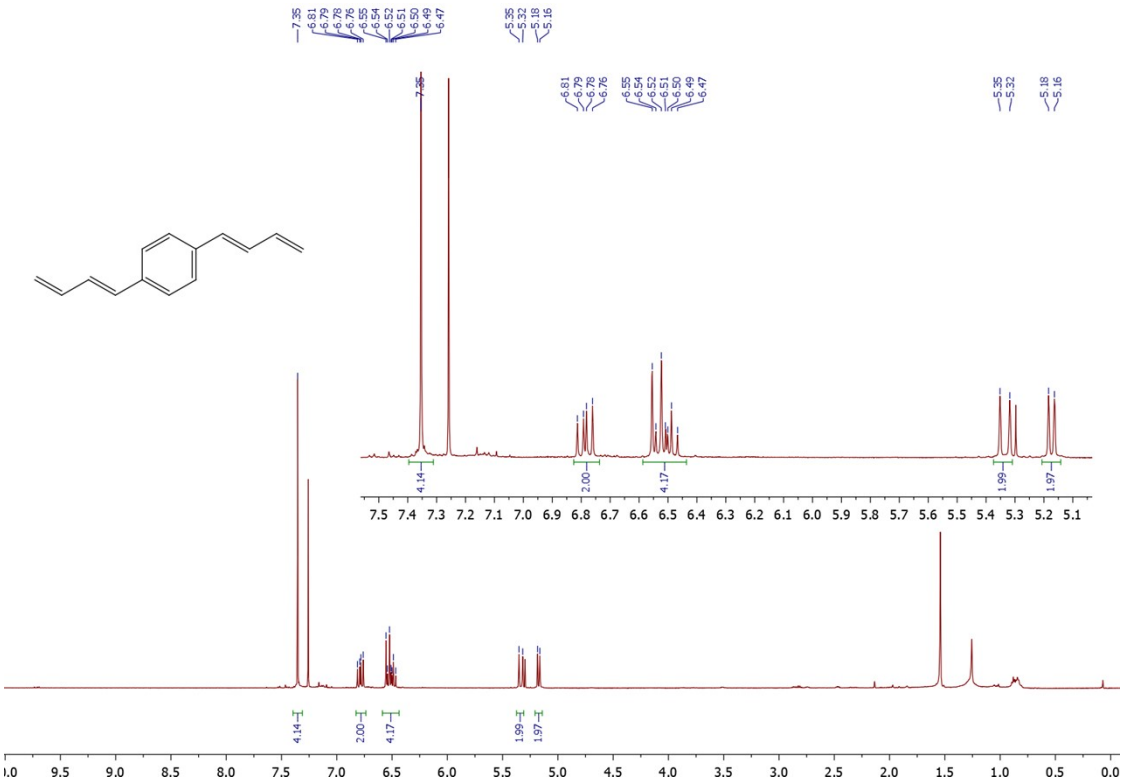


Figure S57. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1,4-di((E)-buta-1,3-dien-1-yl)benzene (**16**).

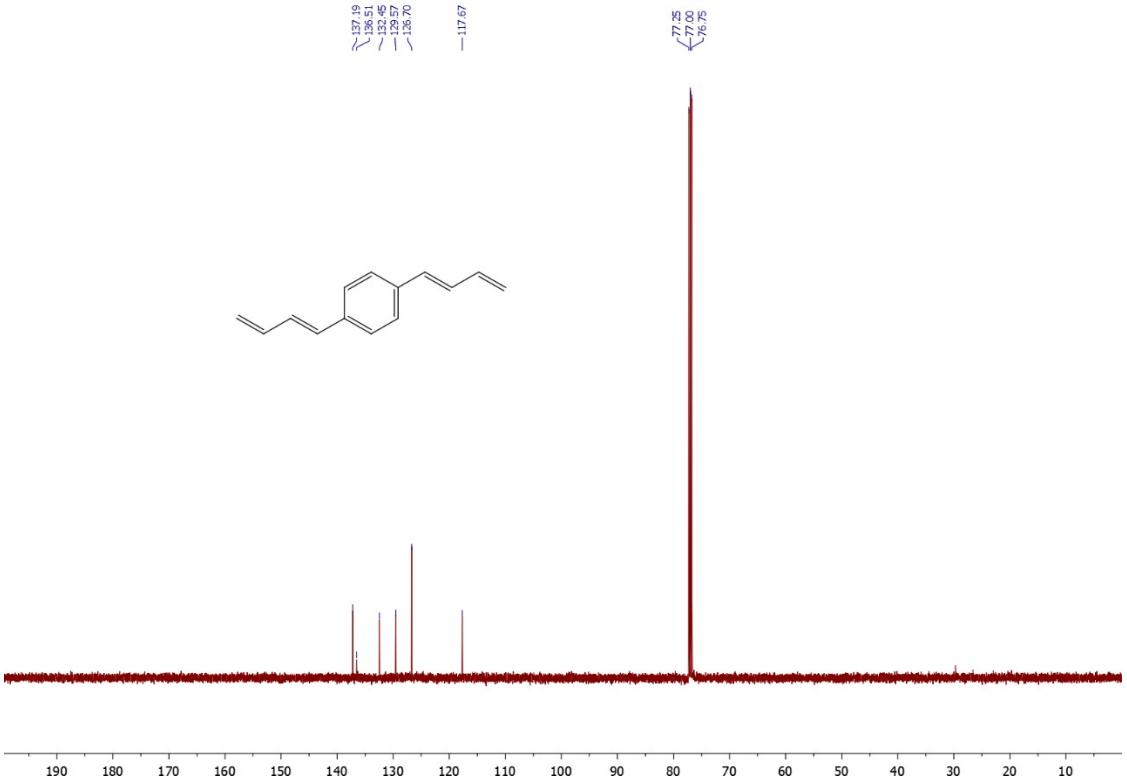


Figure S58. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 1,4-di((E)-buta-1,3-dien-1-yl)benzene (**16**).

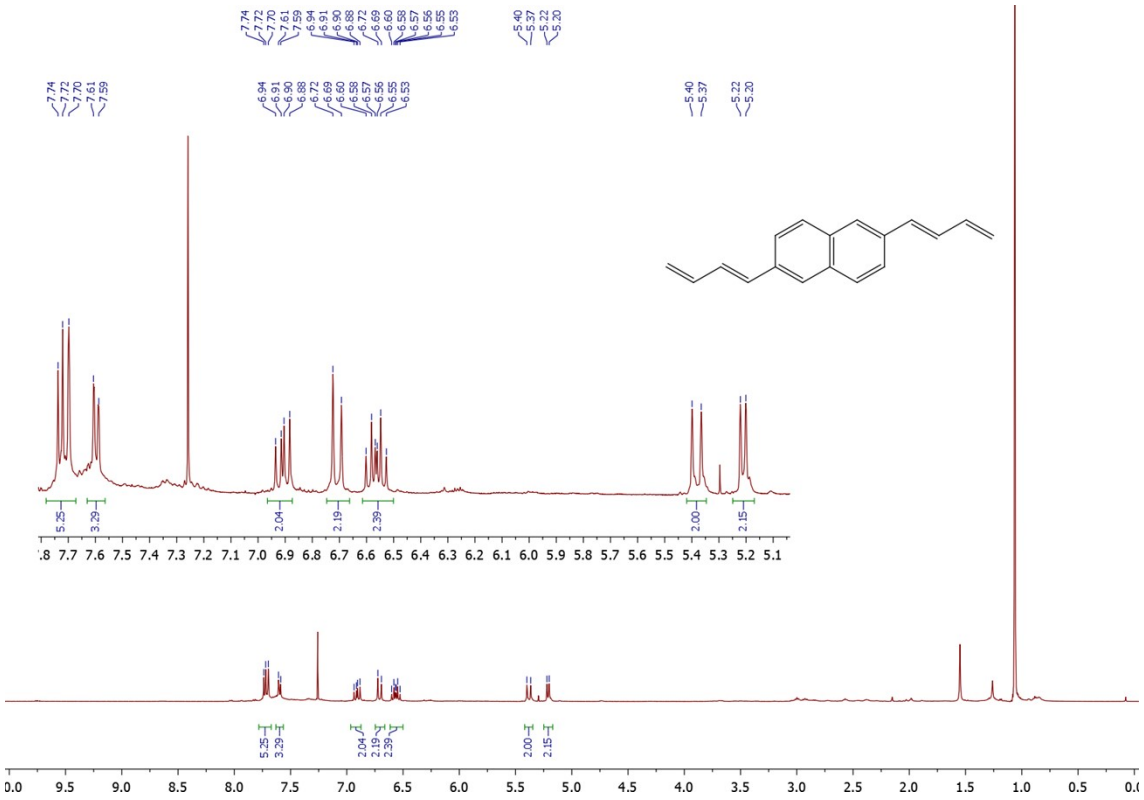


Figure S59. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 2,6-di((E)-buta-1,3-dien-1-yl)naphthalene (**17**).

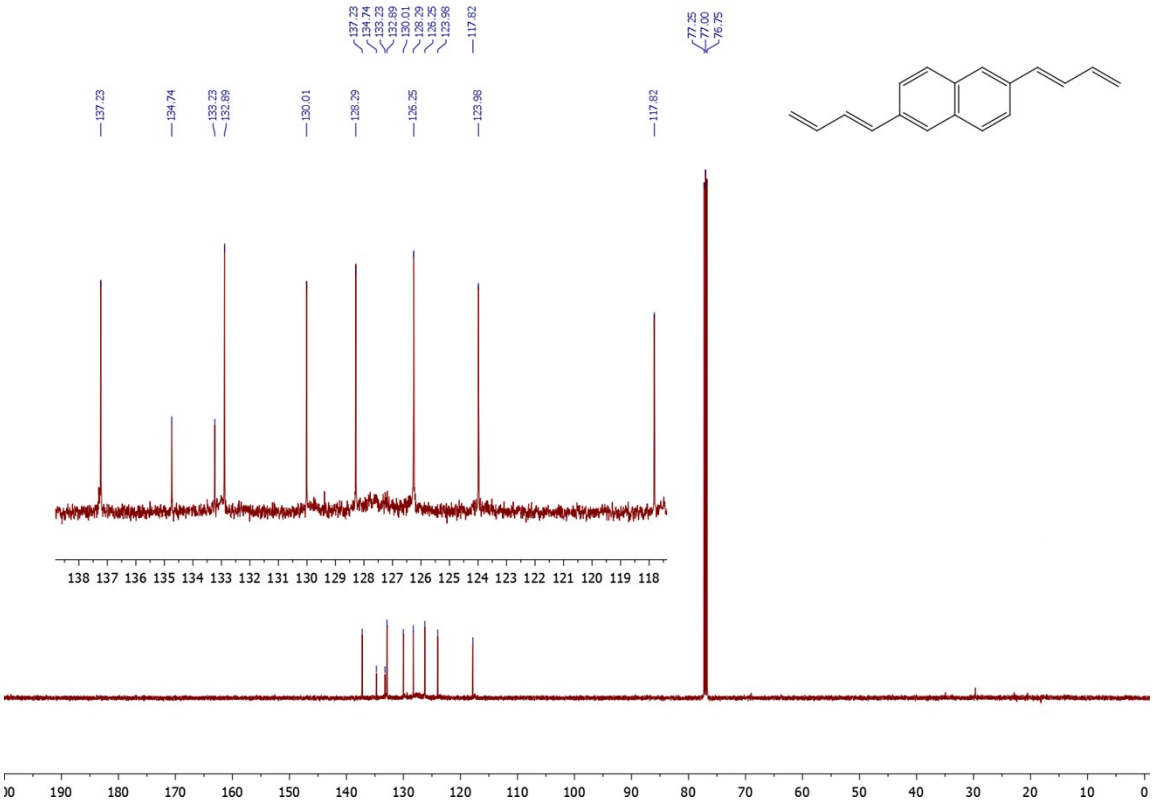


Figure S60. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 2,6-di((E)-buta-1,3-dien-1-yl)naphthalene (**17**).

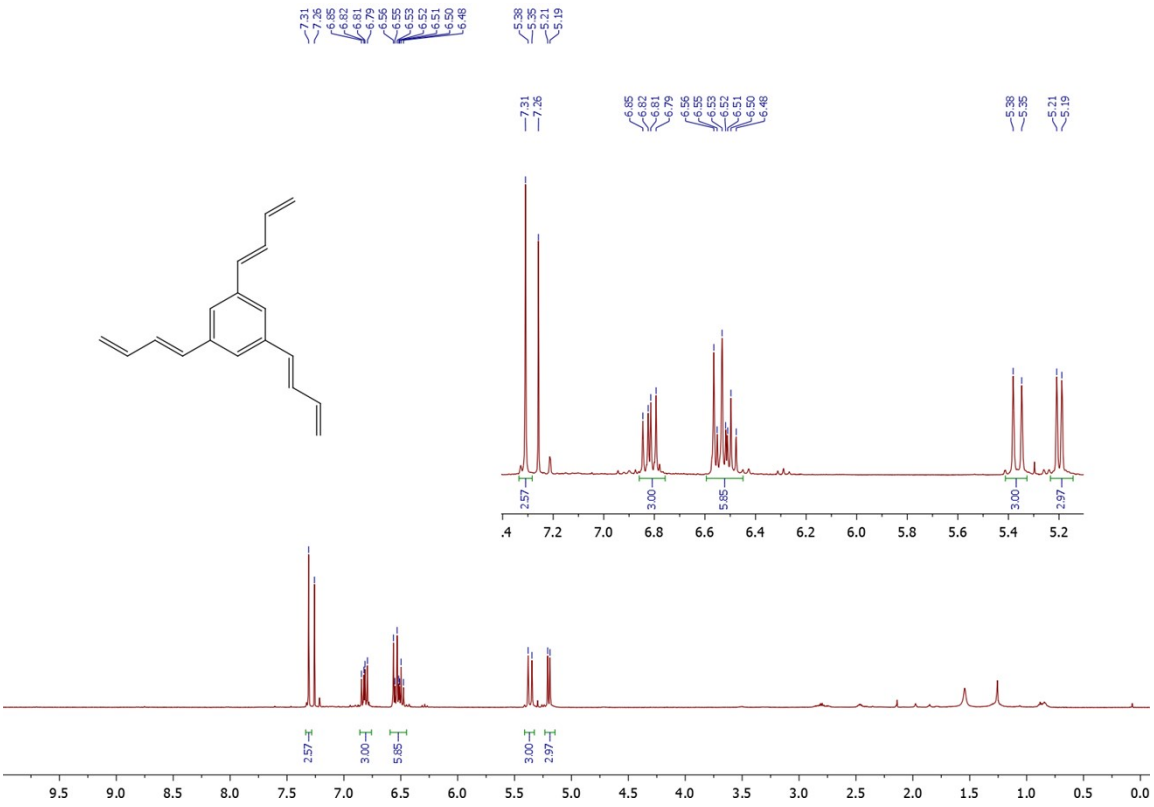


Figure S61. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1,3,5-tri((E)-buta-1,3-dien-1-yl)benzene (**18**).

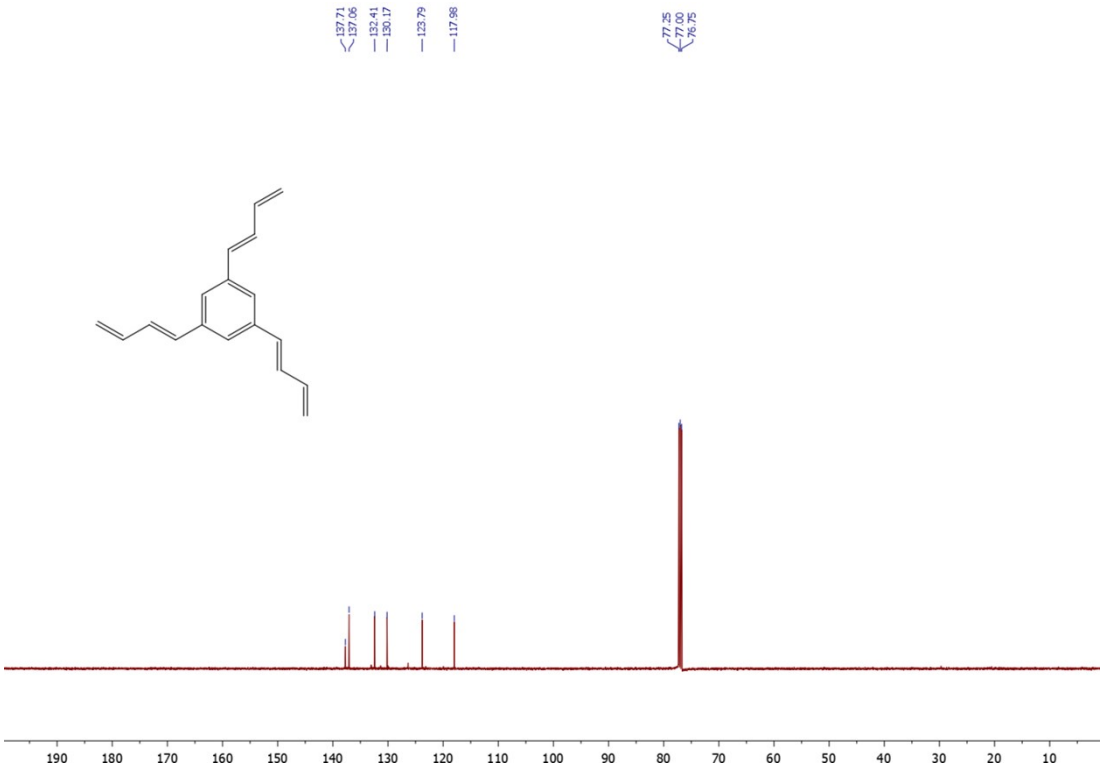


Figure S62. ^{13}C NMR (126 MHz, $CDCl_3$, 293 K) spectrum of 1,3,5-tri((E)-buta-1,3-dien-1-yl)benzene (**18**).

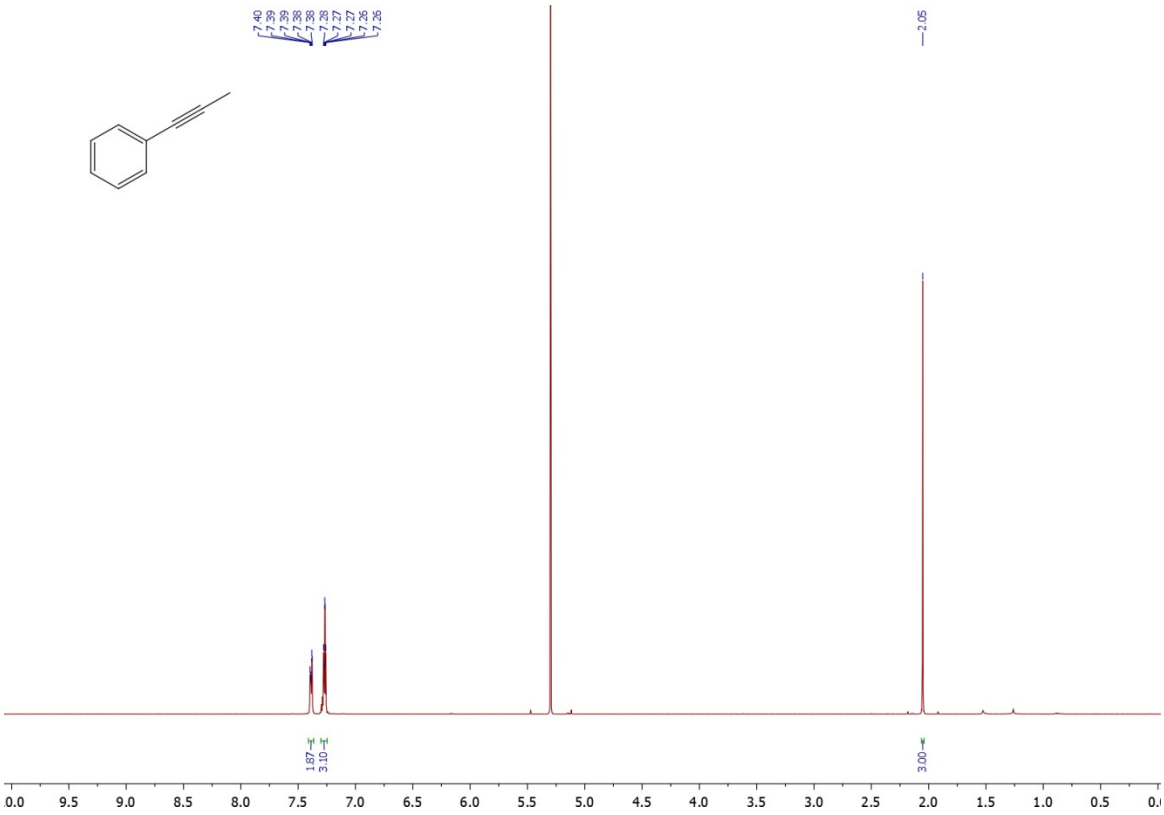


Figure S63. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of prop-1-yn-1-ylbenzene (**19**).

