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Electronic Supporting Information

A K-Arylacetylide Complex for Catalytic Terminal Alkyne Functionalization using KO^{t}Bu as a Precatalyst

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Contents:

I. Experimental Section

General consideration:

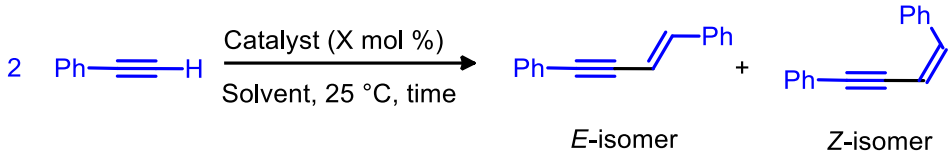
All solvents used in the experiments were distilled from calcium hydride under inert condition prior to use. All chemicals were purchased and used as received. The ^{1}H, ^{13}C, ^{19}F NMR spectra were recorded on 400 and 500 MHz spectrometers in $CDCl_3$ with residual undeuterated solvent ($CDCl_3$, 7.26/77.0) as an internal standard. Chemical shifts (δ) are given in ppm, and J values are given in Hz. All chemical shifts were reported in ppm using tetramethylsilane as a reference. Chemical shifts (δ) downfield from the reference standard were assigned positive values. Open-column chromatography and thin-layer chromatography (TLC) were performed on silica gel (Merck silica gel 100-200 mesh). Evaporation of solvents were performed under reduced pressure using a rotary evaporator. High-resolution mass spectra (HRMS) were obtained on a Bruker maXis impact. ESI-mass spectra were recorded on a water Micro-MS mass spectrometer. EPR spectroscopic measurements were performed in Bruker (X-band) spectrometer. ICPMS quantitative characterizations were carried out using Varian 280-MS ICP mass spectrometer. All the glassware and NMR tubes used for experiments were kept in oven at 120 °C for overnight (12h). X-ray crystallographic measurements were performed in Agilent X-ray diffractometer.

Reaction procedure for optimization study of dimerization of terminal alkynes

Inside a nitrogen filled glovebox, 7.5 mol% of base was taken in an oven dried pressure tube and dissolved in 800 µL of dry solvent. After stirring for 5 min, 0.852 mmol of phenylacetylene was added to base-solvent mixture. Then the pressure tube was taken out from the glovebox and the final reaction mixture was stirred for overnight at 25 °C. After completion of the reaction, general workup was performed using water and ethylacetate. Product was extracted using 30 mL ethylacetate and dried over anhydrous sodium sulphate. The solvent was removed under reduced pressure using a rotary evaporator. Crude product was purified by column

chromatography on silica gel using hexane/ethylacetate mixture to yield the pure desired products.

Table S1. Optimization of terminal alkyne dimerization under transition metal free condition at room temperature in absence of crown ether (Method A).[a]



Sl. No.	Catalyst (mol %)	Solvent	Time (h).	Isolated yield% (E:Z)
1	KO^{t}Bu (5)	DMSO	15	61 (90:10)
2	KO^{t}Bu (7.5)	DMSO	15	87 (91:9)
3	KO^{t}Bu (10)	DMSO	15	85 (91:9)
4	KO^{t}Bu (200)	DMSO	15	0
5	NaOMe (7.5)	DMSO	15	30
6	NaO^{t}Bu (7.5)	DMSO	15	38
7	KOMe (7.5)	DMSO	15	36
8	KOH (7.5)	DMSO	15	18
9	K_3PO_4 (7.5)	DMSO	15	0
10	K_2CO_3(7.5)	DMSO	15	0
11	Na_2CO_3(7.5)	DMSO	15	0
12	Cs_2CO_3(7.5)	DMSO	15	0
13	LiO^{t}Bu(7.5)	DMSO	15	<2
14	KO^{t}Bu(7.5)	DMAc	15	17
15	KO^{t}Bu(30)	DMAc	15	38
16	KO^{t}Bu(7.5)	DMF	15	49
17	KO^{t}Bu(7.5)	Acetonitrile	15	0
18	KO^{t}Bu(7.5)	THF	15	0
19	KO^{t}Bu(7.5)	Toluene	15	0
20	**KO^{t}Bu (7.5) (Sigma-Aldrich, 99.99% Sublimed grade)**	**DMSO**	**15**	**90(90:10)**

[a]Reaction condition: Phenylacetylene (0.85 mmol), Catalyst (0.032 mmol), Solvent (1 mL).