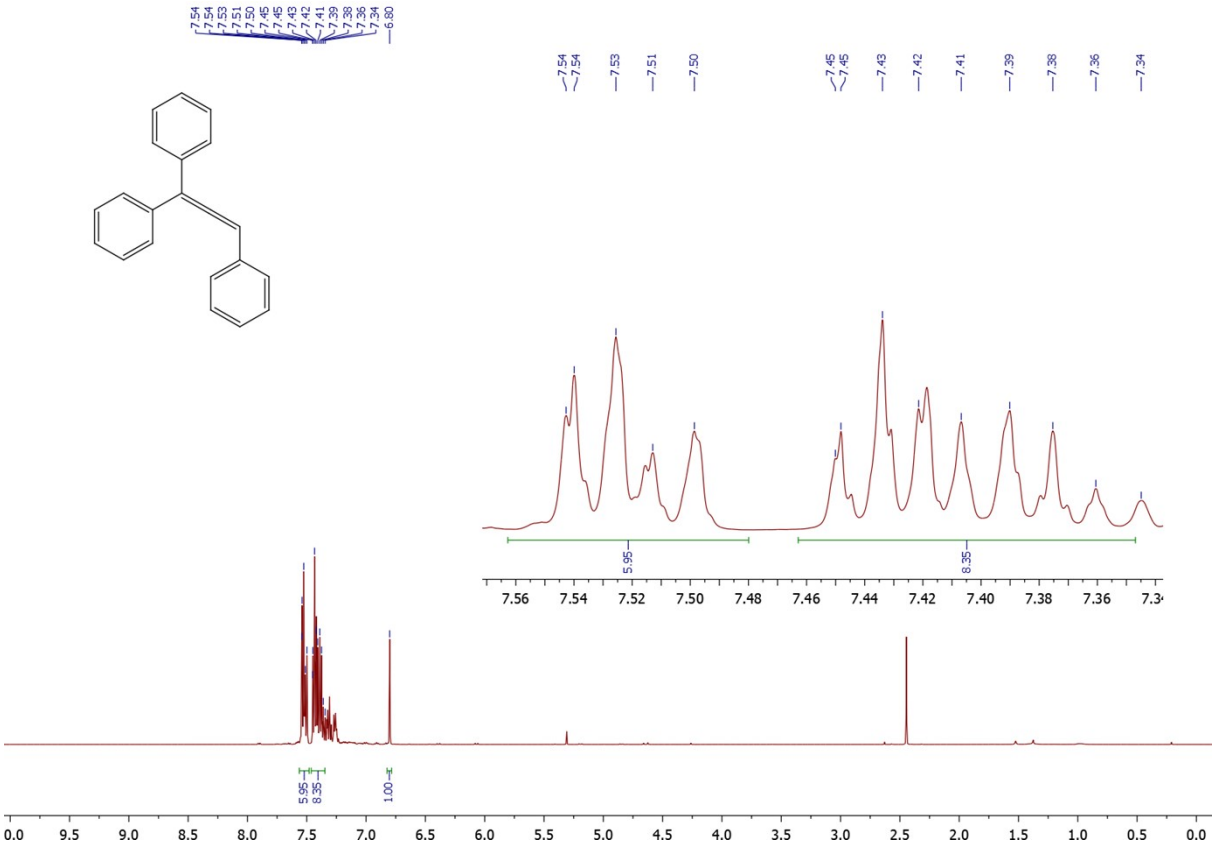


Figure S64. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) spectrum of 1,1,3-triphenylpropa-1,2-diene (**20**).

Computational Methods:

Periodic DFT calculations were performed with Vienna Ab Initio Simulation Package (VASP) (*72*, *73*)version 5, using PBE functional and zero damping DFT-D3. Energy cutoff (ENCUT) 400 eV, EDIFF = 1.00e-07. Bulk γ-Al_2O_3 (Digne's model) was previously optimized (ISIF = 3) with 800 eV energy cutoff (that has little effect on geometry). 110 surface of cubic alumina (100 notation for Digne's model) is the same as used in previous work (illustrated discussion can be found in ESI of that paper). 100 surface of cubic alumina was reproduced by 001 surface of Digne's model. Both surfaces are modelled containing 4 layers, of which 2 top layers are optimised and 2 bottom are frozen in geometry of bulk. 2x2 cell is used in calculations with adsorbed molecules. Butyne was used as adsorbate for the modelling.

Nonperiodic DFT-calculations were performed with ORCA 5.0.1 software. (*74*, *75*)

As it was previously reported by Khivantsev *et al*. (44), there are 2 microscopic surfaces observable on macroscopic 110 cut, namely, 111 and 100. Since 111 surface is completely covered with oxygen atoms and contains no Lewis acidic Al-sites, the reaction was investigated on 100 surface. This dehydrated surface contains few different Al(V) centres, whereas only one Al-site shows significant adsorption with butyne (the respective Al-site is highlighted in the Fig. S69). In this case butyne is oriented so that methyl groups of butyne are located above the "caves" on the surface). 3×2×1 k-points were applied (unit cell parameters mentioned before coordinates, approx. 11.1×16.7×26)

Table S3. Butyne adsorption on 001 surface (Al_V)

System	Total energy (eV)	Relative energy (kcal/mol)
Butyne1-Al_2O_3-001 (phys)	-1241.22809476	8.1
Butyne2-Al_2O_3-001 (best)	-1241.57888189	0.0
Butyne3-Al_2O_3-001	-1241.10292388	11.0

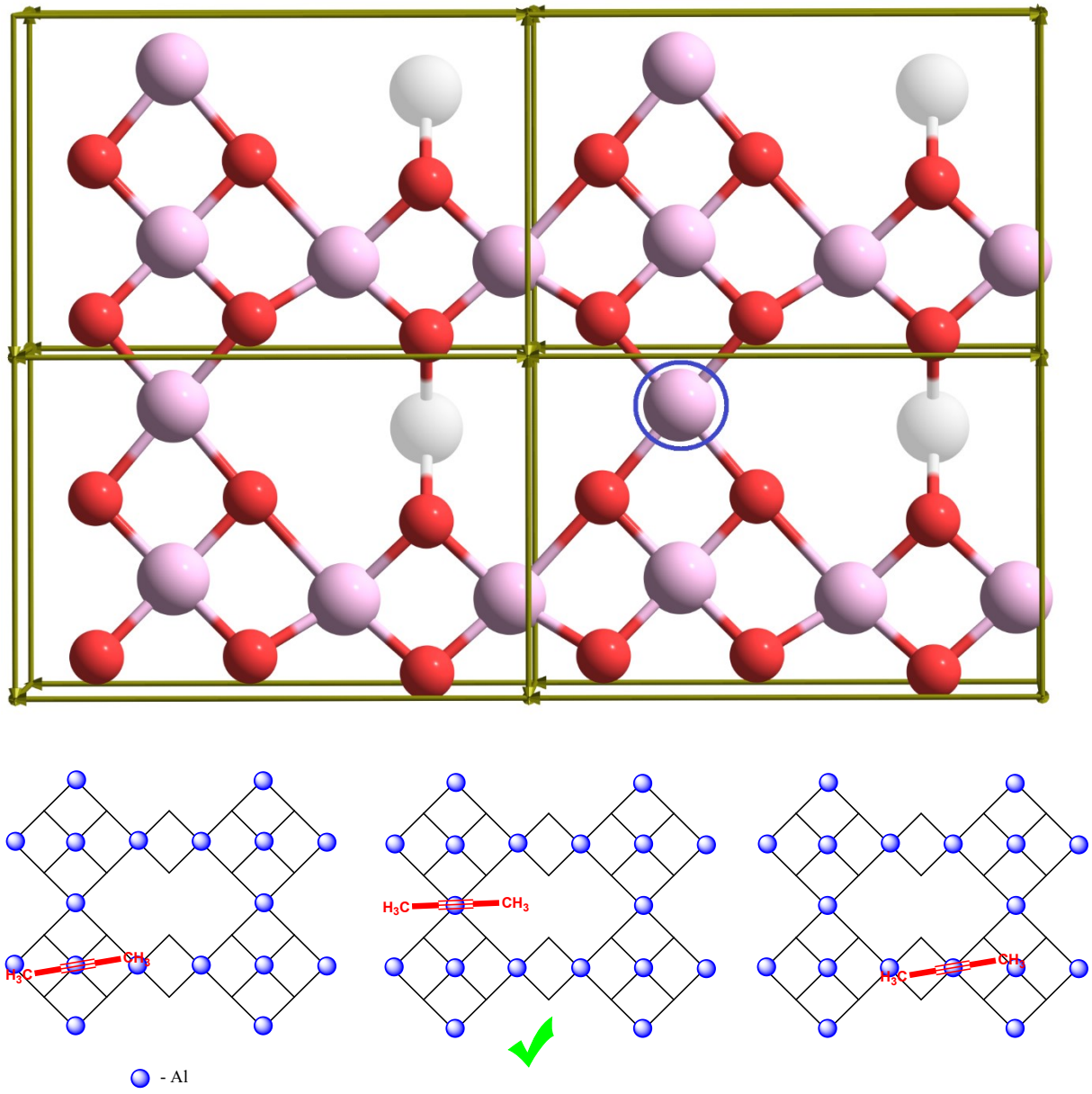


Figure S65. 100 termination of alumina. Lower layers (starting from the first sublayer are omitted for clarity). Al sites between the top and the first sublayer are coloured white. The reactive Al-site (discussed in Fig.4C) is depicted with blue circle.

Absolute and relative energies of the discussed structures.

Table S4. Butyne vs Butadiene gas

System	Total energy (eV)	Relative energy (kcal/mol)
Butyne	-56.65056292	0.00
Butadiene	-57.06427596	-9.56

Table S5. Butyne vs Butadiene on 001 surface

System	Total energy (eV)	Relative energy (kcal/mol)
Butyne	-1241.57888189	0.00
Butadiene	-1241.70634443	-2.94

Table S6. Adsorption of Butyne on 001 surface

System	Total energy (eV)	Relative energy (kcal/mol)
Butyne (gas)	-56.65056292	
Clean 001 surface	-1184.00339453	
Butyne*	-1241.57888189	
Adsorption energy	0.924924	21.4

Table S7. Butyne on different 110 surfaces

System	Total energy (eV)	Comment
Surface with 2-coordinated oxygens (A)	-1183.04258016	Used further
Surface with 3-coordinaed oxygens (B)	-1179.98153467	

Table S8. Reaction on 110 surface (depicted in Fig. 4A)

System	Total energy (eV)	Relative energy (kcal/mol)
Butyne-Al_2O_3-110	-1183.04258016	0.0
TS1 Butyne-Al_2O_3-110	-1182.44725149	13.7
TS2 Butyne-Al_2O_3-110	-1182.01230256	23.8
Allyl1-Al_2O_3-H-110	-1183.37814822	-7.7
Allyl2-Al_2O_3-H-110	-1183.63950333	-13.7
TS Allyl-to-Cumulene-110_3	-1182.35675655	15.8
Cumulene-Al_2O_3-110	-1182.70605987	7.8

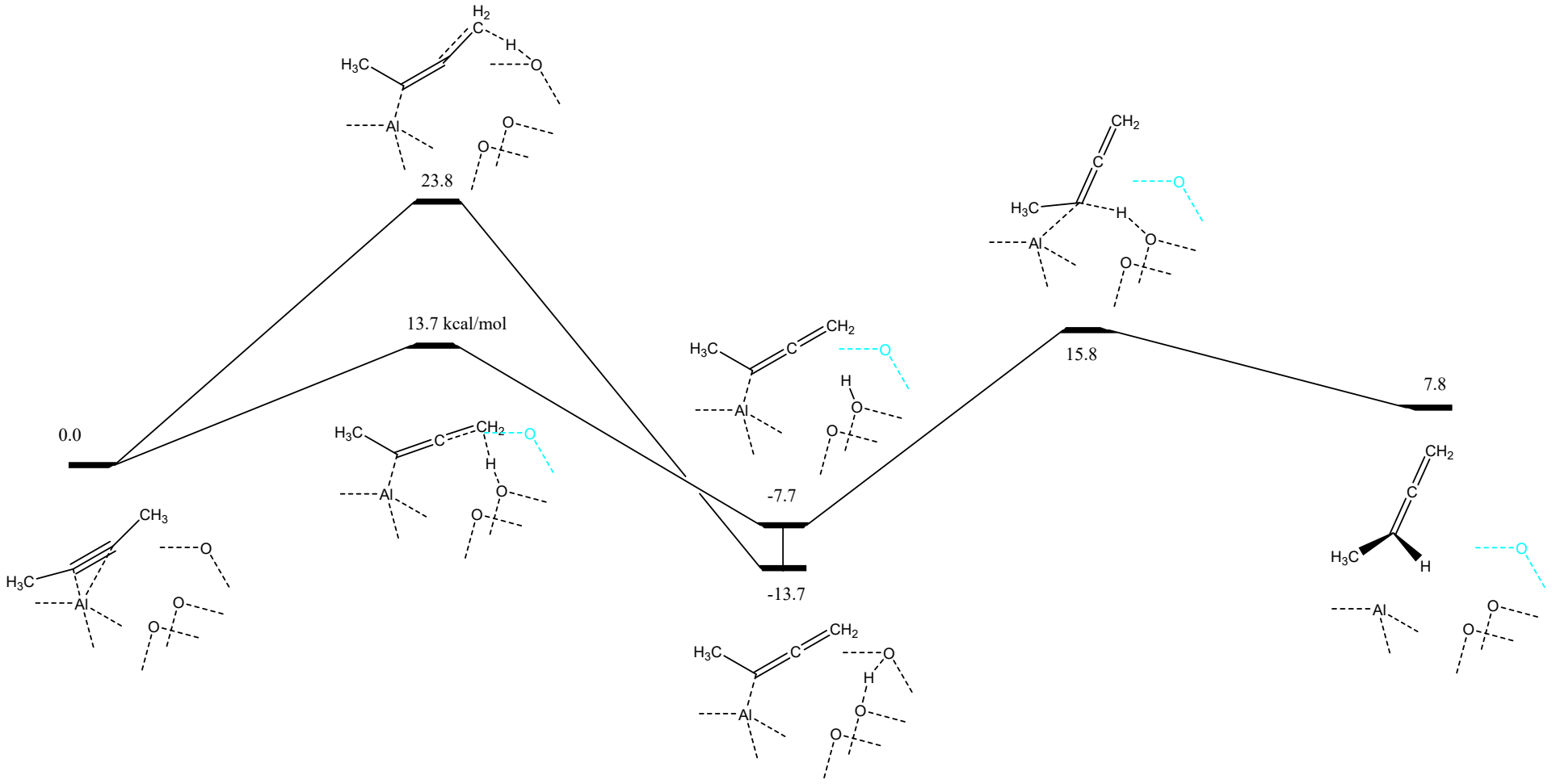


Figure S66. 110 termination Suggested mechanism of Butyne-to-Cumulene transformation on 110 surface of Al_2O_3 (related to Fig. 4A and 4B)

Table S9. Butyne deprotonation on clean 001 surface (Al_V)

System	Total energy (eV)	Relative energy (kcal/mol)
Butyne2-Al_2O_3-001 (best)	-1241.57888189	0.0
TS Butyne2-Al_2O_3-001	-1240.21434799	31.5
Allyl2-Al_2O_3-H-001	-1240.45612179	25.9

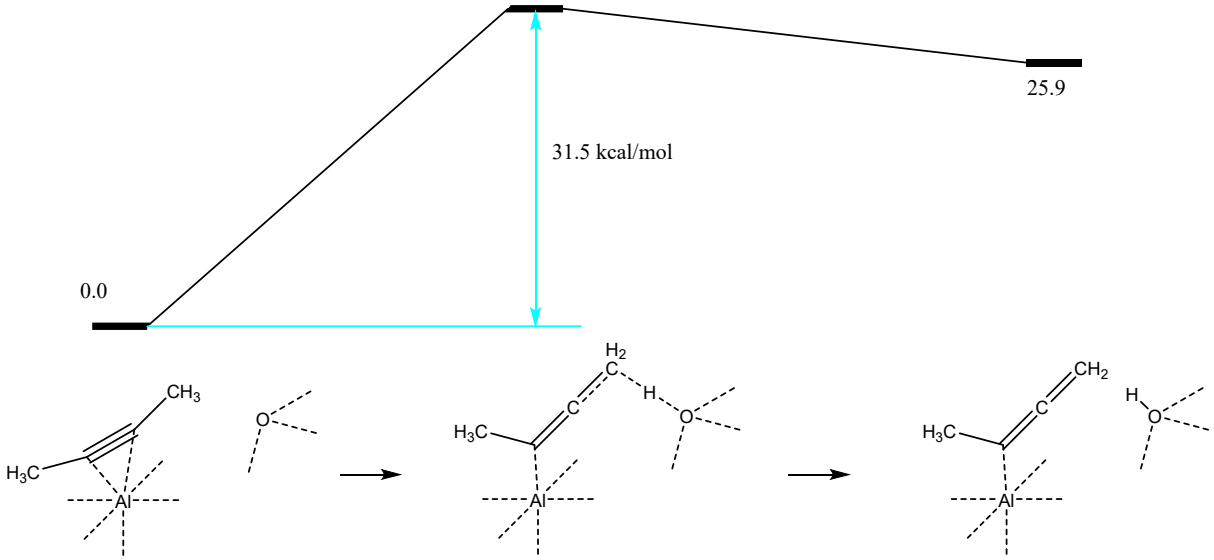


Figure S67. The deprotonation of butyne on 001 alumina surface (related to Fig. 4C)

Table S10. Butyne deprotonation on hydroxylated 001 surface (Al_V)

System	Total energy (eV)	Relative energy (kcal/mol)
Butyne2-Al_2O_3-OH-001	-1241.57888189	0.0
TSA Butyne2-Al_2O_3-OH-001	-1250.03709400	14.5
TSB Butyne2-Al_2O_3-OH-001	-1250.18908963	11.0
AllylA-Al_2O_3H-OH-001	-1250.45281879	4.9

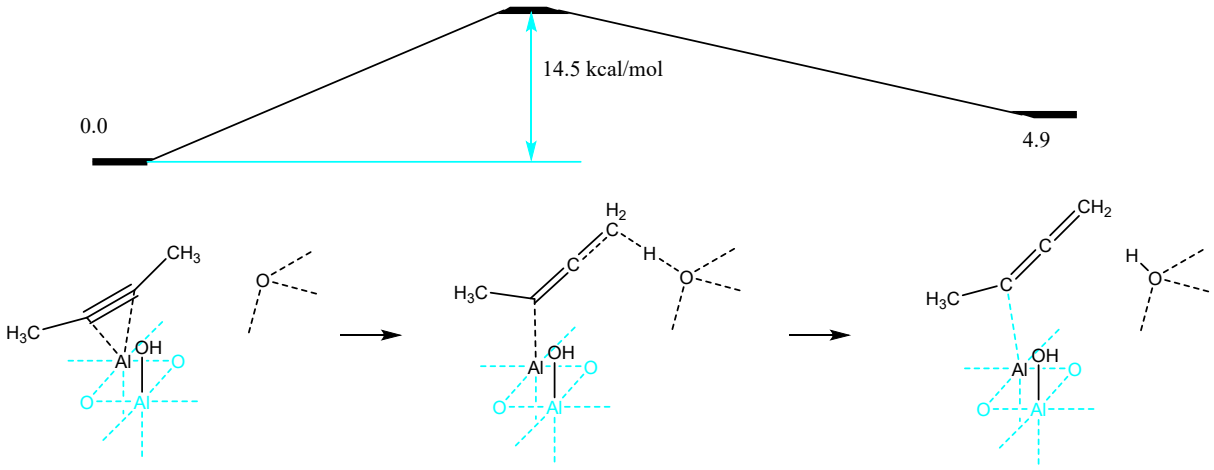
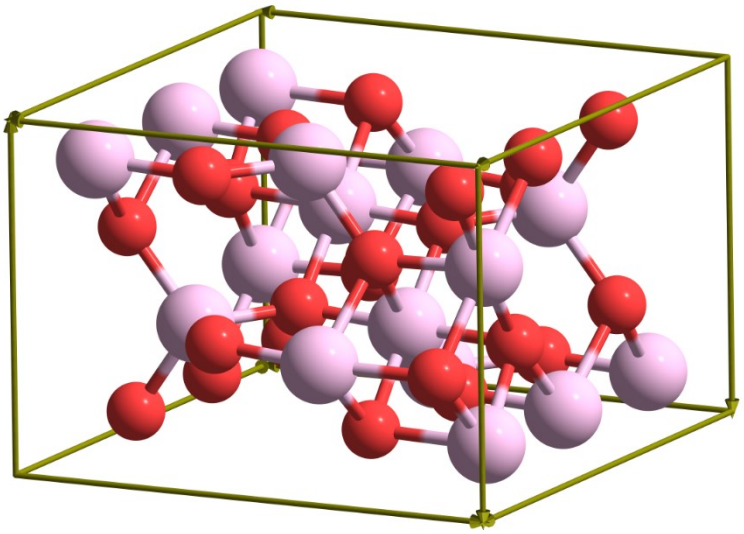


Figure S68. The deprotonation of butyne on hydroxylated 001 alumina surface (related to Fig. 4D)

Coordinates

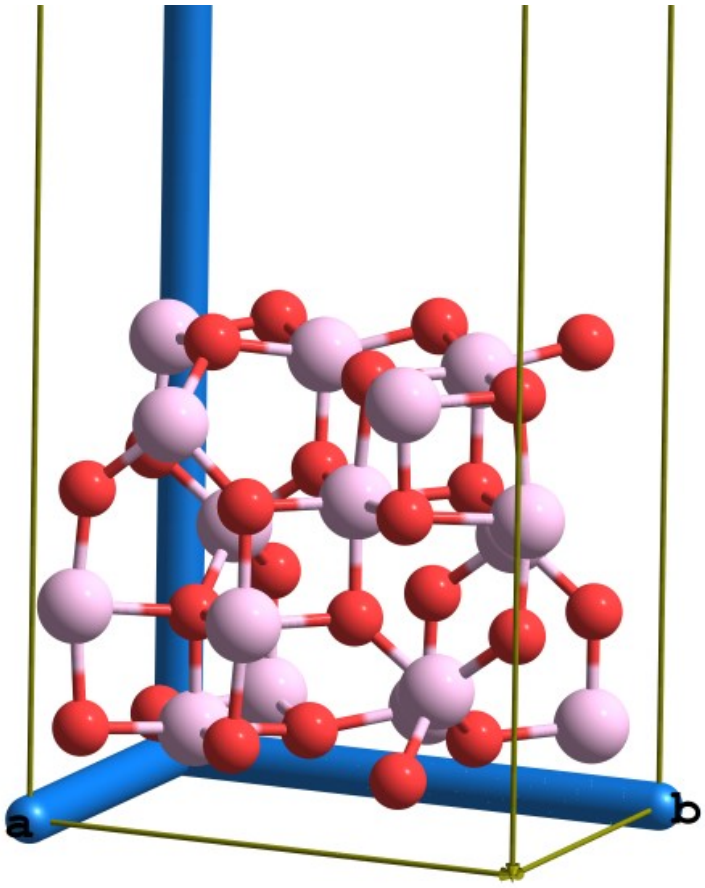
$Al_{16}O_{24}$ (Bulk)



5.558020991	0.000000000	0.000000000
0.000000000	8.351892505	0.000000000
0.000000000	0.000000000	8.034857440
4.92738	3.39122	7.21265
3.37043	7.66610	4.93061
1.98500	3.39225	6.86348
0.74753	7.65893	5.11426
0.62708	7.56688	0.81726
2.18406	3.49054	3.09923
3.56951	7.56818	1.16640
4.80705	3.48353	2.91545
0.62712	4.95531	0.81718
2.18431	0.68034	3.09931
3.56958	4.95455	1.16630
4.80676	0.68773	2.91533
4.92734	0.77969	7.21275
3.37035	4.85579	4.93070
1.98498	0.77857	6.86323
0.74741	4.86323	5.11417
4.90219	6.26110	7.03935
2.01772	6.26105	7.14345
0.65257	2.08544	0.99047
3.53696	2.08577	0.88630
3.40706	2.08565	5.14175
0.73920	2.08552	5.04164
2.14762	6.26119	2.88801
4.81513	6.26127	2.98808
2.04099	0.62710	4.92518
0.65038	4.83158	6.92943
3.51351	4.80308	3.10480
4.90408	0.65580	1.10022
3.51347	7.71944	3.10475
4.90418	3.51499	1.10028
2.04096	3.54349	4.92510
0.65033	7.69072	6.92949
2.10179	6.26094	1.00762
4.86853	6.26131	1.00682
3.43134	6.26101	5.98916
3.45277	2.08584	7.02217
0.68599	2.08537	7.02320
2.12331	2.08549	2.04073
4.83190	2.08560	4.00633
0.72255	6.26108	4.02332

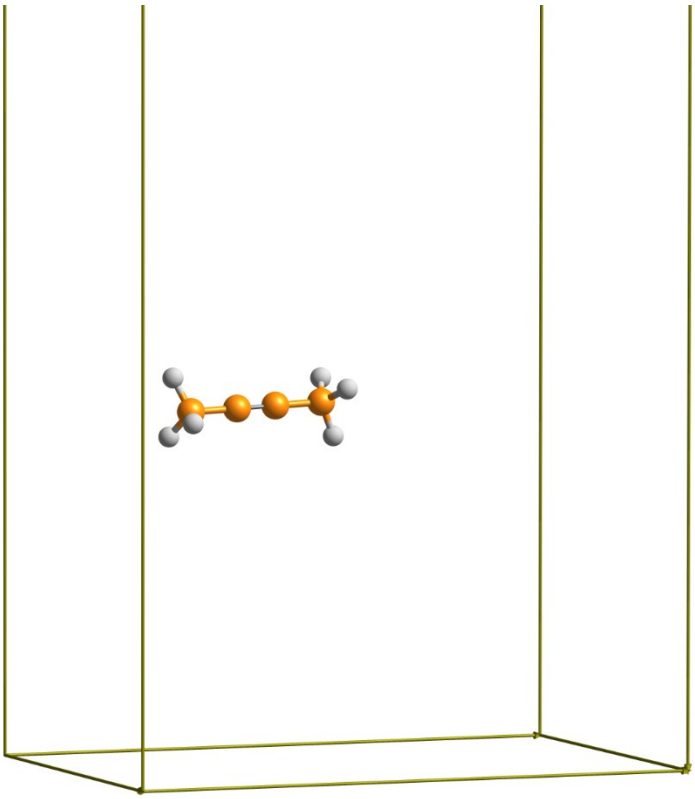
$Al_{16}O_{24}$ (100-surface)

5.558000000	0.000000000	0.000000000
0.000000000	8.351900000	0.000000000
0.000000000	0.000000000	26.000000000
0.39545	1.75649	1.18978
3.18673	1.75607	1.19055
0.43097	4.50284	1.28299
0.43108	7.36203	1.28324
3.20824	5.93252	2.22364
4.59841	0.29825	3.28771
4.59836	3.21456	3.28771
0.35882	5.93269	4.18926
1.80746	1.75624	4.20627
3.11872	4.45786	5.11546
3.11765	7.40757	5.11485
4.26510	1.75529	6.29537
1.45616	0.38700	7.01788
1.45006	3.11808	7.01716
4.63877	5.93102	7.11970
1.79003	5.93148	7.12248
1.71198	3.06206	1.00008
1.71203	0.45050	1.00008
4.62187	5.93286	1.06915
1.73749	5.93252	1.17328
4.65444	3.06331	1.34927
4.65449	0.44967	1.34927
3.23253	1.75632	3.07084
0.33392	7.33063	3.09826
0.33365	4.53475	3.09826
0.34204	1.75640	3.17089
3.26899	7.33756	3.28213
3.26922	4.52740	3.28213
4.38501	3.12821	5.13923
4.38407	0.38428	5.13828
1.84566	5.93145	5.21235
1.75680	3.19690	5.24664
1.75505	0.31551	5.24516
4.50631	5.93328	5.29848
3.12806	4.66293	7.11769
3.11811	7.21182	7.11486
0.23619	1.75206	7.22505
2.73588	1.75655	7.32952
0.50918	7.19411	7.45765
0.51362	4.66546	7.45678



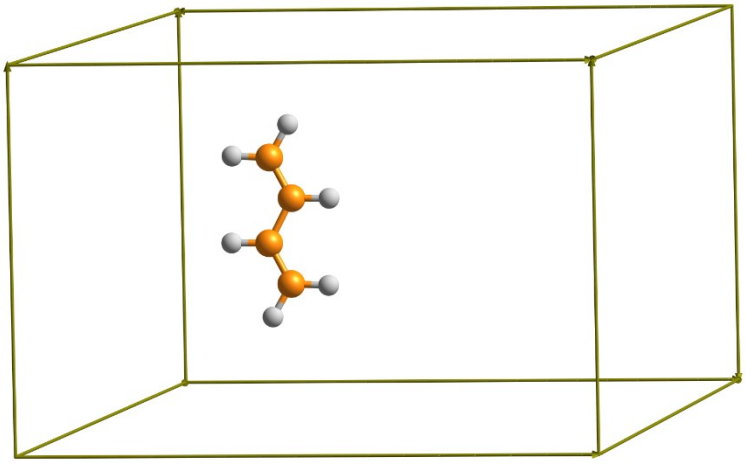
Butyne (gas)

11.116000000	0.000000000	0.000000000
0.000000000	16.703800000	0.000000000
0.000000000	0.000000000	26.000000000
4.87831	6.45911	10.30984
4.95624	5.24890	10.26491
5.05001	3.79862	10.21196
4.78422	7.90920	10.36913
4.78802	3.34501	11.18091
4.36839	3.38069	9.45424
6.07088	3.47265	9.95708
4.63731	8.34389	9.36761
3.93816	8.22915	10.99803
5.69969	8.35213	10.79258



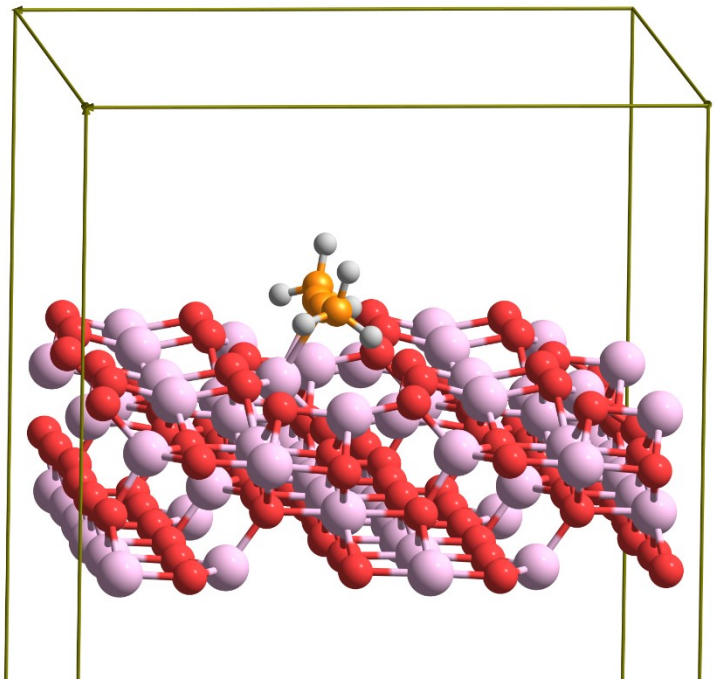
Butadiene (gas)

11.116000000	0.000000000	0.000000000
0.000000000	16.703800000	0.000000000
0.000000000	0.000000000	26.000000000
5.29671	5.55369	10.07329
4.12236	6.19903	9.96144
7.75836	5.56583	10.30280
6.58408	6.21239	10.19733
5.31008	4.45728	10.07236
4.07349	7.29089	9.95722
3.17825	5.66086	9.86834
6.57192	7.30861	10.20270
7.80703	4.47371	10.30083
8.70260	6.10388	10.39454



Butyne adsorbed on 110-A (Surface with 2-coordinated oxygens, $Al_{64}O_{96}C_4H_6$)

16.703785010	0.000000000	0.000000000
0.000000000	16.069714880	0.000000000
0.000000000	0.000000000	26.000000000
14.61297	12.05818	12.29559
6.26108	4.02332	12.29559
6.26108	12.05818	12.29559
14.61297	4.02332	12.29559
10.43726	15.05806	12.25903
2.08537	7.02320	12.25903
2.08537	15.05806	12.25903
10.43726	7.02320	12.25903
13.18347	14.96429	12.22342
4.83158	6.92943	12.22342
4.83158	14.96429	12.22342
13.18347	6.92943	12.22342
16.04261	14.96435	12.22337
7.69072	6.92949	12.22337
7.69072	14.96435	12.22337
16.04261	6.92949	12.22337
11.86688	9.13514	10.91920
3.51499	1.10028	10.91920
3.51499	9.13514	10.91920
11.86688	1.10028	10.91920
9.00769	9.13508	10.91910
0.65580	1.10022	10.91910
0.65580	9.13508	10.91910
9.00769	1.10022	10.91910
14.61320	9.04168	10.88355
6.26131	1.00682	10.88355
6.26131	9.04168	10.88355
14.61320	1.00682	10.88355
10.43749	12.04119	10.84692
2.08560	4.00633	10.84692
2.08560	12.04119	10.84692
10.43749	4.00633	10.84692
13.18739	11.11051	9.44328
4.87965	3.07846	9.43145
4.89471	11.12250	9.43451
13.23180	3.07552	9.43604
15.98020	11.12206	9.43419
7.64188	3.07562	9.43608
7.68789	11.11066	9.44376
15.99378	3.07845	9.43112
10.43788	15.19437	9.01521
2.08519	7.19447	8.98671
2.08563	15.22649	8.98857
10.43545	7.19423	9.01442
14.60117	14.15048	9.32111
6.26202	6.11795	9.32420
6.27424	14.15079	9.32121
14.61147	6.11769	9.32465
10.43765	10.30064	8.07252
2.08426	2.44722	8.42571
2.08576	10.49448	8.44178
10.43654	2.42156	8.42195
14.62504	8.92672	8.34698



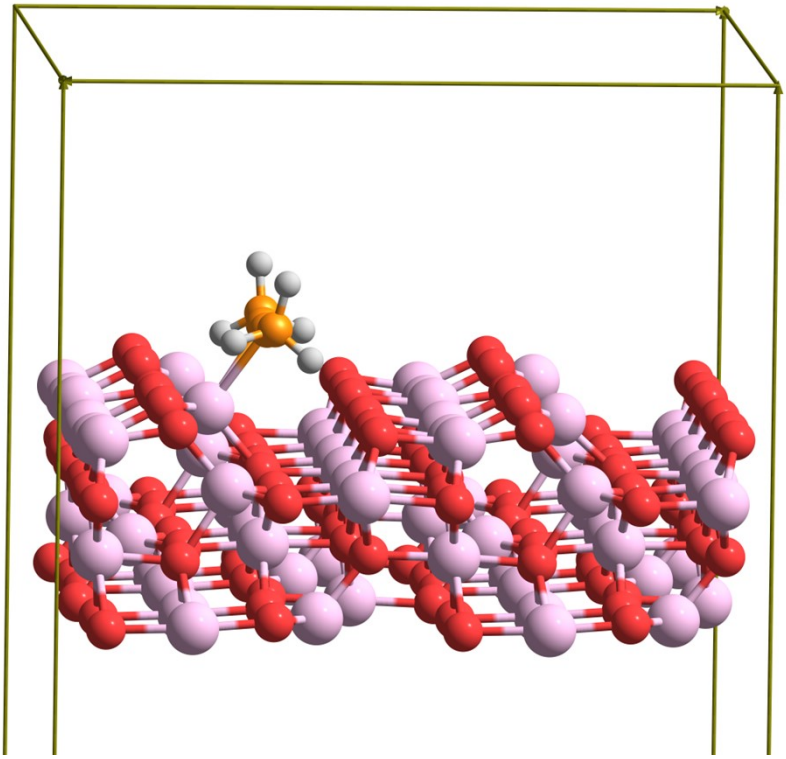
6.26203	0.88620	8.33238
6.25015	8.92673	8.34719
14.61140	0.88616	8.33236
8.94435	13.15884	8.34777
0.57468	5.13041	8.32936
0.57202	13.16640	8.32911
8.93226	5.11712	8.33745
11.93046	13.15812	8.34694
3.59515	5.13009	8.32872
3.59966	13.16694	8.32875
11.94040	5.11694	8.33874
7.65893	5.11426	12.32057
7.65893	13.14912	12.32057
16.01082	5.11426	12.32057
16.01082	13.14912	12.32057
4.86323	5.11417	12.32045
4.86323	13.14903	12.32045
13.21512	5.11417	12.32045
13.21512	13.14903	12.32045
2.08552	5.04164	12.31224
2.08552	13.07650	12.31224
10.43741	5.04164	12.31224
10.43741	13.07650	12.31224
2.08544	0.99047	12.22561
2.08544	9.02533	12.22561
10.43733	0.99047	12.22561
10.43733	9.02533	12.22561
4.95531	0.81718	12.20016
4.95531	8.85204	12.20016
13.30720	0.81718	12.20016
13.30720	8.85204	12.20016
7.56688	0.81726	12.20012
7.56688	8.85212	12.20012
15.91877	0.81726	12.20012
15.91877	8.85212	12.20012
3.39122	7.21265	10.94240
3.39122	15.24751	10.94240
11.74311	7.21265	10.94240
11.74311	15.24751	10.94240
0.77969	7.21275	10.94236
0.77969	15.24761	10.94236
9.13158	7.21275	10.94236
9.13158	15.24761	10.94236
6.26110	7.03935	10.91721
6.26110	15.07421	10.91721
14.61299	7.03935	10.91721
14.61299	15.07421	10.91721
6.26127	2.98808	10.83015
6.26127	11.02294	10.83015
14.61316	2.98808	10.83015
14.61316	11.02294	10.83015
3.48353	2.91545	10.82207
3.48353	10.95031	10.82207
11.83542	2.91545	10.82207
11.83542	10.95031	10.82207
0.68773	2.91533	10.82178
0.68773	10.95019	10.82178
9.03962	2.91533	10.82178

9.03962	10.95019	10.82178
4.89916	1.15836	9.60382
4.89692	9.19225	9.60409
13.25189	1.15703	9.60449
13.25599	9.18108	9.60419
7.62224	1.15727	9.60438
7.61886	9.18104	9.60423
15.97501	1.15863	9.60359
15.97798	9.19188	9.60418
2.08525	0.96548	9.37883
2.08563	9.00044	9.37979
10.43732	0.95342	9.38786
10.43727	9.00710	9.35056
2.08517	5.04592	9.38429
2.08595	13.07745	9.38319
10.43620	5.05607	9.39515
10.43772	13.14564	9.42561
7.54737	4.89612	9.34411
7.55151	12.92965	9.35046
15.89824	4.89872	9.34297
15.89803	12.93851	9.34561
4.97523	4.89888	9.34274
4.97726	12.93890	9.34538
13.32610	4.89594	9.34412
13.32356	12.92946	9.34959
0.63599	3.29620	7.99276
0.63282	11.33093	7.99516
8.99520	3.28952	7.99885
9.01711	11.34220	8.02411
3.53304	3.29572	7.99313
3.53852	11.33108	7.99516
11.87791	3.28960	7.99930
11.85841	11.34137	8.02334
6.26248	2.67681	8.18100
6.27279	10.71169	8.18087
14.61082	2.67667	8.18085
14.60289	10.71147	8.18090
6.26899	7.26079	8.01604
6.25734	15.29283	8.01867
14.60483	7.26049	8.01659
14.61790	15.29275	8.01875
3.43211	6.77443	7.92495
3.42970	14.81029	7.92448
11.77358	6.75672	7.92475
11.78563	14.80532	7.93168
0.73705	6.77498	7.92621
0.74136	14.80983	7.92487
9.09905	6.75690	7.92269
9.08904	14.80598	7.93262
11.05207	9.22944	6.08930
9.82486	9.23539	6.08749
12.48827	9.03800	5.96054
8.38698	9.06339	5.94694
12.71259	8.77689	4.91469
13.04481	9.95188	6.22054
12.77113	8.17485	6.59894
7.83950	9.96902	6.25129
8.16039	8.86021	4.88873

8.09296	8.17712	6.54640

Butyne adsorbed on 110-B (Surface with 3-coordinated oxygens, $Al_{64}O_{96}C_4H_6$, not used further)

16.703785010	0.000000000	0.000000000
0.000000000	16.069714880	0.000000000
0.000000000	0.000000000	26.000000000
0.62710	4.92518	13.61403
3.54349	4.92510	13.61400
6.26094	1.00762	13.67484
2.08549	2.04073	13.69635
4.81765	3.08709	15.08481
7.70565	3.08691	15.08487
6.26146	5.96939	15.00801
2.08602	7.00231	15.09565
0.62710	12.96004	13.61403
3.54349	12.95996	13.61400
6.26094	9.04248	13.67484
2.08549	10.07559	13.69635
4.81765	11.12195	15.08481
6.26146	14.00425	15.00801
2.08602	15.03717	15.09565
7.70565	11.12177	15.08487
8.97899	4.92518	13.61403
11.89538	4.92510	13.61400
14.61283	1.00762	13.67484
10.43738	2.04073	13.69635
13.16954	3.08709	15.08481
16.05754	3.08691	15.08487
14.61335	5.96939	15.00801
10.43791	7.00231	15.09565
8.97899	12.96004	13.61403
11.89538	12.95996	13.61400
14.61283	9.04248	13.67484
10.43738	10.07559	13.69635
13.16954	11.12195	15.08481
16.05754	11.12177	15.08487
14.61335	14.00425	15.00801
0.66005	1.06196	16.48065
10.43791	15.03717	15.09565
3.46487	1.11130	16.59652
6.25052	1.04883	16.53237
2.07440	4.06616	16.60203
4.80931	6.86361	17.44534
7.71329	6.86060	17.44383
2.08857	6.91029	17.67906
6.25591	4.36383	17.78824
0.69494	9.14212	16.58028
3.48589	9.12968	16.54569
6.26202	9.13903	16.55560
2.08700	12.11433	16.59693
4.81047	14.89789	17.43183
7.69373	14.90629	17.42969
2.08175	14.94867	17.67607
6.25918	12.29903	17.99154
9.03217	1.10437	16.57384
11.81822	1.10492	16.58241



14.59865	1.05933	16.54759
10.43509	4.07692	16.60404
13.15708	6.86506	17.45294
16.07008	6.86441	17.45116
10.43353	6.91550	17.68031
14.61156	4.36090	17.78851
9.03634	9.13025	16.54789
11.82882	9.14234	16.57871
14.61359	9.09290	16.53703
10.43511	12.11273	16.59211
13.14662	14.89427	17.45759
16.06180	14.89489	17.45438
10.41494	14.94132	17.68060
14.60507	12.39775	17.78966
2.08594	0.88784	15.14188
4.93931	1.13797	15.09353
7.58405	1.13800	15.09311
2.08566	5.13175	14.96611
7.67306	4.91525	14.95228
4.84974	4.91531	14.95219
0.68034	3.09931	13.75735
3.49054	3.09923	13.75710
6.26119	2.88801	13.72066
6.26105	7.14345	13.59076
3.39225	6.86348	13.55804
0.77857	6.86323	13.55802
2.08594	8.92270	15.14188
4.93931	9.17283	15.09353
7.58405	9.17286	15.09311
2.08566	13.16661	14.96611
7.67306	12.95011	14.95228
4.84974	12.95017	14.95219
0.68034	11.13417	13.75735
3.49054	11.13409	13.75710
6.26119	10.92287	13.72066
6.26105	15.17831	13.59076
3.39225	14.89834	13.55804
0.77857	14.89809	13.55802
10.43783	0.88784	15.14188
13.29120	1.13797	15.09353
15.93594	1.13800	15.09311
10.43755	5.13175	14.96611
16.02495	4.91525	14.95228
13.20163	4.91531	14.95219
9.03223	3.09931	13.75735
11.84243	3.09923	13.75710
14.61308	2.88801	13.72066
14.61294	7.14345	13.59076
11.74414	6.86348	13.55804
9.13046	6.86323	13.55802
10.43783	8.92270	15.14188
13.29120	9.17283	15.09353
15.93594	9.17286	15.09311
10.43755	13.16661	14.96611
16.02495	12.95011	14.95228
13.20163	12.95017	14.95219
9.03223	11.13417	13.75735
11.84243	11.13409	13.75710

14.61308	10.92287	13.72066
14.61294	15.17831	13.59076
11.74414	14.89834	13.55804
9.13046	14.89809	13.55802
2.05645	0.70137	17.78174
4.89950	5.32998	18.21557
7.61694	5.32555	18.21105
2.07804	5.22159	17.93518
4.87290	0.63019	17.70137
7.63133	0.63523	17.69604
3.39148	7.09044	16.42266
0.78134	7.09707	16.42795
6.26097	6.95282	16.42905
0.68309	2.91143	16.41130
3.48026	2.93077	16.43062
6.25841	3.03618	16.56399
2.09491	8.74198	17.80757
4.90635	13.37917	18.18997
7.60427	13.38919	18.18737
2.07672	13.25619	17.94508
4.88133	8.65920	17.69449
7.64188	8.65655	17.69557
3.38236	15.12521	16.42201
0.76701	15.10837	16.41176
6.25225	15.03964	16.39859
0.68599	10.96453	16.43140
3.47603	10.95638	16.43029
6.26135	11.07283	16.55688
10.42768	0.70343	17.80571
13.25345	5.32493	18.20781
15.97004	5.32408	18.20625
10.43576	5.22749	17.94047
13.22561	0.62403	17.70281
15.98359	0.62013	17.67809
11.74124	7.09649	16.42946
9.13156	7.09125	16.42207
14.61298	6.96178	16.43020
9.03944	2.92971	16.42903
11.83473	2.92864	16.43196
14.60967	3.03030	16.56634
10.42864	8.74453	17.80795
13.24515	13.35483	18.21801
15.96345	13.35742	18.21719
10.42645	13.24763	17.94622
13.23627	8.66404	17.70159
15.99021	8.66311	17.70133
11.73239	15.11753	16.43451
9.12528	15.12823	16.41932
14.60164	14.98346	16.43499
9.04630	10.95585	16.42927
11.83692	10.96478	16.43122
14.61181	11.06708	16.56756
5.68990	11.02411	19.82683
6.91810	11.01988	19.81844
8.36989	10.95858	19.93391
4.24159	10.94862	19.98792
8.84690	11.80663	19.41595
8.64098	11.01023	21.00007