General reaction procedure for dimerization of terminal alkynes in DMSO (Method A).

Inside a nitrogen filled glovebox, 7.5 mol% (0.032 mmol) of KO^{t}Bu was taken in an oven dried pressure tube and dissolved in 1 mL of dry DMSO. After 5 min stirring, 0.852 mmol of terminal alkyne was added to KO^{t}Bu-DMSO solution resulting in a sharp color change. Subsequently, the pressure tube was taken out from the glovebox and the final reaction mixture was stirred for 15 h at 25 °C. After completion of the reaction, workup was performed using water and ethylacetate. Product was extracted using 30 mL ethylacetate and dried over anhydrous sodium sulphate. The solvent was removed under reduced pressure using a rotary evaporator. Crude product was purified by column chromatography on silica gel using hexane/ethylacetate mixture to yield the pure desired products.

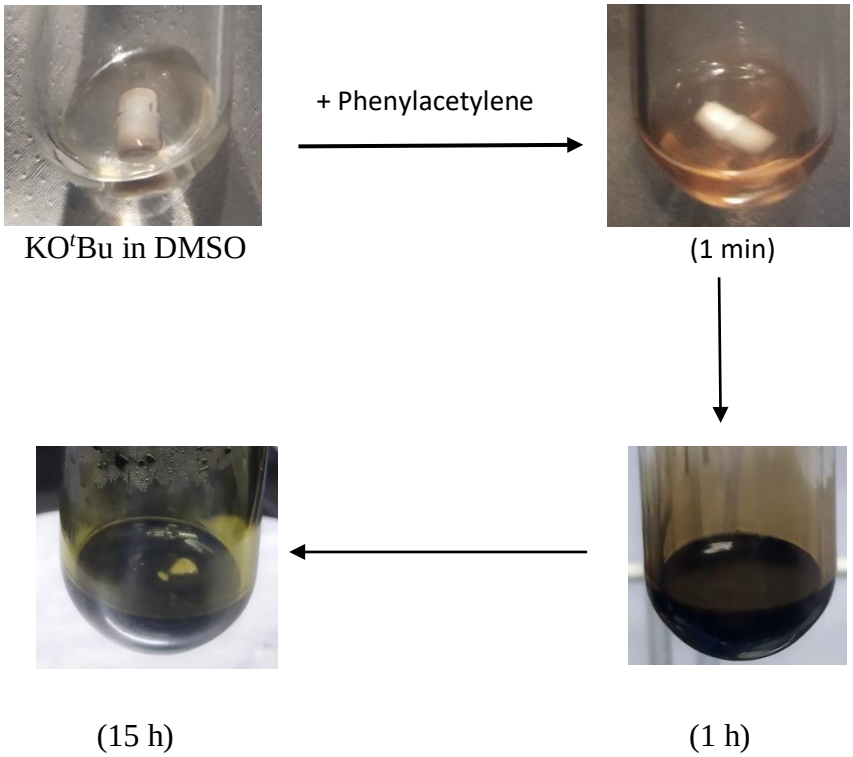
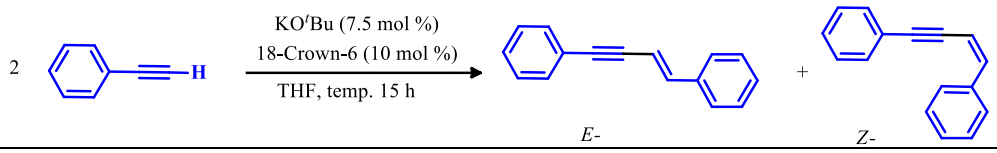


Table S2. Alkyne dimerization under transition metal free condition at room temperature in presence of 18-crown-6 in THF (Method B).[a]