8.74921	10.02162	19.50395
4.02293	10.68937	21.03581
3.76280	11.90791	19.73955
3.81993	10.16895	19.33881

TS1 Butyne-Al_2O_3-110 (Lewis pair provided by triad oxygen, $Al_{64}O_{96}C_4H_6$)

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6.26108	12.05818	12.29559	0		
14.61297	4.02332	12.29559	0		
10.43726	15.05806	12.25903	0		
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2.08537	15.05806	12.25903	0		
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4.83158	14.96429	12.22342	0		
13.18347	6.92943	12.22342	0		
16.04261	14.96435	12.22337	0		
7.69072	6.92949	12.22337	0		
7.69072	14.96435	12.22337	0		
16.04261	6.92949	12.22337	0		
11.86688	9.13514	10.91920	0	0	0
3.51499	1.10028	10.91920	0	0	0
3.51499	9.13514	10.91920	0	0	0
11.86688	1.10028	10.91920	0	0	0
9.00769	9.13508	10.91910	0	0	0
0.65580	1.10022	10.91910	0	0	0
0.65580	9.13508	10.91910	0	0	0
9.00769	1.10022	10.91910	0	0	0
14.61320	9.04168	10.88355	0	0	0
6.26131	1.00682	10.88355	0	0	0
6.26131	9.04168	10.88355	0	0	0
14.61320	1.00682	10.88355	0	0	0
10.43749	12.04119	10.84692	0	0	0
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2.08560	12.04119	10.84692	0	0	0
10.43749	4.00633	10.84692	0	0	0
13.17556	11.10901	9.43717	0	0	0
4.87270	3.07433	9.43046	0	0	0
4.89582	11.12216	9.43463	0	0	0
13.23123	3.07942	9.43907	0	0	0
15.97123	11.11677	9.42960	0	0	0
7.63164	3.06691	9.44324	0	0	0
7.69567	11.10879	9.43526	0	0	0
15.99313	3.07770	9.43135	0	0	0
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2.08283	7.19405	8.99006	0	0	0
2.08045	15.22087	8.99491	0	0	0
10.47472	7.18514	9.10695	0	0	0
14.59777	14.14836	9.32126	0	0	0
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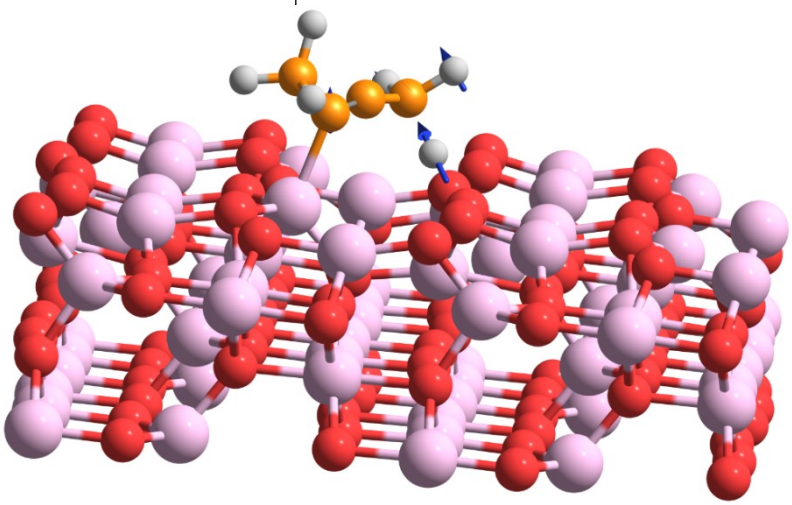

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10.43887	2.40564	8.41318	0	0	0
14.60451	8.92209	8.34035	0	0	0
6.25672	0.88270	8.33111	0	0	0
6.24600	8.92736	8.34869	0	0	0
14.60804	0.88715	8.33231	0	0	0
8.94030	13.15139	8.35118	0	0	0
0.57100	5.12906	8.32735	0	0	0
0.56729	13.16419	8.32875	0	0	0
8.93559	5.09605	8.37642	0	0	0
11.92402	13.15456	8.35799	0	0	0
3.58686	5.12566	8.32747	0	0	0
3.59552	13.16520	8.32707	0	0	0
11.94654	5.12474	8.31918	0	0	0
7.65893	5.11426	12.32057	0	0	0
7.65893	13.14912	12.32057	0	0	0
16.01082	5.11426	12.32057	0	0	0
16.01082	13.14912	12.32057	0	0	0
4.86323	5.11417	12.32045	0	0	0
4.86323	13.14903	12.32045	0	0	0
13.21512	5.11417	12.32045	0	0	0
13.21512	13.14903	12.32045	0	0	0
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2.08552	13.07650	12.31224	0	0	0
10.43741	5.04164	12.31224	0	0	0
10.43741	13.07650	12.31224	0	0	0
2.08544	0.99047	12.22561	0	0	0
2.08544	9.02533	12.22561	0	0	0
10.43733	0.99047	12.22561	0	0	0
10.43733	9.02533	12.22561	0	0	0
4.95531	0.81718	12.20016	0	0	0
4.95531	8.85204	12.20016	0	0	0
13.30720	0.81718	12.20016	0	0	0
13.30720	8.85204	12.20016	0	0	0
7.56688	0.81726	12.20012	0	0	0
7.56688	8.85212	12.20012	0	0	0
15.91877	0.81726	12.20012	0	0	0
15.91877	8.85212	12.20012	0	0	0
3.39122	7.21265	10.94240	0	0	0
3.39122	15.24751	10.94240	0	0	0
11.74311	7.21265	10.94240	0	0	0
11.74311	15.24751	10.94240	0	0	0
0.77969	7.21275	10.94236	0	0	0
0.77969	15.24761	10.94236	0	0	0
9.13158	7.21275	10.94236	0	0	0
9.13158	15.24761	10.94236	0	0	0
6.26110	7.03935	10.91721	0	0	0
6.26110	15.07421	10.91721	0	0	0
14.61299	7.03935	10.91721	0	0	0
14.61299	15.07421	10.91721	0	0	0
6.26127	2.98808	10.83015	0	0	0
6.26127	11.02294	10.83015	0	0	0
14.61316	2.98808	10.83015	0	0	0
14.61316	11.02294	10.83015	0	0	0

3.48353	2.91545	10.82207	0	0	0	
3.48353	10.95031	10.82207	0	0	0	
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11.83542	10.95031	10.82207	0	0	0	
0.68773	2.91533	10.82178	0	0	0	
0.68773	10.95019	10.82178	0	0	0	
9.03962	2.91533	10.82178	0	0	0	
9.03962	10.95019	10.82178	0	0	0	
4.89840	1.15874	9.60357	0	0	0	
4.89496	9.18751	9.60555	0	0	0	
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13.25131	9.17469	9.60951	0	0	0	
7.62123	1.15696	9.60302	0	0	0	
7.61664	9.17348	9.60390	0	0	0	
15.97328	1.15996	9.60231	0	0	0	
15.97309	9.18912	9.60152	0	0	0	
2.08355	0.96384	9.38033	0	0	0	
2.08449	8.99932	9.37983	0	0	0	
10.43447	0.94888	9.38811	0	0	0	
10.43091	9.00417	9.35309	0	0	0	
2.08116	5.04292	9.38288	0	0	0	
2.08199	13.07947	9.38384	0	0	0	
10.43607	5.08067	9.40634	0	0	0	
10.43230	13.16263	9.43844	0	0	0	
7.53549	4.89057	9.35071	0	0	0	
7.54625	12.93096	9.35663	0	0	0	
15.89580	4.89715	9.34280	0	0	0	
15.89302	12.93520	9.34301	0	0	0	
4.96663	4.89304	9.34280	0	0	0	
4.97181	12.93866	9.34522	0	0	0	
13.31956	4.90186	9.34138	0	0	0	
13.32085	12.93239	9.35734	0	0	0	
0.63215	3.29428	7.99116	0	0	0	
0.62809	11.33024	7.99369	0	0	0	
9.00139	3.29305	8.00501	0	0	0	
9.01704	11.34267	8.04923	0	0	0	
3.52848	3.29106	7.99154	0	0	0	
3.53304	11.32994	7.99629	0	0	0	
11.86744	3.29676	7.99961	0	0	0	
11.84885	11.34507	8.04960	0	0	0	
6.26147	2.67498	8.17968	0	0	0	
6.26897	10.70781	8.18196	0	0	0	
14.60576	2.67898	8.18135	0	0	0	
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6.25130	15.29065	8.01905	0	0	0	
14.59515	7.25549	8.01631	0	0	0	
14.61199	15.29405	8.02009	0	0	0	
3.43173	6.77186	7.92744	0	0	0	
3.42300	14.80970	7.92513	0	0	0	
11.72523	6.75750	7.91314	0	0	0	
11.77622	14.80169	7.93220	0	0	0	
0.73829	6.77273	7.92483	0	0	0	
0.73521	14.80976	7.92896	0	0	0	
9.07302	6.76407	8.00280	0	0	0	
9.08246	14.80275	7.93672	0	0	0	
10.51375	9.62367	6.02266	-0.004681	0.027272	-0.352547	
9.46233	8.96142	5.83279	0.040254	0.136586	-0.001458	

11.57624	10.28826	5.20547	0.189956	0.046244	0.045254
8.33854	8.14922	5.89248	-0.232473	0.105127	-0.175264
11.43204	10.07018	4.13922	0.077043	0.010370	0.012326
11.56433	11.37575	5.35548	0.032679	0.009912	0.021069
12.56833	9.93907	5.52124	0.038484	0.005633	0.047387
7.37115	8.65303	5.75705	-0.002802	0.136766	-0.128626
8.40844	7.25223	5.25825	-0.038368	0.220612	-0.327482
8.52854	7.54725	6.98442	-0.473657	0.304184	-0.444407

TS2 Butyne-Al_2O_3-110 (Lewis pair provided by non-triad oxygen, $Al_{64}O_{96}C_4H_6$)

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6.261080	12.058180	12.295590	0	0	0
14.612970	4.023320	12.295590	0	0	0
10.437260	15.058060	12.259030	0	0	0
2.085370	7.023200	12.259030	0	0	0
2.085370	15.058060	12.259030	0	0	0
10.437260	7.023200	12.259030	0	0	0
13.183470	14.964290	12.223420	0	0	0
4.831580	6.929430	12.223420	0	0	0
4.831580	14.964290	12.223420	0	0	0
13.183470	6.929430	12.223420	0	0	0
16.042610	14.964350	12.223370	0	0	0
7.690720	6.929490	12.223370	0	0	0
7.690720	14.964350	12.223370	0	0	0
16.042610	6.929490	12.223370	0	0	0
11.866880	9.135140	10.919200	0	0	0
3.514990	1.100280	10.919200	0	0	0
3.514990	9.135140	10.919200	0	0	0
11.866880	1.100280	10.919200	0	0	0
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0.655800	1.100220	10.919100	0	0	0
0.655800	9.135080	10.919100	0	0	0
9.007690	1.100220	10.919100	0	0	0
14.613200	9.041680	10.883550	0	0	0
6.261310	1.006820	10.883550	0	0	0
6.261310	9.041680	10.883550	0	0	0
14.613200	1.006820	10.883550	0	0	0
10.437490	12.041190	10.846920	0	0	0
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2.085600	12.041190	10.846920	0	0	0
10.437490	4.006330	10.846920	0	0	0
13.158820	11.096410	9.420480	0	0	0
4.893210	3.075600	9.432070	0	0	0
4.883370	11.144680	9.450140	0	0	0
13.239680	3.076730	9.435460	0	0	0
15.959360	11.118710	9.431400	0	0	0
7.654380	3.061850	9.435130	0	0	0
7.695080	11.146850	9.461090	0	0	0
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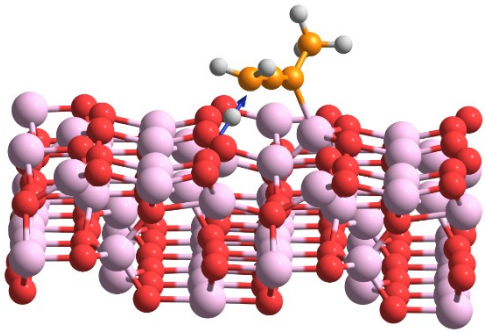

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10.471190 2.413560 8.422100	0	0	0
14.606230 8.919380 8.336980	0	0	0
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13.307200 0.817180 12.200160	0	0	0
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7.566880 0.817260 12.200120	0	0	0
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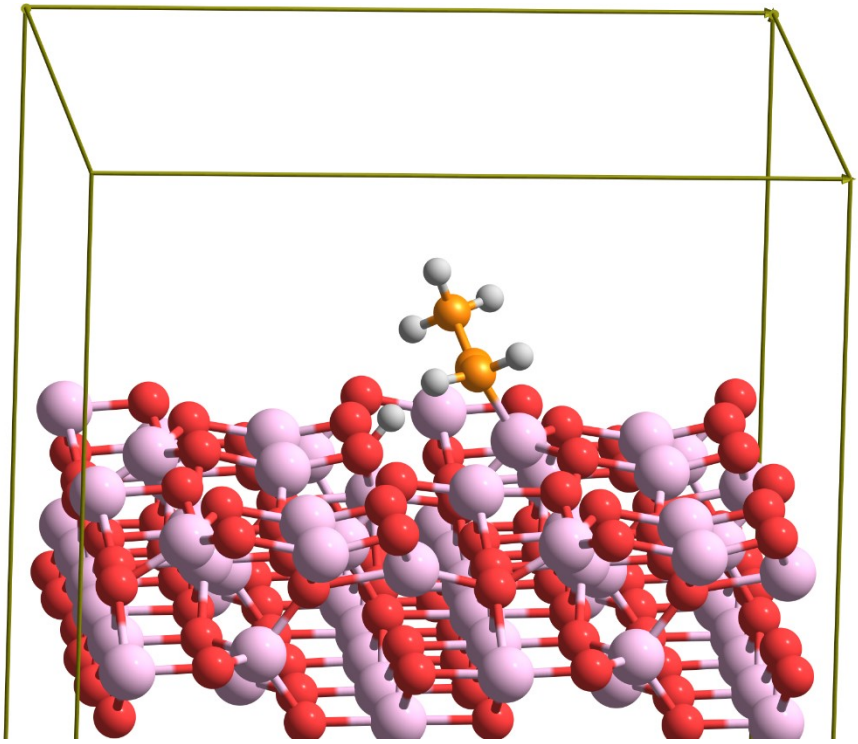
11.835420 2.915450 10.822070	0	0	0
11.835420 10.950310 10.822070	0	0	0
0.687730 2.915330 10.821780	0	0	0
0.687730 10.950190 10.821780	0	0	0
9.039620 2.915330 10.821780	0	0	0
9.039620 10.950190 10.821780	0	0	0
4.902500 1.162210 9.601420	0	0	0
4.905800 9.175070 9.591170	0	0	0
13.256940 1.159490 9.601860	0	0	0
13.252590 9.169440 9.605530	0	0	0
7.623490 1.154420 9.604710	0	0	0
7.607420 9.189910 9.596340	0	0	0
15.980970 1.159230 9.605060	0	0	0
15.976340 9.192360 9.601520	0	0	0
2.090700 0.965250 9.380750	0	0	0
2.097250 9.001910 9.385920	0	0	0
10.451220 0.951730 9.393320	0	0	0
10.421960 9.012550 9.365470	0	0	0
2.110850 5.058710 9.391650	0	0	0
2.074040 13.078800 9.383450	0	0	0
10.480450 5.031570 9.396270	0	0	0
10.434310 13.166820 9.440620	0	0	0
7.571710 4.888030 9.339150	0	0	0
7.535540 12.962870 9.390420	0	0	0
15.923530 4.907650 9.340890	0	0	0
15.880610 12.937250 9.345340	0	0	0
5.018230 4.905940 9.323510	0	0	0
4.952790 12.953610 9.355270	0	0	0
13.346960 4.895400 9.340390	0	0	0
13.305890 12.917360 9.332650	0	0	0
0.660240 3.302420 7.996400	0	0	0
0.618330 11.333660 7.993330	0	0	0
9.017520 3.271260 8.007010	0	0	0
8.985260 11.388390 8.075140	0	0	0
3.549070 3.303330 8.000500	0	0	0
3.525150 11.329120 8.004390	0	0	0
11.903560 3.289450 7.986390	0	0	0
11.813560 11.318580 8.023640	0	0	0
6.275230 2.676780 8.177910	0	0	0
6.255470 10.768870 8.192690	0	0	0
14.627160 2.678390 8.182250	0	0	0
14.584960 10.702520 8.175690	0	0	0
6.392000 7.309190 7.963970	0	0	0
6.243560 15.293960 8.011520	0	0	0
14.644220 7.253210 8.017000	0	0	0
14.611950 15.293650 8.021510	0	0	0
3.525450 6.798030 7.983200	0	0	0
3.415540 14.812540 7.923230	0	0	0
11.790520 6.765080 7.911350	0	0	0
11.778220 14.784510 7.914740	0	0	0
0.824730 6.764700 7.897870	0	0	0

0.731420	14.812110	7.930300	0	0	0
9.108210	6.723930	7.974050	0	0	0
9.084240	14.832870	7.956830	0	0	0
10.118670	9.439890	6.165180	-0.027066	-0.034452	-0.092351
9.048190	8.773730	5.998080	0.074648	0.025614	0.045741
11.134860	9.978610	5.182840	0.025903	0.021388	0.012733
7.861100	8.079390	5.886590	-0.096595	-0.113995	0.109883
10.989420	9.572280	4.177760	-0.003788	-0.004664	0.013225
11.055720	11.076970	5.135980	-0.001696	0.002901	0.006162
12.158320	9.757540	5.523770	0.001609	0.000816	0.009202
7.063840	8.616870	5.357200	0.028459	-0.006960	-0.031952
7.996640	7.041440	5.541130	0.077438	0.041716	-0.176772
7.298100	7.569390	7.054790	0.491447	0.451821	-0.677248

Allyl1-Al_2O_3-H-110 (Hydrogen bound to triad oxygen, $Al_{64}O_{96}C_4H_6$)

16.703785010	0.000000000	0.000000000
0.000000000	16.069714880	0.000000000
0.000000000	0.000000000	26.000000000
14.61297	12.05818	12.29559
6.26108	4.02332	12.29559
6.26108	12.05818	12.29559
14.61297	4.02332	12.29559
10.43726	15.05806	12.25903
2.08537	7.02320	12.25903
2.08537	15.05806	12.25903
10.43726	7.02320	12.25903
13.18347	14.96429	12.22342
4.83158	6.92943	12.22342
4.83158	14.96429	12.22342
13.18347	6.92943	12.22342
16.04261	14.96435	12.22337
7.69072	6.92949	12.22337
7.69072	14.96435	12.22337
16.04261	6.92949	12.22337
11.86688	9.13514	10.91920
3.51499	1.10028	10.91920
3.51499	9.13514	10.91920
11.86688	1.10028	10.91920
9.00769	9.13508	10.91910
0.65580	1.10022	10.91910
0.65580	9.13508	10.91910
9.00769	1.10022	10.91910
14.61320	9.04168	10.88355
6.26131	1.00682	10.88355
6.26131	9.04168	10.88355
14.61320	1.00682	10.88355
10.43749	12.04119	10.84692
2.08560	4.00633	10.84692
2.08560	12.04119	10.84692
10.43749	4.00633	10.84692
13.15788	11.09565	9.41874
4.86899	3.06873	9.42915
4.90221	11.10835	9.43155
13.23821	3.07743	9.44737
15.96525	11.11828	9.42971
7.62415	3.06711	9.45485



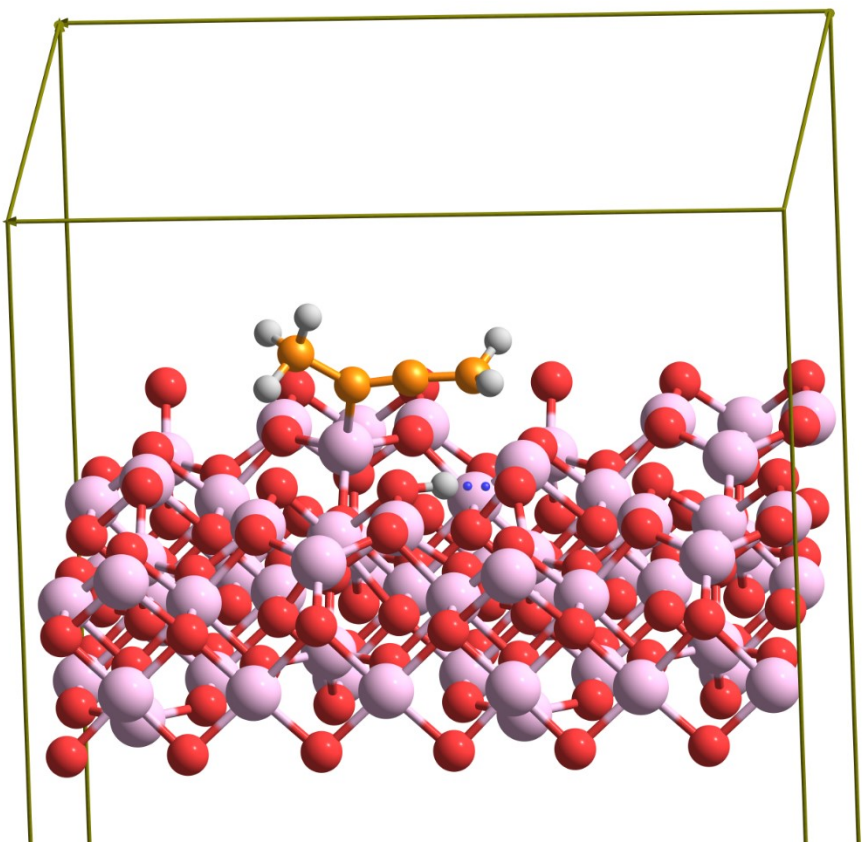
7.69117	11.13545	9.45332
15.99904	3.07474	9.42951
10.46037	15.16363	9.03053
2.09553	7.20234	8.96786
2.08071	15.21293	9.00267
10.56435	7.16245	9.27719
14.57628	14.14093	9.31529
6.23143	6.11857	9.34360
6.25669	14.14736	9.32578
14.62588	6.11929	9.32410
10.37644	10.23590	8.01754
2.08070	2.43214	8.41578
2.08140	10.49862	8.44365
10.44743	2.37741	8.39061
14.60578	8.91929	8.33708
6.26216	0.88154	8.32985
6.36333	8.96067	8.25575
14.61155	0.88598	8.33153
8.93297	13.17270	8.37347
0.57950	5.12705	8.32791
0.55979	13.16696	8.33188
8.94847	5.06721	8.37378
11.90872	13.11964	8.31834
3.58966	5.11636	8.32384
3.59500	13.16153	8.32875
11.95764	5.11963	8.31493
7.65893	5.11426	12.32057
7.65893	13.14912	12.32057
16.01082	5.11426	12.32057
16.01082	13.14912	12.32057
4.86323	5.11417	12.32045
4.86323	13.14903	12.32045
13.21512	5.11417	12.32045
13.21512	13.14903	12.32045
2.08552	5.04164	12.31224
2.08552	13.07650	12.31224
10.43741	5.04164	12.31224
10.43741	13.07650	12.31224
2.08544	0.99047	12.22561
2.08544	9.02533	12.22561
10.43733	0.99047	12.22561
10.43733	9.02533	12.22561
4.95531	0.81718	12.20016
4.95531	8.85204	12.20016
13.30720	0.81718	12.20016
13.30720	8.85204	12.20016
7.56688	0.81726	12.20012
7.56688	8.85212	12.20012
15.91877	0.81726	12.20012
15.91877	8.85212	12.20012
3.39122	7.21265	10.94240
3.39122	15.24751	10.94240
11.74311	7.21265	10.94240
11.74311	15.24751	10.94240
0.77969	7.21275	10.94236
0.77969	15.24761	10.94236
9.13158	7.21275	10.94236
9.13158	15.24761	10.94236

6.26110	7.03935	10.91721
6.26110	15.07421	10.91721
14.61299	7.03935	10.91721
14.61299	15.07421	10.91721
6.26127	2.98808	10.83015
6.26127	11.02294	10.83015
14.61316	2.98808	10.83015
14.61316	11.02294	10.83015
3.48353	2.91545	10.82207
3.48353	10.95031	10.82207
11.83542	2.91545	10.82207
11.83542	10.95031	10.82207
0.68773	2.91533	10.82178
0.68773	10.95019	10.82178
9.03962	2.91533	10.82178
9.03962	10.95019	10.82178
4.90129	1.16209	9.60177
4.91488	9.18653	9.59274
13.24859	1.16440	9.60326
13.25159	9.16027	9.61261
7.62506	1.16350	9.60284
7.63805	9.17906	9.60613
15.97324	1.16352	9.60157
15.97118	9.18270	9.60158
2.08444	0.96266	9.38237
2.08299	8.99752	9.37472
10.44682	0.94472	9.38657
10.44837	8.98557	9.43159
2.08619	5.03973	9.38136
2.07666	13.08109	9.38517
10.42766	5.11408	9.42087
10.44473	13.16903	9.44130
7.54906	4.90455	9.34069
7.54849	12.96053	9.39397
15.90072	4.89478	9.34141
15.88193	12.93628	9.34201
4.96786	4.88585	9.34481
4.96139	12.93796	9.35743
13.32032	4.90569	9.34628
13.30754	12.91328	9.32778
0.63557	3.29172	7.99033
0.62337	11.33004	8.00035
9.02114	3.29446	7.99608
9.00961	11.37646	8.08929
3.53125	3.28380	7.98935
3.52957	11.33334	7.98837
11.85910	3.30691	8.00075
11.82089	11.30031	8.02691
6.26960	2.67953	8.18200
6.27682	10.75784	8.21940
14.60346	2.68206	8.18230
14.58712	10.69821	8.18026
6.30462	7.24946	8.05085
6.24801	15.29122	8.01980
14.58194	7.24930	8.01337
14.61231	15.29565	8.02198
3.43713	6.75757	7.90825
3.42250	14.80820	7.93009

11.69662	6.75610	7.94415
11.79034	14.78037	7.91866
0.73879	6.77134	7.92300
0.73376	14.81280	7.93432
9.10883	6.76852	8.03983
9.09118	14.82228	7.95634
10.03573	9.20035	6.33099
8.76383	9.06786	6.08281
11.17024	8.80858	5.40900
7.44045	9.02174	5.90841
10.81841	8.42971	4.43876
11.82775	9.67467	5.23333
11.77570	8.03465	5.90771
6.93327	9.85692	5.41667
6.90342	8.06880	5.99105
9.12291	7.36947	7.26048

Allyl2-Al_2O_3-H-110 (Hydrogen shared between triad- and non-triad- oxygen, $Al_{64}O_{96}C_4H_6$)

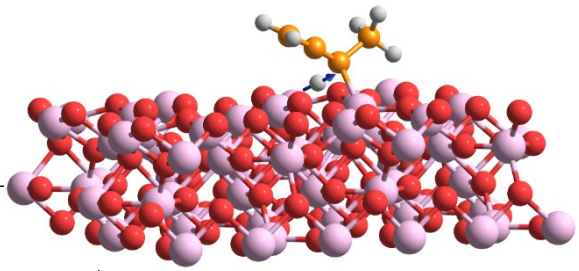
16.703785010	0.000000000	0.000000000
0.000000000	16.069714880	0.000000000
0.000000000	0.000000000	26.000000000
14.61297	12.05818	12.29559
6.26108	4.02332	12.29559
6.26108	12.05818	12.29559
14.61297	4.02332	12.29559
10.43726	15.05806	12.25903
2.08537	7.02320	12.25903
2.08537	15.05806	12.25903
10.43726	7.02320	12.25903
13.18347	14.96429	12.22342
4.83158	6.92943	12.22342
4.83158	14.96429	12.22342
13.18347	6.92943	12.22342
16.04261	14.96435	12.22337
7.69072	6.92949	12.22337
7.69072	14.96435	12.22337
16.04261	6.92949	12.22337
11.86688	9.13514	10.91920
3.51499	1.10028	10.91920
3.51499	9.13514	10.91920
11.86688	1.10028	10.91920
9.00769	9.13508	10.91910
0.65580	1.10022	10.91910
0.65580	9.13508	10.91910
9.00769	1.10022	10.91910
14.61320	9.04168	10.88355
6.26131	1.00682	10.88355
6.26131	9.04168	10.88355
14.61320	1.00682	10.88355
10.43749	12.04119	10.84692
2.08560	4.00633	10.84692
2.08560	12.04119	10.84692
10.43749	4.00633	10.84692
13.16499	11.10252	9.42381
4.87079	3.05561	9.42928
4.90980	11.09945	9.43120



13.23775	3.08003	9.44507
15.97044	11.11971	9.43047
7.62760	3.04648	9.45604
7.69890	11.15773	9.47553
16.00007	3.08046	9.43102
10.46771	15.16393	9.05522
2.14435	7.20282	8.97082
2.08966	15.20697	9.00852
10.46922	7.17951	9.20255
14.58921	14.14384	9.31398
6.23610	6.08411	9.38782
6.25902	14.14555	9.32884
14.62346	6.12436	9.32645
10.38575	10.25816	8.03077
2.08058	2.42553	8.41169
2.09394	10.49874	8.44364
10.45924	2.36527	8.39070
14.60760	8.92534	8.33827
6.26350	0.87154	8.32668
6.48035	9.01196	8.18048
14.61512	0.88841	8.33200
8.94188	13.18386	8.37725
0.59064	5.13586	8.33125
0.57077	13.16494	8.32896
8.96000	5.02564	8.38272
11.92120	13.13298	8.32800
3.59573	5.10424	8.32273
3.60625	13.16042	8.33225
11.94862	5.12322	8.32350
7.65893	5.11426	12.32057
7.65893	13.14912	12.32057
16.01082	5.11426	12.32057
16.01082	13.14912	12.32057
4.86323	5.11417	12.32045
4.86323	13.14903	12.32045
13.21512	5.11417	12.32045
13.21512	13.14903	12.32045
2.08552	5.04164	12.31224
2.08552	13.07650	12.31224
10.43741	5.04164	12.31224
10.43741	13.07650	12.31224
2.08544	0.99047	12.22561
2.08544	9.02533	12.22561
10.43733	0.99047	12.22561
10.43733	9.02533	12.22561
4.95531	0.81718	12.20016
4.95531	8.85204	12.20016
13.30720	0.81718	12.20016
13.30720	8.85204	12.20016
7.56688	0.81726	12.20012
7.56688	8.85212	12.20012
15.91877	0.81726	12.20012
15.91877	8.85212	12.20012
3.39122	7.21265	10.94240
3.39122	15.24751	10.94240
11.74311	7.21265	10.94240
11.74311	15.24751	10.94240
0.77969	7.21275	10.94236

0.77969	15.24761	10.94236
9.13158	7.21275	10.94236
9.13158	15.24761	10.94236
6.26110	7.03935	10.91721
6.26110	15.07421	10.91721
14.61299	7.03935	10.91721
14.61299	15.07421	10.91721
6.26127	2.98808	10.83015
6.26127	11.02294	10.83015
14.61316	2.98808	10.83015
14.61316	11.02294	10.83015
3.48353	2.91545	10.82207
3.48353	10.95031	10.82207
11.83542	2.91545	10.82207
11.83542	10.95031	10.82207
0.68773	2.91533	10.82178
0.68773	10.95019	10.82178
9.03962	2.91533	10.82178
9.03962	10.95019	10.82178
4.90090	1.15643	9.60179
4.93192	9.17727	9.57887
13.25190	1.16587	9.60183
13.25346	9.16460	9.60868
7.62410	1.15380	9.60281
7.65674	9.19662	9.61140
15.97486	1.16569	9.60352
15.97428	9.18271	9.60188
2.08679	0.96102	9.38200
2.09261	8.99648	9.37470
10.45079	0.94408	9.40024
10.43812	8.99326	9.42401
2.09974	5.04648	9.38260
2.08523	13.08030	9.38547
10.43055	5.09416	9.41675
10.45338	13.17273	9.44581
7.54869	4.87356	9.34983
7.56461	12.97840	9.40855
15.90758	4.90647	9.33699
15.89282	12.93751	9.34002
4.97107	4.87189	9.34712
4.96619	12.93658	9.36782
13.32282	4.91059	9.33913
13.31951	12.91968	9.33524
0.64258	3.29879	7.99450
0.63428	11.32858	8.00219
9.02043	3.26036	7.99688
9.01581	11.38959	8.09643
3.53239	3.27885	7.98712
3.53953	11.33374	7.98468
11.86580	3.30217	8.00148
11.83161	11.31580	8.03263
6.26733	2.66846	8.18097
6.29429	10.79820	8.24059
14.60901	2.68587	8.18370
14.59416	10.70325	8.17991
6.52621	7.23963	8.12054
6.25345	15.28321	8.01752
14.58530	7.25239	8.01206

14.62475	15.29837	8.02015
3.51810	6.76094	7.93912
3.43501	14.80880	7.93720
11.63513	6.74110	7.92330
11.80337	14.79559	7.94361
0.80527	6.76847	7.89951
0.74696	14.81016	7.93114
9.02822	6.73292	8.00532
9.10796	14.83255	7.96123
10.11158	9.22258	6.32829
8.84322	9.12932	6.16600
11.28167	8.78243	5.48563
7.48250	9.07477	6.11914
10.95438	8.31677	4.54555
11.93362	9.63834	5.25308
11.86815	8.04582	6.06278
6.98047	9.87864	5.57131
7.05354	8.06846	6.01316
8.04338	7.07860	8.01695



TS Allyl-to-Cumulene-Al_2O_3-110 ($Al_{64}O_{96}C_4H_6$)

16.703785010	0.000000000	0.000000000			
0.000000000	16.069714880	0.000000000			
0.000000000	0.000000000	26.000000000			
30 f/i=	24.268308 THz	152.482276 2PiTHz	809.503596 cm-1		
X	Y	Z	dx	dy	dz
14.612970	12.058180	12.295590	0	0	0
6.261080	4.023320	12.295590	0	0	0
6.261080	12.058180	12.295590	0	0	0
14.612970	4.023320	12.295590	0	0	0
10.437260	15.058060	12.259030	0	0	0
2.085370	7.023200	12.259030	0	0	0
2.085370	15.058060	12.259030	0	0	0
10.437260	7.023200	12.259030	0	0	0
13.183470	14.964290	12.223420	0	0	0
4.831580	6.929430	12.223420	0	0	0
4.831580	14.964290	12.223420	0	0	0
13.183470	6.929430	12.223420	0	0	0
16.042610	14.964350	12.223370	0	0	0
7.690720	6.929490	12.223370	0	0	0
7.690720	14.964350	12.223370	0	0	0
16.042610	6.929490	12.223370	0	0	0
11.866880	9.135140	10.919200	0	0	0
3.514990	1.100280	10.919200	0	0	0
3.514990	9.135140	10.919200	0	0	0
11.866880	1.100280	10.919200	0	0	0
9.007690	9.135080	10.919100	0	0	0
0.655800	1.100220	10.919100	0	0	0
0.655800	9.135080	10.919100	0	0	0
9.007690	1.100220	10.919100	0	0	0
14.613200	9.041680	10.883550	0	0	0
6.261310	1.006820	10.883550	0	0	0
6.261310	9.041680	10.883550	0	0	0
14.613200	1.006820	10.883550	0	0	0
10.437490	12.041190	10.846920	0	0	0
2.085600	4.006330	10.846920	0	0	0

2.085600 12.041190 10.846920	0	0	0
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13.158930 11.081050 9.417070	0	0	0
4.881480 3.076850 9.433440	0	0	0
4.893330 11.120180 9.432740	0	0	0
13.240500 3.070860 9.440990	0	0	0
15.962450 11.118450 9.431290	0	0	0
7.646930 3.097050 9.432040	0	0	0
7.688650 11.117130 9.447250	0	0	0
16.000400 3.078450 9.429850	0	0	0
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2.100910 7.195830 8.990100	0	0	0
2.078400 15.221290 8.996030	0	0	0
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14.563080 14.134860 9.315790	0	0	0
6.249130 6.135990 9.316080	0	0	0
6.266340 14.151330 9.320200	0	0	0
14.625070 6.118390 9.322560	0	0	0
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2.091130 2.442180 8.424410	0	0	0
2.071200 10.497050 8.444960	0	0	0
10.441200 2.415680 8.408980	0	0	0
14.616910 8.915300 8.337570	0	0	0
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6.277280 8.943600 8.327140	0	0	0
14.618970 0.882780 8.332800	0	0	0
8.939800 13.147110 8.359100	0	0	0
0.585290 5.129040 8.324530	0	0	0
0.553820 13.170790 8.336780	0	0	0
8.963190 5.168580 8.336890	0	0	0
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3.588990 13.164650 8.329860	0	0	0
11.970460 5.124640 8.344840	0	0	0
7.658930 5.114260 12.320570	0	0	0
7.658930 13.149120 12.320570	0	0	0
16.010820 5.114260 12.320570	0	0	0
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4.863230 13.149030 12.320450	0	0	0
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7.566880 0.817260 12.200120	0	0	0
7.566880 8.852120 12.200120	0	0	0
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9.131580 15.247610 10.942360	0	0	0
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6.261270 11.022940 10.830150	0	0	0
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9.039620 10.950190 10.821780	0	0	0
4.903660 1.163370 9.600800	0	0	0
4.904490 9.185950 9.599370	0	0	0
13.251620 1.158190 9.603220	0	0	0
13.255290 9.161050 9.609870	0	0	0
7.628790 1.168960 9.601980	0	0	0
7.623360 9.181150 9.605630	0	0	0
15.976120 1.159050 9.603500	0	0	0
15.975140 9.188710 9.602980	0	0	0
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2.093260 5.041530 9.382430	0	0	0
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10.442820 5.098900 9.420330	0	0	0
10.439590 13.146140 9.425160	0	0	0
7.565830 4.935990 9.317450	0	0	0
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13.295800 12.898070 9.305950	0	0	0
0.643890 3.292760 7.991310	0	0	0
0.619120 11.335620 7.999940	0	0	0
9.024000 3.337350 7.999710	0	0	0
9.006790 11.336510 8.054650	0	0	0
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3.525490 11.331400 7.997040	0	0	0
11.875030 3.306500 8.006700	0	0	0
11.801180 11.258840 8.003270	0	0	0
6.275390 2.687170 8.181060	0	0	0
6.267820 10.726380 8.189470	0	0	0

14.613440	2.674820	8.180210	0	0	0
14.586980	10.695860	8.177760	0	0	0
6.315470	7.270130	8.004910	0	0	0
6.255260	15.299700	8.020100	0	0	0
14.625320	7.249700	8.009440	0	0	0
14.602100	15.290480	8.023690	0	0	0
3.459820	6.775080	7.939860	0	0	0
3.420360	14.808970	7.925460	0	0	0
11.806570	6.781410	8.027740	0	0	0
11.778210	14.750990	7.886850	0	0	0
0.765180	6.769210	7.915810	0	0	0
0.730380	14.814550	7.932980	0	0	0
9.208120	6.846540	7.980180	0	0	0
9.087190	14.795390	7.931560	0	0	0
10.056770	8.845700	6.414800	-0.015746	-0.158630	-0.106478
8.994280	9.372640	5.818590	-0.042833	0.074947	-0.026959
11.321940	8.521270	5.615380	0.031357	0.015931	-0.006608
7.889250	9.851590	5.313590	0.025585	0.039555	-0.000193
11.243860	7.491690	5.238260	0.002174	0.004037	0.006920
11.460590	9.202580	4.766380	0.000659	0.019197	0.014758
12.210630	8.526360	6.257990	-0.004794	0.002859	0.016546
7.673560	10.922640	5.336150	-0.089575	-0.010644	0.160389
7.163510	9.187020	4.837220	0.101952	0.013060	-0.151874
9.605510	7.864580	7.190610	0.431148	0.761595	-0.342352

Cumulene-Al_2O_3-110 ($Al_{64}O_{96}C_4H_6$)

16.703785010	0.000000000	0.000000000
0.000000000	16.069714880	0.000000000
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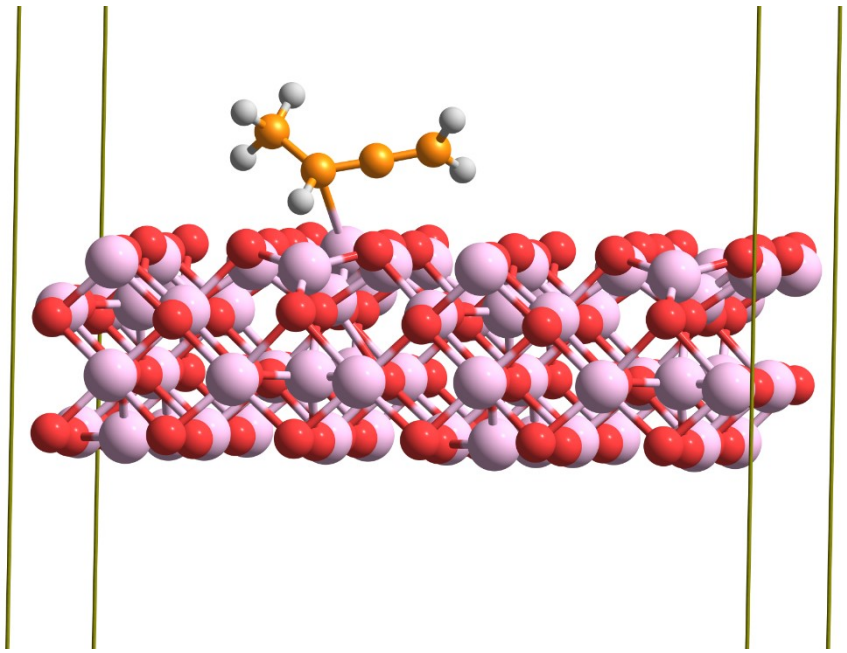
14.61297	12.05818	12.29559
6.26108	4.02332	12.29559
6.26108	12.05818	12.29559
14.61297	4.02332	12.29559
10.43726	15.05806	12.25903
2.08537	7.02320	12.25903
2.08537	15.05806	12.25903
10.43726	7.02320	12.25903
13.18347	14.96429	12.22342
4.83158	6.92943	12.22342
4.83158	14.96429	12.22342
13.18347	6.92943	12.22342
16.04261	14.96435	12.22337
7.69072	6.92949	12.22337
7.69072	14.96435	12.22337
16.04261	6.92949	12.22337
11.86688	9.13514	10.91920
3.51499	1.10028	10.91920
3.51499	9.13514	10.91920
11.86688	1.10028	10.91920
9.00769	9.13508	10.91910
0.65580	1.10022	10.91910
0.65580	9.13508	10.91910
9.00769	1.10022	10.91910
14.61320	9.04168	10.88355
6.26131	1.00682	10.88355
6.26131	9.04168	10.88355



14.61320	1.00682	10.88355
10.43749	12.04119	10.84692
2.08560	4.00633	10.84692
2.08560	12.04119	10.84692
10.43749	4.00633	10.84692
13.18709	11.10767	9.44161
4.87915	3.07742	9.42871
4.89949	11.11383	9.42666
13.23083	3.08122	9.43306
15.97875	11.11848	9.42938
7.64165	3.07771	9.43505
7.69288	11.10826	9.44403
15.99349	3.07981	9.43089
10.44938	15.19674	8.99987
2.08246	7.19774	8.97463
2.08880	15.22429	8.99244
10.40384	7.15581	9.15119
14.60212	14.14959	9.32075
6.25629	6.11797	9.32216
6.27984	14.14610	9.32195
14.61382	6.12324	9.31944
10.44460	10.27637	8.09992
2.08244	2.44689	8.42907
2.08862	10.49506	8.43924
10.43615	2.42866	8.41693
14.61699	8.92217	8.34212
6.26267	0.88401	8.33310
6.27729	8.91545	8.33944
14.61227	0.88843	8.33277
8.95558	13.15407	8.34826
0.57268	5.12944	8.32771
0.57367	13.16554	8.32817
8.92152	5.13201	8.33453
11.93405	13.14808	8.34428
3.59122	5.12809	8.32569
3.60369	13.16555	8.33160
11.93613	5.13895	8.34806
7.65893	5.11426	12.32057
7.65893	13.14912	12.32057
16.01082	5.11426	12.32057
16.01082	13.14912	12.32057
4.86323	5.11417	12.32045
4.86323	13.14903	12.32045
13.21512	5.11417	12.32045
13.21512	13.14903	12.32045
2.08552	5.04164	12.31224
2.08552	13.07650	12.31224
10.43741	5.04164	12.31224
10.43741	13.07650	12.31224
2.08544	0.99047	12.22561
2.08544	9.02533	12.22561
10.43733	0.99047	12.22561
10.43733	9.02533	12.22561
4.95531	0.81718	12.20016
4.95531	8.85204	12.20016
13.30720	0.81718	12.20016
13.30720	8.85204	12.20016
7.56688	0.81726	12.20012