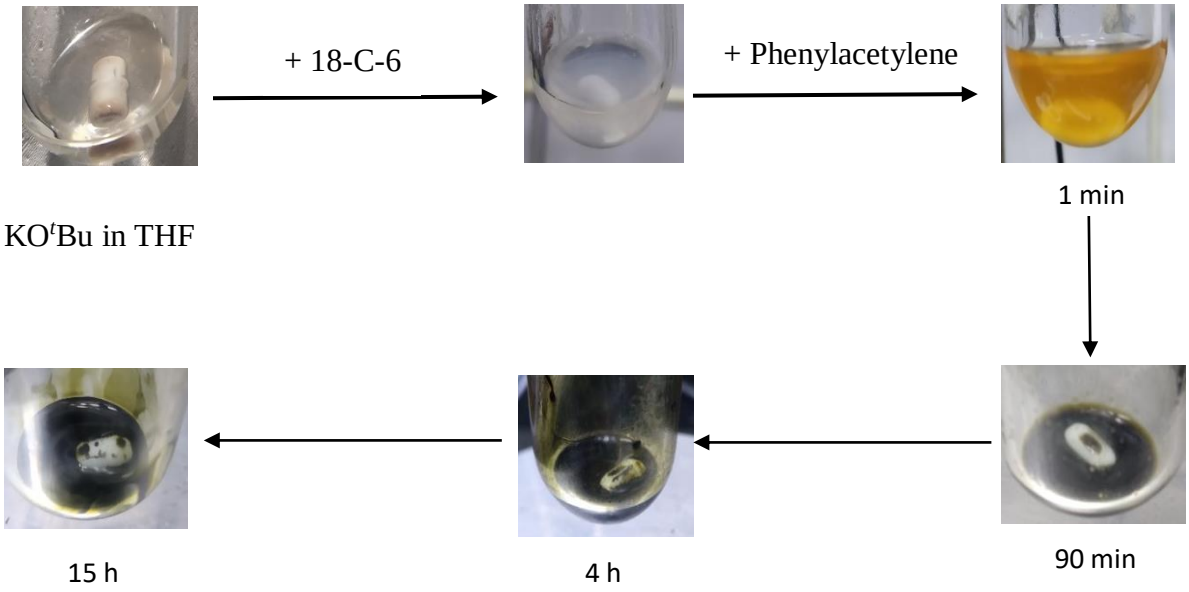


Sl No.	Catalyst	Tarpping agent	Temp.	Yield
1	KO^{t}Bu (7.5)	18-crown-6 (10)	25 ^{o}C	65%
2	**KO^{t}Bu (7.5)**	**18-crown-6 (10)**	**80 ^{o}C**	**83% (85:15)**
3	NaO^{t}Bu (7.5)	15-crown-5	80 ^{o}C	20%
4	KO^{t}Bu (7.5)	-	80 ^{o}C	-

[a]Reaction condition: Phenylacetylene (0.85 mmol), Catalyst (0.032 mmol), 18-crown-6 (0.032 mmol), THF (1 mL).

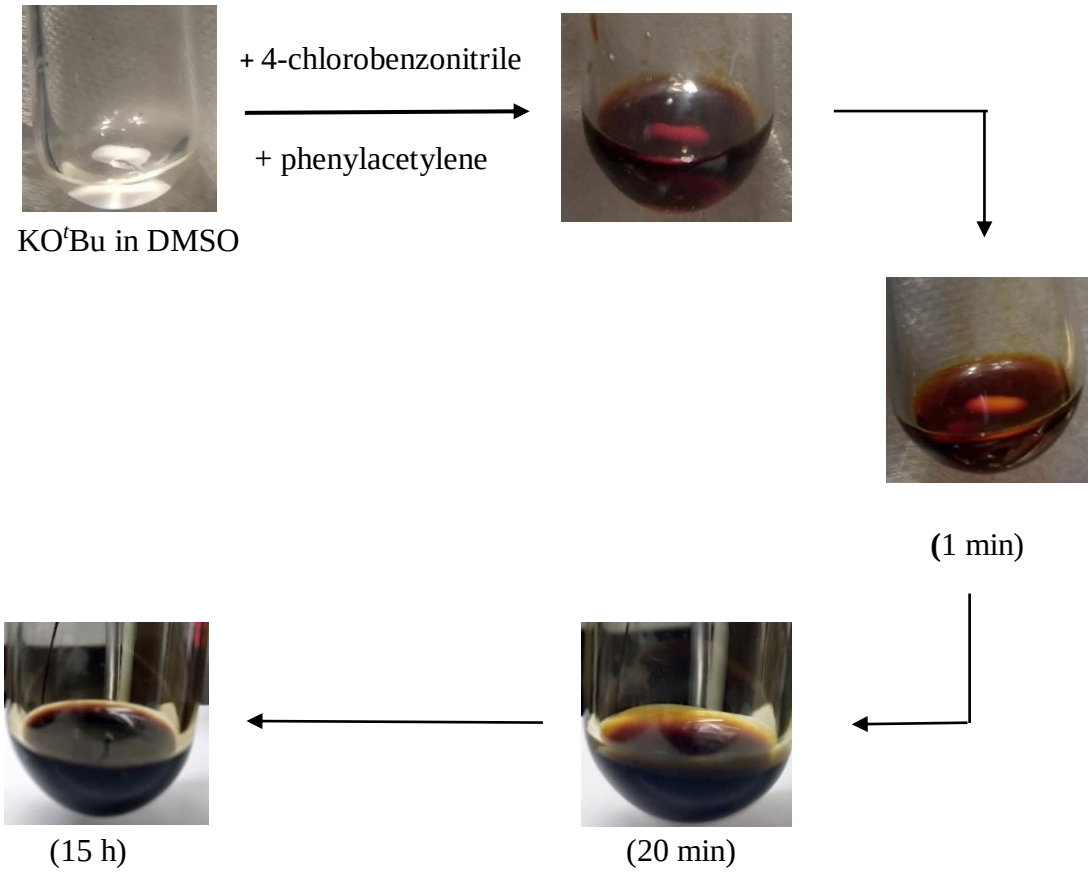
General reaction procedure for dimerization of terminal alkynes in THF (Method B).

Inside a nitrogen filled glovebox, 7.5 mol% (0.032 mmol) of KO^{t}Bu and 7.5 mol% (0.032 mmol) of 18-crown-6 were taken in an oven dried sealed tube and dissolved in 1 mL of dry THF. After 5 min stirring, 0.852 mmol terminal alkyne was added to KO^{t}Bu-18-crown-6-THF solution, resulting in a sharp color change of reaction mixture. Subsequently, the sealed tube was taken out from the glovebox and the final reaction mixture was stirred for 15h at 80°C. After completion of the reaction, workup was performed using water and ethylacetate. Product was extracted using 30 mL ethylacetate and dried over anhydrous sodium sulphate. The solvent was removed under reduced pressure using a rotary evaporator. Crude product was purified by column chromatography on silica gel using hexane/ethylacetate mixture to yield the pure desired products.

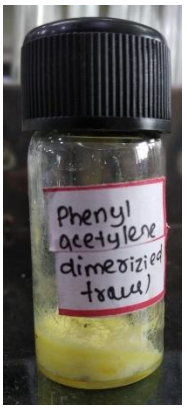


General reaction procedure for coupling between terminal alkynes and aromatic nitriles

Inside a nitrogen filled glovebox, 7.5 mol% (0.032 mmol) of KO^{t}Bu was taken in an oven dried pressure tube and dissolved in 1 mL of dry DMSO. It was next stirred for 5 min followed by addition of 0.426 mmol aromatic nitriles and 0.639 mmol terminal alkyne, respectively. A sharp color change was observed. The sealed tube was taken out from the glovebox and the final reaction mixture was stirred for 15h at 25 °C. After completion of the reaction, workup was performed using water and ethylacetate. Product was extracted using 30 mL ethylacetate and dried over anhydrous sodium sulphate. The solvent was removed under reduced pressure using a rotary evaporator. Crude product was purified by column chromatography on silica gel using triehthylamine/hexane/ethylacetate mixture to yield the pure desired products.



Reaction procedure for gram scale dimerization of phenyl acetylene



Inside a nitrogen filled glovebox, 10 mol% (110 mg) of KO^{t}Bu was taken in an oven dried pressure tube and dissolved in 7 mL of dry DMSO. After stirring for 10 min, 0.02 mol (2g) of phenyl acetylene was added to KO^{t}Bu-DMSO solution resulting in a sharp color change from colorless to deep black color within 2 mins. Then the pressure tube was taken out from the glovebox and the final reaction mixture was stirred for 24 h at 25 °C. After completion of the reaction, general workup was performed using water and ethylacetate. Product was extracted using 80 mL of ethylacetate and dried over anhydrous sodium sulphate. The solvent was removed under reduced pressure using a rotary evaporator. Crude product was purified by

column chromatography on silica gel using hexane/ethylacetate mixture to yield the pure desired products.