7.56688	8.85212	12.20012
15.91877	0.81726	12.20012
15.91877	8.85212	12.20012
3.39122	7.21265	10.94240
3.39122	15.24751	10.94240
11.74311	7.21265	10.94240
11.74311	15.24751	10.94240
0.77969	7.21275	10.94236
0.77969	15.24761	10.94236
9.13158	7.21275	10.94236
9.13158	15.24761	10.94236
6.26110	7.03935	10.91721
6.26110	15.07421	10.91721
14.61299	7.03935	10.91721
14.61299	15.07421	10.91721
6.26127	2.98808	10.83015
6.26127	11.02294	10.83015
14.61316	2.98808	10.83015
14.61316	11.02294	10.83015
3.48353	2.91545	10.82207
3.48353	10.95031	10.82207
11.83542	2.91545	10.82207
11.83542	10.95031	10.82207
0.68773	2.91533	10.82178
0.68773	10.95019	10.82178
9.03962	2.91533	10.82178
9.03962	10.95019	10.82178
4.89957	1.15756	9.60348
4.90376	9.19198	9.60025
13.25112	1.15935	9.60434
13.25430	9.17936	9.60759
7.62361	1.15813	9.60409
7.62225	9.17875	9.61097
15.97498	1.15985	9.60385
15.97506	9.19080	9.60269
2.08415	0.96377	9.38128
2.08600	9.00066	9.37651
10.44161	0.95466	9.37757
10.43090	9.00146	9.39738
2.08217	5.04142	9.38175
2.08772	13.07614	9.38280
10.43222	5.06350	9.40932
10.44501	13.14895	9.42755
7.54303	4.89510	9.34766
7.55912	12.92785	9.34725
15.89707	4.89952	9.34361
15.89790	12.93661	9.34291
4.97029	4.89726	9.34263
4.98479	12.93234	9.34137
13.32508	4.90319	9.34485
13.32578	12.92731	9.34913
0.63325	3.29355	7.99257
0.63392	11.32978	7.99451
8.99643	3.30088	7.99986
9.03311	11.33599	8.03151
3.53166	3.29181	7.99173
3.54149	11.33132	7.99270
11.87238	3.30822	8.00119

11.85667	11.33075	8.02828
6.26315	2.67429	8.17958
6.28613	10.70437	8.17584
14.60892	2.67948	8.18121
14.59706	10.70625	8.17674
6.26253	7.25181	8.01278
6.26516	15.29023	8.02170
14.59873	7.25940	8.00878
14.61947	15.29467	8.02028
3.42639	6.77006	7.91685
3.43518	14.80972	7.93043
11.75788	6.79831	8.00452
11.79336	14.79426	7.91649
0.73028	6.77409	7.92510
0.74696	14.80910	7.92453
9.10854	6.77993	7.97865
9.09893	14.80019	7.92350
10.95385	8.99763	6.25529
9.66192	9.19601	6.00923
12.08302	9.53213	5.40041
8.39617	9.37020	5.73998
11.72160	10.16546	4.58147
12.79672	10.11266	6.00662
12.62347	8.66757	4.98202
7.82011	10.18608	6.19137
7.89671	8.67452	5.06024
11.23827	8.15563	6.95595

Butyne1-Al_2O_3-001 (physisorption to the center of “square”, $Al_{64}O_{96}C_4H_6$)

11.116000000	0.000000000	0.000000000
0.000000000	16.703800000	0.000000000
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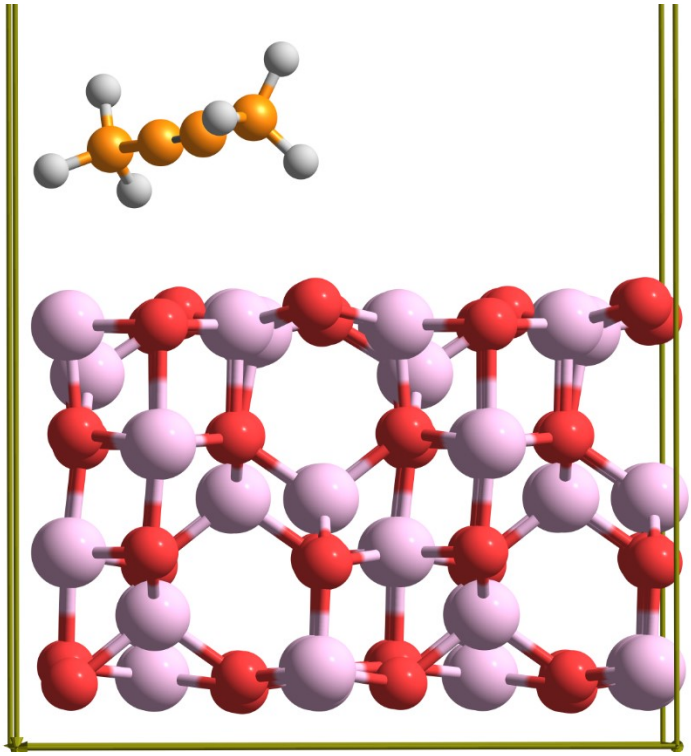
0.39545	1.75649	1.18978
3.18673	1.75607	1.19055
0.43097	4.50284	1.28299
0.43108	7.36203	1.28324
3.20824	5.93252	2.22364
4.59841	0.29825	3.28771
4.59836	3.21456	3.28771
0.35882	5.93269	4.18926
1.80746	1.75624	4.20627
5.95345	10.10839	1.18978
8.74473	10.10797	1.19055
5.98897	12.85474	1.28299
5.98908	15.71393	1.28324
8.76624	14.28442	2.22364
10.15641	8.65015	3.28771
10.15636	11.56646	3.28771
5.91682	14.28459	4.18926
7.36546	10.10814	4.20627
0.39545	10.10839	1.18978
3.18673	10.10797	1.19055
0.43097	12.85474	1.28299
0.43108	15.71393	1.28324
3.20824	14.28442	2.22364
4.59841	8.65015	3.28771



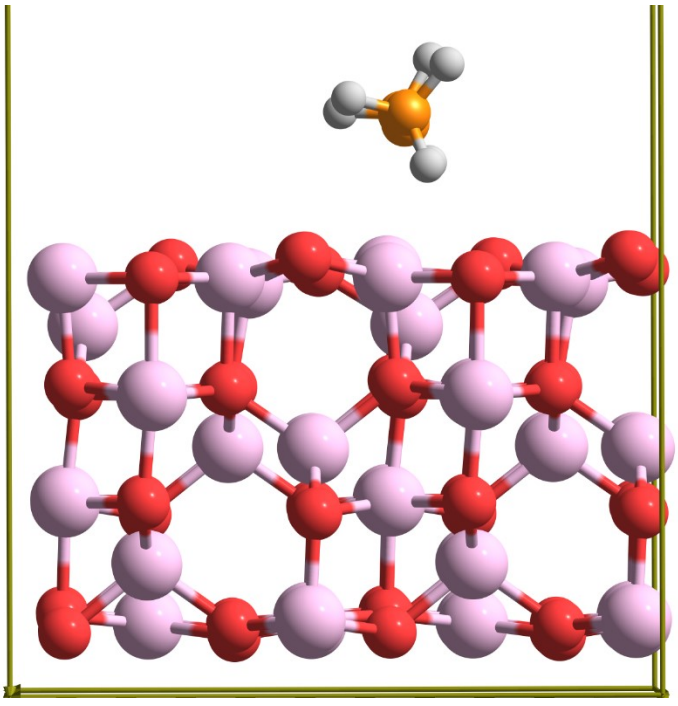
4.59836	11.56646	3.28771
0.35882	14.28459	4.18926
1.80746	10.10814	4.20627
5.95345	1.75649	1.18978
8.74473	1.75607	1.19055
5.98897	4.50284	1.28299
5.98908	7.36203	1.28324
8.76624	5.93252	2.22364
10.15641	0.29825	3.28771
10.15636	3.21456	3.28771
5.91682	5.93269	4.18926
7.36546	1.75624	4.20627
8.67623	4.46340	5.11944
8.66866	7.40383	5.11379
9.83881	1.75986	6.29651
7.04165	0.37356	7.02576
7.00622	3.11454	7.01017
10.18730	5.94151	7.12852
7.35197	5.92078	7.16579
3.12156	12.80967	5.11656
3.11539	15.75967	5.11371
4.27629	10.10134	6.30047
1.46933	8.73260	7.02288
1.45903	11.46639	7.02070
4.63874	14.28176	7.12232
1.78650	14.28240	7.12461
8.67885	12.81136	5.11688
8.67429	15.76199	5.11340
9.83359	10.10607	6.29954
7.03852	8.72009	7.01752
7.00831	11.45764	7.01939
10.19832	14.28221	7.12255
7.34262	14.28037	7.12474
3.11904	4.45682	5.11467
3.11546	7.40550	5.11489
4.27952	1.74943	6.30037
1.47225	0.38286	7.02317
1.46884	3.12078	7.02122
4.64202	5.92118	7.11427
1.78166	5.93051	7.12418
1.71198	3.06206	1.00008
1.71203	0.45050	1.00008
4.62187	5.93286	1.06915
1.73749	5.93252	1.17328
4.65444	3.06331	1.34927
4.65449	0.44967	1.34927
3.23253	1.75632	3.07084
0.33392	7.33063	3.09826
0.33365	4.53475	3.09826
0.34204	1.75640	3.17089
3.26899	7.33756	3.28213
3.26922	4.52740	3.28213
1.71198	11.41396	1.00008
1.71203	8.80240	1.00008
4.62187	14.28476	1.06915
1.73749	14.28442	1.17328
4.65444	11.41521	1.34927
4.65449	8.80157	1.34927

3.23253	10.10822	3.07084
0.33392	15.68253	3.09826
0.33365	12.88665	3.09826
0.34204	10.10830	3.17089
3.26899	15.68946	3.28213
3.26922	12.87930	3.28213
7.26998	3.06206	1.00008
7.27003	0.45050	1.00008
10.17987	5.93286	1.06915
7.29549	5.93252	1.17328
10.21244	3.06331	1.34927
10.21249	0.44967	1.34927
8.79053	1.75632	3.07084
5.89192	7.33063	3.09826
5.89165	4.53475	3.09826
5.90004	1.75640	3.17089
8.82699	7.33756	3.28213
8.82722	4.52740	3.28213
7.26998	11.41396	1.00008
7.27003	8.80240	1.00008
10.17987	14.28476	1.06915
7.29549	14.28442	1.17328
10.21244	11.41521	1.34927
10.21249	8.80157	1.34927
8.79053	10.10822	3.07084
5.89192	15.68253	3.09826
5.89165	12.88665	3.09826
5.90004	10.10830	3.17089
8.82699	15.68946	3.28213
8.82722	12.87930	3.28213
4.38996	3.12683	5.14340
4.38690	0.38065	5.13914
1.84167	5.92983	5.21513
1.75914	3.19578	5.24829
1.75424	0.31595	5.24679
4.49783	5.93122	5.29504
3.11872	4.65945	7.12249
3.10683	7.21180	7.12104
0.25076	1.75333	7.23829
2.75349	1.75600	7.33371
0.49996	7.19363	7.45990
0.50904	4.66309	7.46659
4.39114	11.47952	5.14423
4.38557	8.73240	5.13985
1.84229	14.28197	5.21631
1.76090	11.54829	5.24988
1.75493	8.66736	5.24685
4.50372	14.28488	5.29959
3.12882	13.01954	7.12637
3.10505	15.57064	7.12026
0.24812	10.10023	7.23415
2.75028	10.10713	7.33464
0.49987	15.54434	7.46106
0.51222	13.01415	7.45805
9.94994	3.13149	5.14000
9.94653	0.38493	5.14139
7.39668	5.93191	5.22021
7.31730	3.19461	5.24450

7.31496	0.31706	5.24666
10.06466	5.94216	5.30182
8.69188	4.66343	7.09633
8.65446	7.22936	7.11262
5.81135	1.73799	7.23247
8.31356	1.76532	7.33821
6.05386	7.18468	7.45502
6.06105	4.65450	7.44550
9.94900	11.48384	5.14404
9.94145	8.73710	5.13917
7.40096	14.28231	5.21626
7.31967	11.54863	5.25125
7.31035	8.66848	5.24115
10.06150	14.29160	5.30064
8.69482	13.03046	7.12945
8.65322	15.58331	7.11966
5.80656	10.08675	7.23522
8.30823	10.10963	7.33424
6.05710	15.53847	7.46172
6.07113	13.00800	7.45632
7.86075	6.01865	10.38746
8.57261	5.04073	10.24446
9.41875	3.86013	10.14050
7.01433	7.17300	10.65641
9.52934	3.37849	11.12567
9.00847	3.11755	9.43992
10.42518	4.11346	9.77291
6.21603	7.27314	9.90584
6.53971	7.08553	11.64722
7.59869	8.10729	10.64524

Butyne2-Al_2O_3-001 (strongest found adsorption, $Al_{64}O_{96}C_4H_6$)

11.116000000	0.000000000	0.000000000
0.000000000	16.703800000	0.000000000
0.000000000	0.000000000	26.000000000
0.39545	1.75649	1.18978
3.18673	1.75607	1.19055
0.43097	4.50284	1.28299
0.43108	7.36203	1.28324
3.20824	5.93252	2.22364
4.59841	0.29825	3.28771
4.59836	3.21456	3.28771
0.35882	5.93269	4.18926
1.80746	1.75624	4.20627
5.95345	10.10839	1.18978
8.74473	10.10797	1.19055
5.98897	12.85474	1.28299
5.98908	15.71393	1.28324
8.76624	14.28442	2.22364
10.15641	8.65015	3.28771
10.15636	11.56646	3.28771
5.91682	14.28459	4.18926
7.36546	10.10814	4.20627
0.39545	10.10839	1.18978
3.18673	10.10797	1.19055
0.43097	12.85474	1.28299



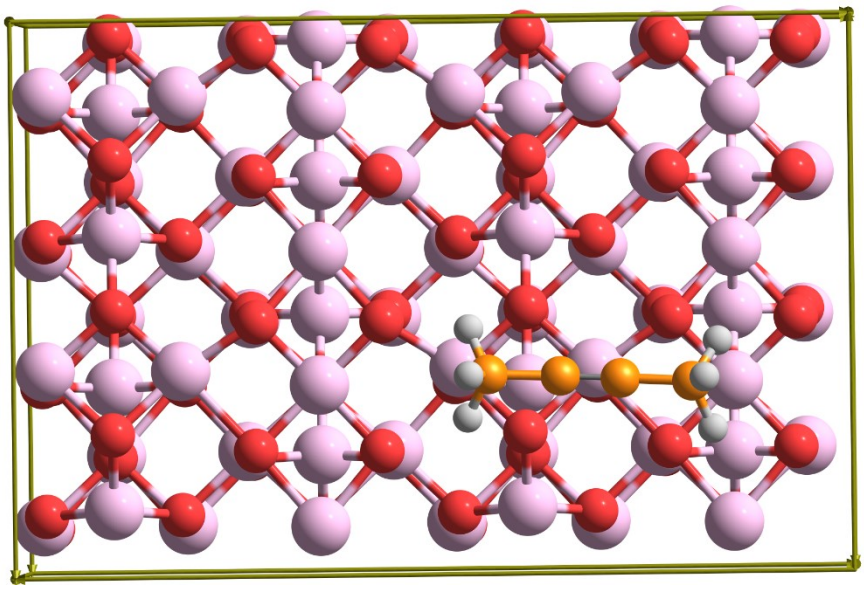
0.43108	15.71393	1.28324
3.20824	14.28442	2.22364
4.59841	8.65015	3.28771
4.59836	11.56646	3.28771
0.35882	14.28459	4.18926
1.80746	10.10814	4.20627
5.95345	1.75649	1.18978
8.74473	1.75607	1.19055
5.98897	4.50284	1.28299
5.98908	7.36203	1.28324
8.76624	5.93252	2.22364
10.15641	0.29825	3.28771
10.15636	3.21456	3.28771
5.91682	5.93269	4.18926
7.36546	1.75624	4.20627
8.68105	4.45973	5.11273
8.67849	7.40573	5.11179
9.84950	1.75749	6.29960
7.04132	0.38033	7.02380
7.03756	3.12024	7.01236
10.18475	5.92974	7.11994
7.33343	5.93071	7.10725
3.12160	12.81121	5.11540
3.11855	15.75919	5.11325
4.28451	10.10826	6.29193
1.47937	8.71452	7.00961
1.46552	11.46251	7.02279
4.64057	14.28300	7.12305
1.78650	14.28238	7.12515
8.67913	12.80992	5.11552
8.67664	15.76116	5.11315
9.84279	10.10361	6.29971
7.04085	8.72919	7.01574
7.02130	11.46683	7.02110
10.19918	14.28306	7.12291
7.34420	14.28223	7.12454
3.12983	4.46453	5.12201
3.12747	7.39907	5.12136
4.29086	1.75228	6.29215
1.48308	0.38625	7.02510
1.47544	3.13650	7.00857
4.62129	5.92405	7.23118
1.76028	5.92935	7.11329
1.71198	3.06206	1.00008
1.71203	0.45050	1.00008
4.62187	5.93286	1.06915
1.73749	5.93252	1.17328
4.65444	3.06331	1.34927
4.65449	0.44967	1.34927
3.23253	1.75632	3.07084
0.33392	7.33063	3.09826
0.33365	4.53475	3.09826
0.34204	1.75640	3.17089
3.26899	7.33756	3.28213
3.26922	4.52740	3.28213
1.71198	11.41396	1.00008
1.71203	8.80240	1.00008
4.62187	14.28476	1.06915

1.73749	14.28442	1.17328
4.65444	11.41521	1.34927
4.65449	8.80157	1.34927
3.23253	10.10822	3.07084
0.33392	15.68253	3.09826
0.33365	12.88665	3.09826
0.34204	10.10830	3.17089
3.26899	15.68946	3.28213
3.26922	12.87930	3.28213
7.26998	3.06206	1.00008
7.27003	0.45050	1.00008
10.17987	5.93286	1.06915
7.29549	5.93252	1.17328
10.21244	3.06331	1.34927
10.21249	0.44967	1.34927
8.79053	1.75632	3.07084
5.89192	7.33063	3.09826
5.89165	4.53475	3.09826
5.90004	1.75640	3.17089
8.82699	7.33756	3.28213
8.82722	4.52740	3.28213
7.26998	11.41396	1.00008
7.27003	8.80240	1.00008
10.17987	14.28476	1.06915
7.29549	14.28442	1.17328
10.21244	11.41521	1.34927
10.21249	8.80157	1.34927
8.79053	10.10822	3.07084
5.89192	15.68253	3.09826
5.89165	12.88665	3.09826
5.90004	10.10830	3.17089
8.82699	15.68946	3.28213
8.82722	12.87930	3.28213
4.39589	3.12677	5.14051
4.39366	0.37829	5.14014
1.83779	5.93102	5.20741
1.76276	3.19523	5.23728
1.76252	0.31686	5.24923
4.51020	5.93303	5.34525
3.07381	4.63872	7.09742
3.06028	7.23565	7.09695
0.26671	1.75587	7.23217
2.76934	1.76336	7.33790
0.48075	7.19116	7.45538
0.48747	4.66290	7.45318
4.39541	11.48599	5.14265
4.39215	8.73699	5.13908
1.84349	14.28259	5.21670
1.76611	11.54707	5.25266
1.75924	8.66831	5.23554
4.50399	14.28661	5.30120
3.12937	13.01949	7.12886
3.10818	15.57119	7.12324
0.26003	10.09262	7.23218
2.76346	10.10261	7.33805
0.50488	15.54557	7.46109
0.51333	13.01239	7.45882
9.95224	3.13045	5.14093

9.94923	0.38300	5.14143
7.40570	5.93137	5.20555
7.32381	3.19494	5.24200
7.31571	0.31554	5.24672
10.05854	5.93366	5.29529
8.67830	4.66360	7.11741
8.66503	7.21428	7.11338
5.81848	1.74994	7.23709
8.32145	1.75693	7.33247
6.07473	7.20497	7.44801
6.08259	4.64842	7.44261
9.95046	11.48217	5.14418
9.94872	8.73477	5.13899
7.40136	14.28247	5.21679
7.31914	11.54869	5.25040
7.31950	8.66939	5.24140
10.06239	14.28717	5.30142
8.68657	13.02040	7.12821
8.66398	15.57224	7.12190
5.81101	10.09749	7.23755
8.31484	10.10931	7.33337
6.06179	15.54394	7.46236
6.07001	13.01341	7.45968
4.28455	6.51419	9.75833
4.31043	5.29181	9.75445
4.35874	3.84601	9.91425
4.27129	7.95883	9.93933
3.85341	3.55838	10.84917
3.87147	3.32394	9.07879
5.40032	3.49618	9.95704
3.93726	8.48286	9.03368
3.59186	8.22626	10.76354
5.27908	8.32544	10.18485

Butyne3-Al_2O_3-001 (one more possible adsorption geometry, $Al_{64}O_{96}C_4H_6$)

11.116000000	0.000000000	0.000000000
0.000000000	16.703800000	0.000000000
0.000000000	0.000000000	26.000000000
0.39545	1.75649	1.18978
3.18673	1.75607	1.19055
0.43097	4.50284	1.28299
0.43108	7.36203	1.28324
3.20824	5.93252	2.22364
4.59841	0.29825	3.28771
4.59836	3.21456	3.28771
0.35882	5.93269	4.18926
1.80746	1.75624	4.20627
5.95345	10.10839	1.18978
8.74473	10.10797	1.19055
5.98897	12.85474	1.28299
5.98908	15.71393	1.28324
8.76624	14.28442	2.22364
10.15641	8.65015	3.28771
10.15636	11.56646	3.28771
5.91682	14.28459	4.18926
7.36546	10.10814	4.20627