Reaction procedure for checking the longevity of the dimerization of phenyl acetylene

Inside a nitrogen filled glovebox, 4 reaction setups were prepared as described below. 7.5 mol% (3.6 mg) of KO^{t}Bu was taken in four oven dried pressure tubes and dissolved in 800 µL of dry DMSO. After stirring for 5 min, 0.852 mmol of phenylacetylene was added to KO^{t}Bu-DMSO solution in each of these four setups and a sharp color change was observed in each case from colorless to deep black color.

Reaction set 1: The reaction was stopped and quenched with ethylacetate and water after 24 h.

Reaction set 2: After 24 h another batch of substrate (.852 mmol of phenylacetylene) was added to the reaction mixture without further addition of catalyst. Finally after another 24 h, the reaction was stopped and quenched with ethylacetate and water.

Reaction set 3: Consecutively 2 times another batch of substrate (0.852 mmol of phenylacetylene) was added to the reaction mixture in 24 h interval. Finally after 3 days, the reaction was stopped and quenched with ethylacetate and water.

Reaction set 4: Consecutively 3 times only substrate (0.852 mmol of phenylacetylene) was added to the reaction mixture in 24 h interval. Finally after 4 days, the reaction was stopped and quenched with ethylacetate and water.

Product was isolated at the end of each reaction set and the yield for each cycle varies within the range of 90-71%.

ICPMS measurement:

The quantitative results of reagent grade KOtBu (98% purity), obtained from the ICPMS are given below:

Blank: 53.85 ppb (Pd), 22.31 ppb (Pt)

Sample: 60.00 ppb (Pd), 90 ppb (Pt)

Cyclic Voltammogram:

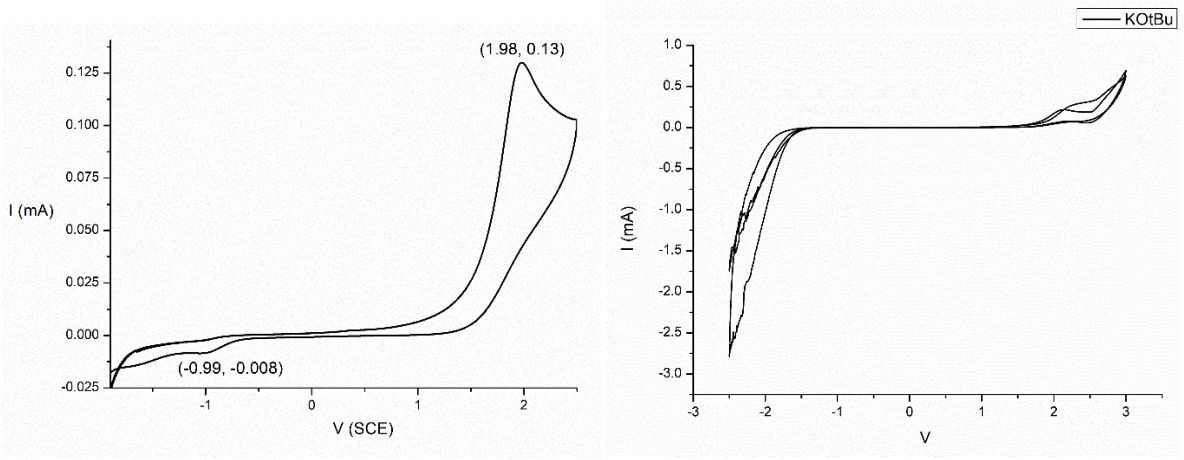


Figure S1. a) CV of phenylacetylene and KO^{t}Bu mixture in THF; **b)** CV of KO^{t}Bu in THF.

^{1}H NMR spectroscopic characterization for proton abstraction of arylacetylene with KO^{t}Bu in presence of 18-crown-6

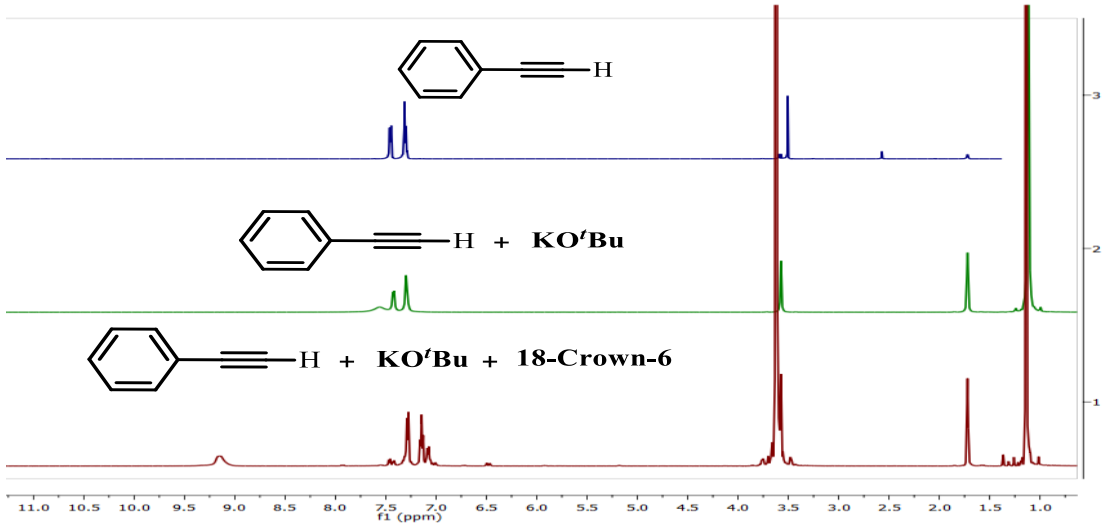


Figure S2a. Stack plots of ^{1}H NMR spectra (in THF-d_8) revealing abstraction of phenylacetylene proton by addition KO^{t}Bu with 18-crown-6.

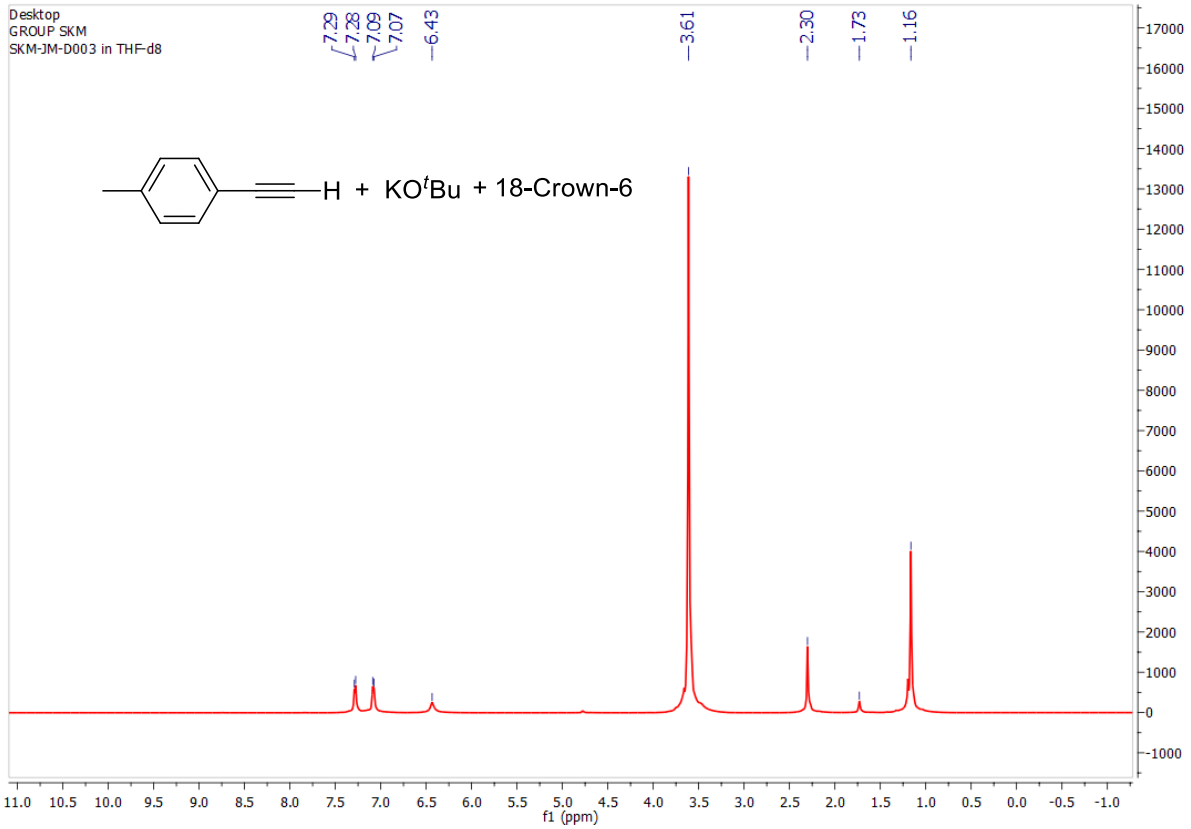
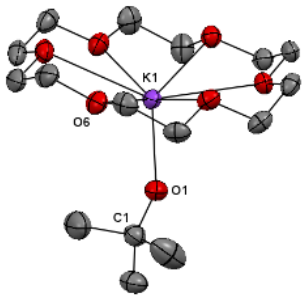