0.39545	10.10839	1.18978
3.18673	10.10797	1.19055
0.43097	12.85474	1.28299
0.43108	15.71393	1.28324
3.20824	14.28442	2.22364
4.59841	8.65015	3.28771
4.59836	11.56646	3.28771
0.35882	14.28459	4.18926
1.80746	10.10814	4.20627
5.95345	1.75649	1.18978
8.74473	1.75607	1.19055
5.98897	4.50284	1.28299
5.98908	7.36203	1.28324
8.76624	5.93252	2.22364
10.15641	0.29825	3.28771
10.15636	3.21456	3.28771
5.91682	5.93269	4.18926
7.36546	1.75624	4.20627
8.67487	4.45436	5.11453
8.67919	7.40384	5.11503
9.83625	1.75413	6.30020
7.01648	0.39834	7.01905
7.03710	3.13485	7.02552
10.19878	5.93125	7.12103
7.34374	5.93316	7.12159
3.11507	12.80928	5.11298
3.12094	15.75777	5.11621
4.29072	10.11718	6.29813
1.47224	8.74622	7.02161
1.47705	11.48366	7.02310
4.63819	14.27996	7.11432
1.77967	14.28589	7.12154
8.66459	12.79519	5.11806
8.68004	15.75383	5.11721
9.84742	10.10317	6.29348
7.01947	8.75437	7.00385
7.06362	11.48766	7.09086
10.19262	14.27801	7.12309
7.33468	14.28810	7.11570
3.11655	4.45784	5.11472
3.12294	7.40785	5.11676
4.27953	1.75961	6.29967
1.46282	0.39000	7.02032
1.47030	3.12670	7.02251
4.64176	5.93482	7.12081
1.78656	5.93343	7.12425
1.71198	3.06206	1.00008
1.71203	0.45050	1.00008
4.62187	5.93286	1.06915
1.73749	5.93252	1.17328
4.65444	3.06331	1.34927
4.65449	0.44967	1.34927
3.23253	1.75632	3.07084
0.33392	7.33063	3.09826
0.33365	4.53475	3.09826
0.34204	1.75640	3.17089
3.26899	7.33756	3.28213
3.26922	4.52740	3.28213

1.71198	11.41396	1.00008
1.71203	8.80240	1.00008
4.62187	14.28476	1.06915
1.73749	14.28442	1.17328
4.65444	11.41521	1.34927
4.65449	8.80157	1.34927
3.23253	10.10822	3.07084
0.33392	15.68253	3.09826
0.33365	12.88665	3.09826
0.34204	10.10830	3.17089
3.26899	15.68946	3.28213
3.26922	12.87930	3.28213
7.26998	3.06206	1.00008
7.27003	0.45050	1.00008
10.17987	5.93286	1.06915
7.29549	5.93252	1.17328
10.21244	3.06331	1.34927
10.21249	0.44967	1.34927
8.79053	1.75632	3.07084
5.89192	7.33063	3.09826
5.89165	4.53475	3.09826
5.90004	1.75640	3.17089
8.82699	7.33756	3.28213
8.82722	4.52740	3.28213
7.26998	11.41396	1.00008
7.27003	8.80240	1.00008
10.17987	14.28476	1.06915
7.29549	14.28442	1.17328
10.21244	11.41521	1.34927
10.21249	8.80157	1.34927
8.79053	10.10822	3.07084
5.89192	15.68253	3.09826
5.89165	12.88665	3.09826
5.90004	10.10830	3.17089
8.82699	15.68946	3.28213
8.82722	12.87930	3.28213
4.38728	3.13076	5.13986
4.38994	0.38519	5.14214
1.84420	5.93290	5.21543
1.75650	3.19629	5.24672
1.75971	0.31541	5.24695
4.50374	5.93127	5.29813
3.11214	4.65224	7.12085
3.12648	7.20276	7.12401
0.25018	1.75965	7.23438
2.75349	1.75439	7.33239
0.51340	7.20010	7.45842
0.50457	4.67004	7.45934
4.38438	11.48400	5.13514
4.39187	8.73698	5.14039
1.84123	14.28677	5.21302
1.75377	11.55042	5.24338
1.76241	8.66589	5.24728
4.49742	14.28642	5.29307
3.09921	12.99792	7.11325
3.12167	15.55055	7.12263
0.25874	10.11197	7.23162
2.76065	10.10868	7.32763

0.50769	15.55272	7.45832
0.49799	13.02304	7.45987
9.94659	3.12666	5.14030
9.95004	0.37982	5.14198
7.40217	5.92958	5.21367
7.31450	3.19513	5.24569
7.32103	0.31582	5.24806
10.06214	5.92471	5.29896
8.66068	4.63880	7.11926
8.69194	7.18696	7.12530
5.80949	1.76910	7.23353
8.31257	1.75213	7.33545
6.06875	7.20306	7.44609
6.06029	4.67369	7.46278
9.95081	11.47813	5.13879
9.95428	8.72709	5.13874
7.40247	14.28610	5.20956
7.31580	11.53717	5.27168
7.31693	8.65557	5.23503
10.06047	14.27365	5.30054
8.65232	12.99188	7.12326
8.68592	15.54244	7.12343
5.81716	10.11565	7.22756
8.33236	10.07910	7.31003
6.06677	15.56398	7.45276
6.04128	13.03938	7.42911
7.26675	12.02031	10.26666
7.20906	10.81067	10.20369
7.16468	9.35497	10.21898
7.33843	13.46120	10.46108
6.52726	13.98668	9.93388
7.25677	13.71678	11.53177
8.29751	13.87333	10.10427
8.03503	8.93487	9.68815
7.18696	8.97182	11.24967
6.24472	8.97141	9.74442

TS Butyne2-Al_2O_3-001 (without hydroxyls, H goes to surface O, $Al_{64}O_{96}C_4H_6$)

11.116000000	0.000000000	0.000000000			
0.000000000	16.703800000	0.000000000			
0.000000000	0.000000000	26.000000000			
150 f/i= 25.266310 THz 158.752910 2PiTHz 842.793369 cm-1					
X	Y	Z	dx	dy	dz
0.395450	1.756490	1.189780	0	0	0
3.186730	1.756070	1.190550	0	0	0
0.430970	4.502840	1.282990	0	0	0
0.431080	7.362030	1.283240	0	0	0
3.208240	5.932520	2.223640	0	0	0
4.598410	0.298250	3.287710	0	0	0
4.598360	3.214560	3.287710	0	0	0
0.358820	5.932690	4.189260	0	0	0
1.807460	1.756240	4.206270	0	0	0
5.953450	10.108390	1.189780	0	0	0
8.744730	10.107970	1.190550	0	0	0
5.988970	12.854740	1.282990	0	0	0
5.989080	15.713930	1.283240	0	0	0

8.766240 14.284420 2.223640	0	0	0
10.156410 8.650150 3.287710	0		
10.156360 11.566460 3.287710	0		
5.916820 14.284590 4.189260	0		
7.365460 10.108140 4.206270	0		
0.395450 10.108390 1.189780	0		
3.186730 10.107970 1.190550	0		
0.430970 12.854740 1.282990	0		
0.431080 15.713930 1.283240	0		
3.208240 14.284420 2.223640	0		
4.598410 8.650150 3.287710	0		
4.598360 11.566460 3.287710	0		
0.358820 14.284590 4.189260	0		
1.807460 10.108140 4.206270	0		
5.953450 1.756490 1.189780	0		
8.744730 1.756070 1.190550	0		
5.988970 4.502840 1.282990	0		
5.989080 7.362030 1.283240	0		
8.766240 5.932520 2.223640	0	0	0
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1.783370 14.288524 7.133048	0.003417	-0.017793	-0.001505
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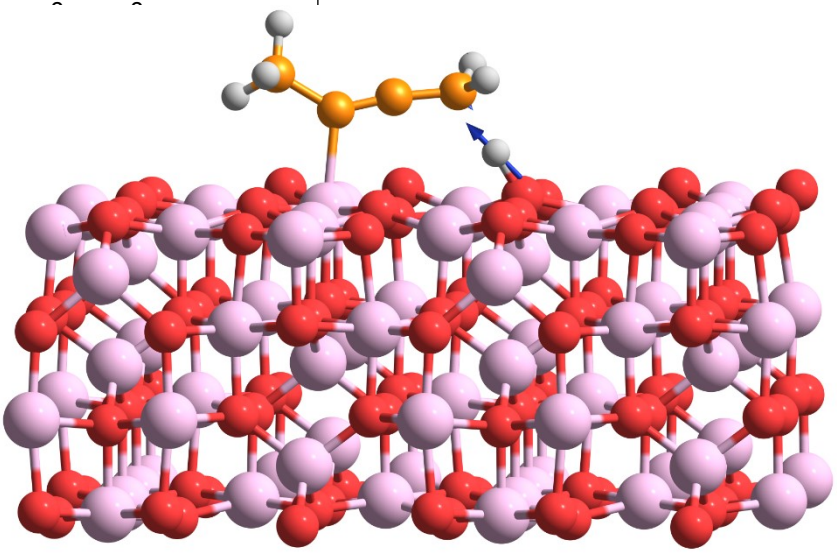

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0.452014	4.671964	7.456850	0.009897	-0.008153	0.004418
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6.107437	15.592719	7.455099	0.000954	0.006953	0.002891
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3.236633	9.441002	8.448752	0.203530	-0.522981	0.563477
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Allyl2-Al_2O_3-H-001 (lowest found structure, $Al_{64}O_{96}C_4H_6$)

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3.18673	1.75607	1.19055
0.43097	4.50284	1.28299
0.43108	7.36203	1.28324
3.20824	5.93252	2.22364
4.59841	0.29825	3.28771
4.59836	3.21456	3.28771
0.35882	5.93269	4.18926
1.80746	1.75624	4.20627
5.95345	10.10839	1.18978

8.74473	10.10797	1.19055
5.98897	12.85474	1.28299
5.98908	15.71393	1.28324
8.76624	14.28442	2.22364
10.15641	8.65015	3.28771
10.15636	11.56646	3.28771
5.91682	14.28459	4.18926
7.36546	10.10814	4.20627
0.39545	10.10839	1.18978
3.18673	10.10797	1.19055
0.43097	12.85474	1.28299
0.43108	15.71393	1.28324
3.20824	14.28442	2.22364
4.59841	8.65015	3.28771
4.59836	11.56646	3.28771
0.35882	14.28459	4.18926
1.80746	10.10814	4.20627
5.95345	1.75649	1.18978
8.74473	1.75607	1.19055
5.98897	4.50284	1.28299
5.98908	7.36203	1.28324
8.76624	5.93252	2.22364
10.15641	0.29825	3.28771
10.15636	3.21456	3.28771
5.91682	5.93269	4.18926
7.36546	1.75624	4.20627
8.68105	4.45973	5.11273
8.67849	7.40573	5.11179
3.12160	12.81121	5.11540
3.11855	15.75919	5.11325
8.67913	12.80992	5.11552
8.67664	15.76116	5.11315
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3.12747	7.39907	5.12136
9.83415	1.77848	6.29853
4.45130	10.10248	6.23830
9.90119	10.10093	6.29934
4.26926	1.76794	6.29533
7.00113	0.44735	7.00988
7.02626	3.16015	7.02013
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7.31550	5.94777	7.09870
1.45409	8.60618	6.98218
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1.78850	14.30068	7.13494
7.12308	8.72510	7.03689
7.13446	11.51296	7.04328
10.21001	14.34798	7.12003
7.35721	14.29423	7.12770
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4.62016	5.96757	7.37944
1.73828	5.91988	7.12355
1.71198	3.06206	1.00008
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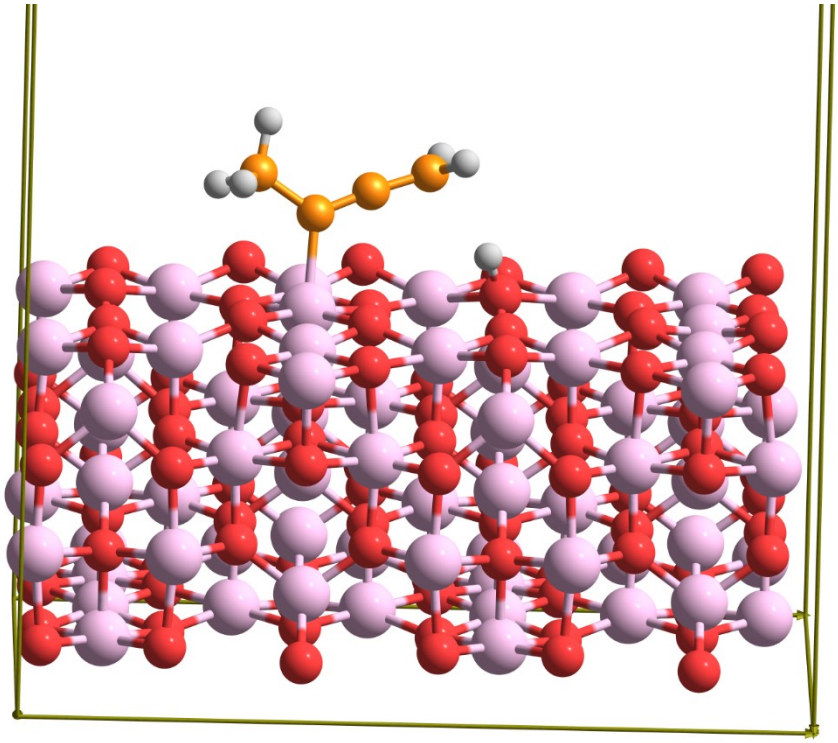
1.73749	5.93252	1.17328



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0.34204	1.75640	3.17089
3.26899	7.33756	3.28213
3.26922	4.52740	3.28213
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4.62187	14.28476	1.06915
1.73749	14.28442	1.17328
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3.23253	10.10822	3.07084
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0.33365	12.88665	3.09826
0.34204	10.10830	3.17089
3.26899	15.68946	3.28213
3.26922	12.87930	3.28213
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7.27003	0.45050	1.00008
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7.29549	5.93252	1.17328
10.21244	3.06331	1.34927
10.21249	0.44967	1.34927
8.79053	1.75632	3.07084
5.89192	7.33063	3.09826
5.89165	4.53475	3.09826
5.90004	1.75640	3.17089
8.82699	7.33756	3.28213
8.82722	4.52740	3.28213
7.26998	11.41396	1.00008
7.27003	8.80240	1.00008
10.17987	14.28476	1.06915
7.29549	14.28442	1.17328
10.21244	11.41521	1.34927
10.21249	8.80157	1.34927
8.79053	10.10822	3.07084
5.89192	15.68253	3.09826
5.89165	12.88665	3.09826
5.90004	10.10830	3.17089
8.82699	15.68946	3.28213
8.82722	12.87930	3.28213
4.39589	3.12677	5.14051
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1.76276	3.19523	5.23728
1.76252	0.31686	5.24923
4.51020	5.93303	5.34525
4.39541	11.48599	5.14265
4.39215	8.73699	5.13908
1.84349	14.28259	5.21670
1.76611	11.54707	5.25266
1.75924	8.66831	5.23554
4.50399	14.28661	5.30120
9.95224	3.13045	5.14093
9.94923	0.38300	5.14143

7.40570	5.93137	5.20555
7.32381	3.19494	5.24200
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10.05854	5.93366	5.29529
9.95046	11.48217	5.14418
9.94872	8.73477	5.13899
7.40136	14.28247	5.21679
7.31914	11.54869	5.25040
7.31950	8.66939	5.24140
10.06239	14.28717	5.30142
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2.94641	7.30457	7.02944
0.24209	1.81542	7.23233
2.74978	1.73446	7.33078
0.42041	7.17722	7.45869
0.44742	4.67096	7.46193
2.96250	12.87988	7.11992
3.19704	15.46117	7.15938
0.37437	10.11640	7.22059
2.93389	10.04978	7.40650
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0.43180	13.08083	7.47145
8.66501	4.66643	7.10929
8.66409	7.22600	7.10452
5.79716	1.78502	7.23044
8.30593	1.75881	7.32940
6.10428	7.25339	7.42400
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8.61132	12.95325	7.11716
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5.90134	10.13845	7.25366
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6.11067	15.59295	7.45315
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3.72329	7.25896	9.77873
4.11836	6.09452	9.36252
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3.33879	8.49419	10.10592
3.97906	5.05880	11.28935
3.69446	4.03744	9.84616
5.33129	4.54176	10.23659
3.24819	9.76683	8.31301
2.27722	8.74121	10.22683
4.06134	9.22170	10.49192

Allyl3-Al_2O_3-H-001 (result of “Butyne3” dehydrogenation, $Al_{64}O_{96}C_4H_6$)

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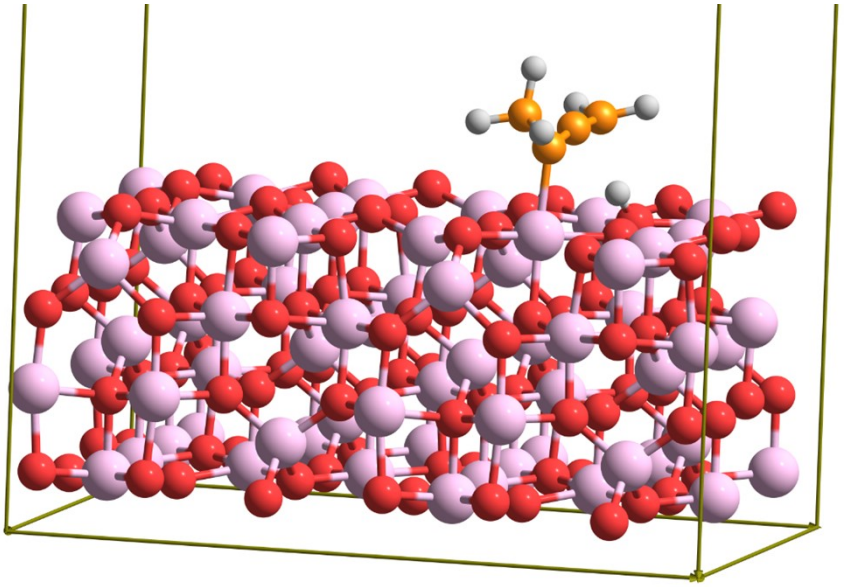
3.18673	1.75607	1.19055
0.43097	4.50284	1.28299
0.43108	7.36203	1.28324
3.20824	5.93252	2.22364
4.59841	0.29825	3.28771
4.59836	3.21456	3.28771

0.35882	5.93269	4.18926
1.80746	1.75624	4.20627
5.95345	10.10839	1.18978
8.74473	10.10797	1.19055
5.98897	12.85474	1.28299
5.98908	15.71393	1.28324
8.76624	14.28442	2.22364
10.15641	8.65015	3.28771
10.15636	11.56646	3.28771
5.91682	14.28459	4.18926
7.36546	10.10814	4.20627
0.39545	10.10839	1.18978
3.18673	10.10797	1.19055
0.43097	12.85474	1.28299
0.43108	15.71393	1.28324
3.20824	14.28442	2.22364
4.59841	8.65015	3.28771
4.59836	11.56646	3.28771
0.35882	14.28459	4.18926
1.80746	10.10814	4.20627
5.95345	1.75649	1.18978
8.74473	1.75607	1.19055
5.98897	4.50284	1.28299
5.98908	7.36203	1.28324
8.76624	5.93252	2.22364
10.15641	0.29825	3.28771
10.15636	3.21456	3.28771
5.91682	5.93269	4.18926
7.36546	1.75624	4.20627
8.68105	4.45973	5.11273
8.67849	7.40573	5.11179
3.12160	12.81121	5.11540
3.11855	15.75919	5.11325
8.67913	12.80992	5.11552
8.67664	15.76116	5.11315
3.12983	4.46453	5.12201
3.12747	7.39907	5.12136
9.83415	1.77848	6.29853
4.45130	10.10248	6.23830
9.90119	10.10093	6.29934
4.26926	1.76794	6.29533
7.00113	0.44735	7.00988
7.02626	3.16015	7.02013
10.16460	5.90893	7.12389
7.31550	5.94777	7.09870
1.45409	8.60618	6.98218
1.44613	11.59895	7.00591
4.70919	14.36290	7.11995
1.78850	14.30068	7.13494
7.12308	8.72510	7.03689
7.13446	11.51296	7.04328
10.21001	14.34798	7.12003
7.35721	14.29423	7.12770
1.41297	0.46645	7.00592
1.50999	3.19271	7.02143
4.62016	5.96757	7.37944
1.73828	5.91988	7.12355
1.71198	3.06206	1.00008



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4.65449	0.44967	1.34927
3.23253	1.75632	3.07084
0.33392	7.33063	3.09826
0.33365	4.53475	3.09826
0.34204	1.75640	3.17089
3.26899	7.33756	3.28213
3.26922	4.52740	3.28213
1.71198	11.41396	1.00008
1.71203	8.80240	1.00008
4.62187	14.28476	1.06915
1.73749	14.28442	1.17328
4.65444	11.41521	1.34927
4.65449	8.80157	1.34927
3.23253	10.10822	3.07084
0.33392	15.68253	3.09826
0.33365	12.88665	3.09826
0.34204	10.10830	3.17089
3.26899	15.68946	3.28213
3.26922	12.87930	3.28213
7.26998	3.06206	1.00008
7.27003	0.45050	1.00008
10.17987	5.93286	1.06915
7.29549	5.93252	1.17328
10.21244	3.06331	1.34927
10.21249	0.44967	1.34927
8.79053	1.75632	3.07084
5.89192	7.33063	3.09826
5.89165	4.53475	3.09826
5.90004	1.75640	3.17089
8.82699	7.33756	3.28213
8.82722	4.52740	3.28213
7.26998	11.41396	1.00008
7.27003	8.80240	1.00008
10.17987	14.28476	1.06915
7.29549	14.28442	1.17328
10.21244	11.41521	1.34927
10.21249	8.80157	1.34927
8.79053	10.10822	3.07084
5.89192	15.68253	3.09826
5.89165	12.88665	3.09826
5.90004	10.10830	3.17089
8.82699	15.68946	3.28213
8.82722	12.87930	3.28213
4.39589	3.12677	5.14051
4.39366	0.37829	5.14014
1.83779	5.93102	5.20741
1.76276	3.19523	5.23728
1.76252	0.31686	5.24923
4.51020	5.93303	5.34525
4.39541	11.48599	5.14265
4.39215	8.73699	5.13908
1.84349	14.28259	5.21670
1.76611	11.54707	5.25266
1.75924	8.66831	5.23554

4.50399	14.28661	5.30120
9.95224	3.13045	5.14093
9.94923	0.38300	5.14143
7.40570	5.93137	5.20555
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10.05854	5.93366	5.29529
9.95046	11.48217	5.14418
9.94872	8.73477	5.13899
7.40136	14.28247	5.21679
7.31914	11.54869	5.25040
7.31950	8.66939	5.24140
10.06239	14.28717	5.30142
2.99077	4.58492	7.08002
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0.24209	1.81542	7.23233
2.74978	1.73446	7.33078
0.42041	7.17722	7.45869
0.44742	4.67096	7.46193
2.96250	12.87988	7.11992
3.19704	15.46117	7.15938
0.37437	10.11640	7.22059
2.93389	10.04978	7.40650
0.54418	15.59799	7.44790
0.43180	13.08083	7.47145
8.66501	4.66643	7.10929
8.66409	7.22600	7.10452
5.79716	1.78502	7.23044
8.30593	1.75881	7.32940
6.10428	7.25339	7.42400
6.09029	4.66378	7.46246
8.61132	12.95325	7.11716
8.72632	15.51747	7.14061
5.90134	10.13845	7.25366
8.39581	10.10866	7.33630
6.11067	15.59295	7.45315
6.04215	13.06052	7.46665
3.72329	7.25896	9.77873
4.11836	6.09452	9.36252
4.28296	4.87816	10.24720
3.33879	8.49419	10.10592
3.97906	5.05880	11.28935
3.69446	4.03744	9.84616
5.33129	4.54176	10.23659
3.24819	9.76683	8.31301
2.27722	8.74121	10.22683
4.06134	9.22170	10.49192

Butyne2-Al_2O_3-OH-001 ($Al_{64}O_{97}C_4H_7$)

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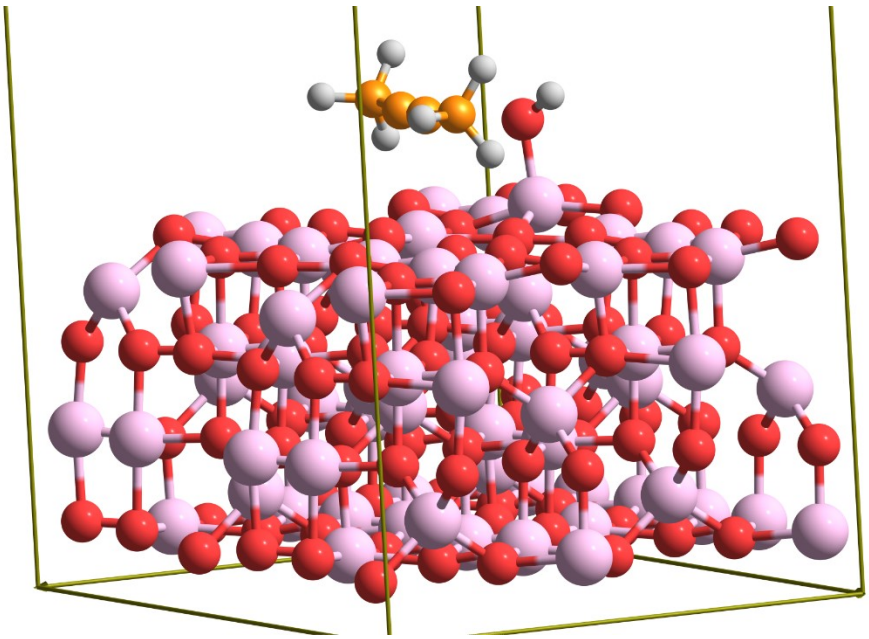
0.43097	4.50284	1.28299
0.43108	7.36203	1.28324

3.20824	5.93252	2.22364
4.59841	0.29825	3.28771
4.59836	3.21456	3.28771
0.35882	5.93269	4.18926
1.80746	1.75624	4.20627
5.95345	10.10839	1.18978
8.74473	10.10797	1.19055
5.98897	12.85474	1.28299
5.98908	15.71393	1.28324
8.76624	14.28442	2.22364
10.15641	8.65015	3.28771
10.15636	11.56646	3.28771
5.91682	14.28459	4.18926
7.36546	10.10814	4.20627
0.39545	10.10839	1.18978
3.18673	10.10797	1.19055
0.43097	12.85474	1.28299
0.43108	15.71393	1.28324
3.20824	14.28442	2.22364
4.59841	8.65015	3.28771
4.59836	11.56646	3.28771
0.35882	14.28459	4.18926
1.80746	10.10814	4.20627
5.95345	1.75649	1.18978
8.74473	1.75607	1.19055
5.98897	4.50284	1.28299
5.98908	7.36203	1.28324
8.76624	5.93252	2.22364
10.15641	0.29825	3.28771
10.15636	3.21456	3.28771
5.91682	5.93269	4.18926
7.36546	1.75624	4.20627
8.68537	4.46901	5.12222
8.67436	7.40310	5.11758
9.85383	1.75851	6.30385
7.05351	0.36251	7.02316
7.01899	3.10116	7.00717
10.25346	5.89932	7.09243
7.34023	5.92707	7.10484
3.12660	12.80834	5.12410
3.11531	15.76107	5.11661
4.27448	10.08131	6.29343
1.48323	8.66248	7.01112
1.44938	11.42779	7.01980
4.64588	14.27699	7.12170
1.79227	14.27461	7.12566
8.68415	12.81232	5.12323
8.67259	15.76351	5.11605
9.84304	10.09926	6.30432
7.06963	8.69231	7.00916
6.99272	11.43477	7.01169
10.21121	14.27487	7.12163
7.34846	14.27496	7.12625
3.08180	4.50863	5.14402
3.07050	7.35427	5.13654
4.28281	1.76155	6.29163
1.49421	0.37831	7.02522
1.47183	3.13811	7.00967



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4.62187	5.93286	1.06915
1.73749	5.93252	1.17328
4.65444	3.06331	1.34927
4.65449	0.44967	1.34927
3.23253	1.75632	3.07084
0.33392	7.33063	3.09826
0.33365	4.53475	3.09826
0.34204	1.75640	3.17089
3.26899	7.33756	3.28213
3.26922	4.52740	3.28213
1.71198	11.41396	1.00008
1.71203	8.80240	1.00008
4.62187	14.28476	1.06915
1.73749	14.28442	1.17328
4.65444	11.41521	1.34927
4.65449	8.80157	1.34927
3.23253	10.10822	3.07084
0.33392	15.68253	3.09826
0.33365	12.88665	3.09826
0.34204	10.10830	3.17089
3.26899	15.68946	3.28213
3.26922	12.87930	3.28213
7.26998	3.06206	1.00008
7.27003	0.45050	1.00008
10.17987	5.93286	1.06915
7.29549	5.93252	1.17328
10.21244	3.06331	1.34927
10.21249	0.44967	1.34927
8.79053	1.75632	3.07084
5.89192	7.33063	3.09826
5.89165	4.53475	3.09826
5.90004	1.75640	3.17089
8.82699	7.33756	3.28213
8.82722	4.52740	3.28213
7.26998	11.41396	1.00008
7.27003	8.80240	1.00008
10.17987	14.28476	1.06915
7.29549	14.28442	1.17328
10.21244	11.41521	1.34927
10.21249	8.80157	1.34927
8.79053	10.10822	3.07084
5.89192	15.68253	3.09826
5.89165	12.88665	3.09826
5.90004	10.10830	3.17089
8.82699	15.68946	3.28213
8.82722	12.87930	3.28213
4.37793	3.14195	5.14343
4.38818	0.38421	5.13553
1.85205	5.92844	5.14211
1.75986	3.18896	5.23818
1.75491	0.31169	5.24071
4.51243	5.93606	5.33599
3.10560	4.65504	7.12847
3.03808	7.24809	7.12821

0.26982	1.74025	7.22651
2.76778	1.76291	7.33315
0.44870	7.18632	7.48217
0.47988	4.62841	7.42250
4.39622	11.47535	5.14539
4.36085	8.71761	5.13635
1.84511	14.27669	5.21422
1.76831	11.54751	5.25343
1.74005	8.66902	5.23041
4.50609	14.28981	5.29768
3.15784	13.03957	7.13227
3.09084	15.58842	7.11250
0.25642	10.06543	7.23130
2.75665	10.09705	7.33582
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0.52936	12.99497	7.45331
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9.94316	0.38705	5.13712
7.40469	5.92442	5.19548
7.32640	3.19683	5.23907
7.30709	0.31317	5.23763
10.04655	5.94717	5.27965
8.71051	4.69727	7.10834
8.61163	7.26516	7.08654
5.81629	1.72969	7.22894
8.31907	1.76233	7.32490
6.05839	7.18466	7.42477
6.09996	4.63399	7.43478
9.95320	11.48273	5.14573
9.93938	8.74016	5.13160
7.40225	14.27803	5.21463
7.32188	11.55099	5.24879
7.30738	8.66684	5.22079
10.06342	14.29533	5.29852
8.71879	13.04933	7.13286
8.63590	15.60034	7.11032
5.80949	10.06068	7.22778
8.31071	10.11593	7.32471
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6.08462	12.99520	7.45355
1.94399	5.76838	9.46028
4.62764	6.57185	9.85653
4.58966	5.34589	9.87054
4.51604	3.90566	10.01129
4.60215	8.01721	9.96988
3.91459	3.65234	10.89730
4.04931	3.44610	9.12825
5.52105	3.47205	10.12572
4.08786	8.47261	9.11030
4.08395	8.31246	10.89570
5.62120	8.43087	9.99848
1.64079	6.52781	9.98449

TS1 Butyne2-Al_2O_3-OH-001 (with hydroxyl on nearest Al, H goes to surface O, $Al_{64}O_{97}C_4H_7$)

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0.000000000	16.703800000	0.000000000

0.000000000 0.000000000 26.000000000					
36 f/i= 30.295649 THz 190.353180 2PiTHz 1010.554060 cm-1					
X	Y	Z	dx	dy	dz
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3.186730	1.756070	1.190550	0	0	0
0.430970	4.502840	1.282990	0	0	0
0.431080	7.362030	1.283240	0	0	0
3.208240	5.932520	2.223640	0	0	0
4.598410	0.298250	3.287710	0	0	0
4.598360	3.214560	3.287710			
0.358820	5.932690	4.189260			
1.807460	1.756240	4.206270			
5.953450	10.108390	1.189780			
8.744730	10.107970	1.190550			
5.988970	12.854740	1.282990			
5.989080	15.713930	1.283240			
8.766240	14.284420	2.223640			
10.156410	8.650150	3.287710			
10.156360	11.566460	3.287710			
5.916820	14.284590	4.189260			
7.365460	10.108140	4.206270			
0.395450	10.108390	1.189780			
3.186730	10.107970	1.190550			
0.430970	12.854740	1.282990			
0.431080	15.713930	1.283240			
3.208240	14.284420	2.223640			
4.598410	8.650150	3.287710			
4.598360	11.566460	3.287710			
0.358820	14.284590	4.189260	0	0	0
1.807460	10.108140	4.206270	0	0	0
5.953450	1.756490	1.189780	0	0	0
8.744730	1.756070	1.190550	0	0	0
5.988970	4.502840	1.282990	0	0	0
5.989080	7.362030	1.283240	0	0	0
8.766240	5.932520	2.223640	0	0	0
10.156410	0.298250	3.287710	0	0	0
10.156360	3.214560	3.287710	0	0	0
5.916820	5.932690	4.189260	0	0	0
7.365460	1.756240	4.206270	0	0	0
8.668680	4.469890	5.110300	0	0	0
8.679640	7.408550	5.109920	0	0	0
9.794410	1.766640	6.299020	0	0	0
3.123070	12.799280	5.116540	0	0	0
3.122610	15.749640	5.121720	0	0	0
4.386690	10.082030	6.243270	0	0	0
8.680450	12.803150	5.109230	0	0	0
8.677640	15.754490	5.118510	0	0	0
9.898280	10.105740	6.302550	0	0	0
3.075610	4.502390	5.129610	0	0	0
3.069130	7.361820	5.111610	0	0	0
4.231970	1.776460	6.293440	0	0	0
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6.979750	3.134460	7.017110	0	0	0
10.238480	5.884150	7.094870	0	0	0
7.331110	5.944930	7.114820	0	0	0
1.455740	8.611230	6.983980	0	0	0
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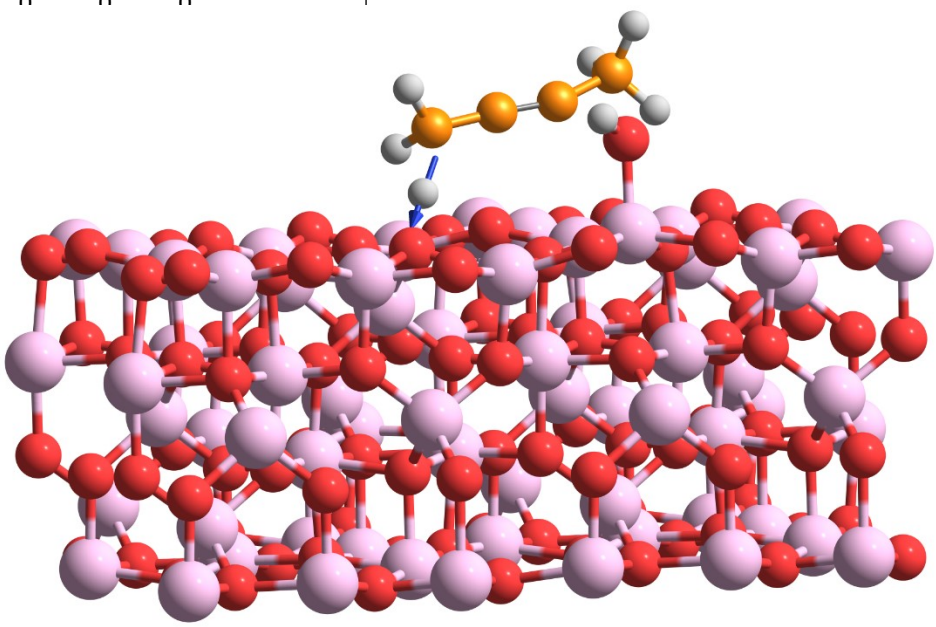

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7.269980 3.062060 1.000080	0	0	0
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8.826990 15.689460 3.282130	0	0	0
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4.958910 9.544310 9.224690	-0.115593	0.039370	-0.140392

1.539440 6.521770 9.911550	0.017883 0.001138 0.002262

TS2 Butyne2-Al_2O_3-OH-001 (with hydroxyl on nearest Al, H goes to OH, $Al_{64}O_{97}C_4H_7$)

11.116000000 0.000000000 0.000000000 0.000000000 16.703800000 0.000000000 0.000000000 0.000000000 26.000000000	
36 f/i= 17.782483 THz 111.730636 2PiTHz 593.159768 cm-1	
X Y Z	dx dy dz
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3.186730 1.756070 1.190550	0 0 0
0.430970 4.502840 1.282990	
0.431080 7.362030 1.283240	
3.208240 5.932520 2.223640	
4.598410 0.298250 3.287710	
4.598360 3.214560 3.287710	
0.358820 5.932690 4.189260	
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5.953450 10.108390 1.189780	
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4.598360 11.566460 3.287710	0 0 0
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7.365460 1.756240 4.206270	0 0 0
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4.273080 10.102030 6.290730	0 0 0
8.671310 12.808040 5.113990	0 0 0
8.682400 15.757340 5.121870	0 0 0
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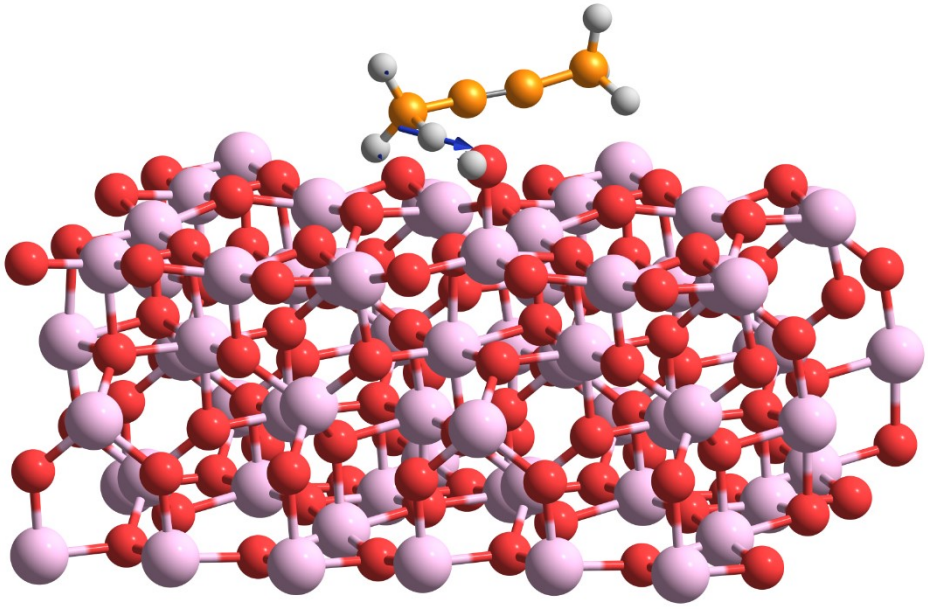

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4.654490 0.449670 1.349270	0	0	0
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1.712030 8.802400 1.000080	0	0	0
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0.415230	4.667350	7.416640	0	0	0
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Allyl2-Al_2O_3H-OH-001 (with hydroxyl on nearest Al, H goes to surface O, $Al_{64}O_{97}C_4H_7$)

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0.43108	7.36203	1.28324
3.20824	5.93252	2.22364
4.59841	0.29825	3.28771
4.59836	3.21456	3.28771
0.35882	5.93269	4.18926
1.80746	1.75624	4.20627
5.95345	10.10839	1.18978
8.74473	10.10797	1.19055
5.98897	12.85474	1.28299
5.98908	15.71393	1.28324
8.76624	14.28442	2.22364
10.15641	8.65015	3.28771
10.15636	11.56646	3.28771
5.91682	14.28459	4.18926
7.36546	10.10814	4.20627
0.39545	10.10839	1.18978
3.18673	10.10797	1.19055
0.43097	12.85474	1.28299
0.43108	15.71393	1.28324
3.20824	14.28442	2.22364
4.59841	8.65015	3.28771
4.59836	11.56646	3.28771
0.35882	14.28459	4.18926
1.80746	10.10814	4.20627
5.95345	1.75649	1.18978
8.74473	1.75607	1.19055
5.98897	4.50284	1.28299
5.98908	7.36203	1.28324
8.76624	5.93252	2.22364
10.15641	0.29825	3.28771
10.15636	3.21456	3.28771
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7.36546	1.75624	4.20627
8.67050	4.45954	5.09472
8.66134	7.39974	5.13183
9.86863	1.72470	6.30032
3.14912	12.83630	5.12855
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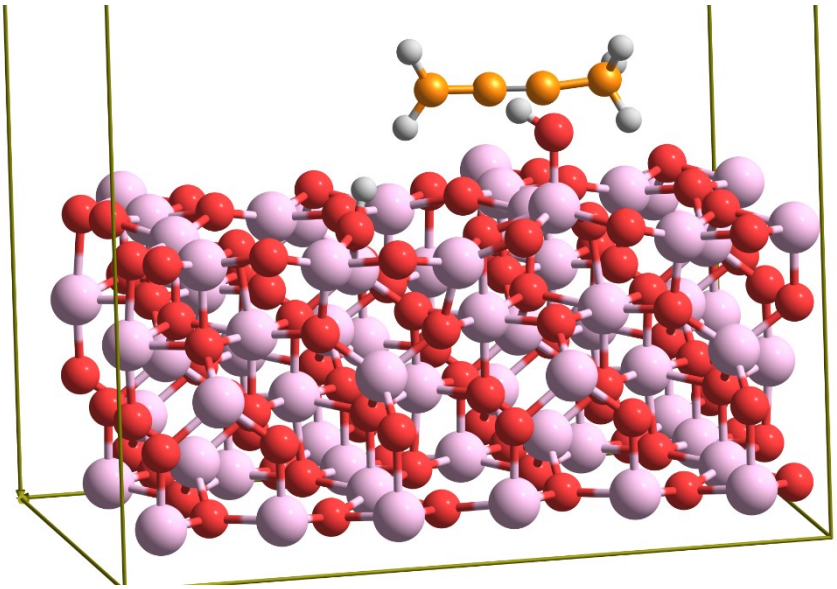

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7.37202	5.93778	7.13128
1.15343	8.35838	6.86860
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1.79193	14.26653	7.13270
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7.04854	11.43406	7.03191
10.19528	14.28364	7.12298
7.35217	14.26412	7.12802
1.53801	0.31859	7.02878
1.47875	3.02688	7.01825
4.74988	5.75480	7.16945
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1.71203	0.45050	1.00008
4.62187	5.93286	1.06915
1.73749	5.93252	1.17328
4.65444	3.06331	1.34927
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3.23253	1.75632	3.07084
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0.33365	4.53475	3.09826
0.34204	1.75640	3.17089
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1.71198	11.41396	1.00008
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4.62187	14.28476	1.06915
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8.82699	7.33756	3.28213
8.82722	4.52740	3.28213
7.26998	11.41396	1.00008

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10.21244	11.41521	1.34927
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5.90004	10.10830	3.17089
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8.82722	12.87930	3.28213
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1.84805	5.93032	5.13558
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1.74265	0.30827	5.23118
4.50990	5.96750	5.34872
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4.32604	8.74467	5.14471
1.84215	14.25738	5.22133
1.83619	11.50915	5.30362
1.69259	8.68809	5.21231
4.50875	14.31178	5.30524
9.95483	3.12474	5.15971
9.94270	0.36830	5.13247
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7.33809	3.18156	5.25696
7.30777	0.30927	5.24013
10.04751	5.90266	5.30199
9.97899	11.47786	5.16238
9.96166	8.71746	5.15484
7.40261	14.27133	5.21938
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2.79362	1.74941	7.34071
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3.02453	15.64876	7.10120
0.29319	9.97040	7.22547
2.94832	10.38031	7.43105
0.47655	15.48595	7.47448
0.53231	12.95720	7.45772
8.74358	4.69708	7.14919
8.47286	7.36470	7.06933
5.83111	1.70687	7.23245
8.34172	1.73593	7.33570
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6.17420	4.58487	7.46413
8.72518	13.04220	7.14236
8.62837	15.59440	7.11329
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8.33669	10.13070	7.34103
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4.91682	8.03723	10.19181
3.94267	3.74344	11.05725
4.15908	3.55488	9.29951
5.58162	3.54872	10.36740
3.17991	10.08270	8.32976
4.80194	8.54940	11.14912
5.14189	8.62536	9.30212
2.37752	6.54570	10.07840

References.

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