Figure S2b. ^{1}H NMR spectrum of 1:1:1 mixture of KO^{t}Bu, 18-crown-6 and 4-ethynyltoluene in THF-d_8.

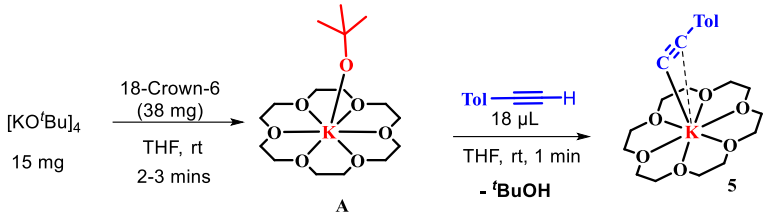
Synthesis of K-[18-Crown-6]-O^{t}Bu (A):

Inside a nitrogen filled glovebox, 15 mg (0.133 mmol) of KO^{t}Bu and 38 mg (0.147 mmol) of 18-crown-6 were taken in a 5 mL vial with 1.2 mL THF. The reaction mixture was stirred for 2-3 min. which offered a clear solution. The clean solution was kept at -36 °C for crystallization inside the glovebox. After overnight standing, colorless crystals were obtained. A suitable crystal was analyzed by solid state structure and NMR spectroscopy. All data were matched with previous report.[8]



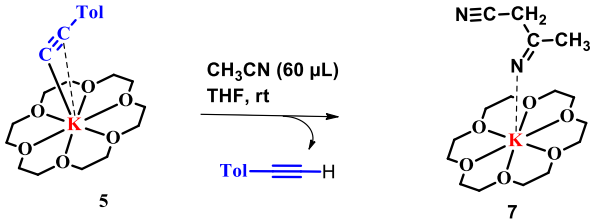
Synthesis of intermediate 5:

Inside a nitrogen filled glovebox, 15 mg (0.133 mmol) KO^tBu and 38 mg (0.147 mmol) 18-crown-6 were taken in a 5 mL vial with 1.2 mL THF. The reaction mixture was stirred for 2-3 min which offered a clear solution. 18 µL (0.133 mmol) 4-ethynyltoluene was added which resulted in a light brownish solution. The brown solution was kept at -36 °C for crystallization inside the glovebox. Colorless crystals were obtained on overnight standing. A suitable crystal was coated with precooled inert oil and was analyzed by solid state structure. Also it was characterized by NMR spectroscopy.



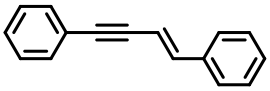
Synthesis of complex 7:

Inside a nitrogen filled glovebox, 20 mg crystalline material of **5** was treated with 60 µL of dry acetonitrile in a 5 mL vial. The reaction mixture was diluted with 1.2 mL of THF which offered a clear reddish yellow solution. 600 µL hexane was added to this clear solution and the clear solution was kept at -36 °C for crystallization inside the glovebox. Yellow colored crystals were obtained on overnight standing. The crystals were coated with precooled inert oil and analysed in single crystal X-ray diffractometer at 100K. Also it was characterized by NMR spectroscopy.



II. The analytical and spectral characterization data of the products

(*E*)-but-1-en-3-yne-1,4-diyldibenzene (2aa):[1]

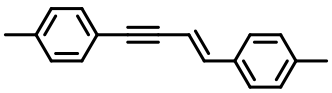


Prepared according to general procedure described above by reacting phenylacetylene (94 µL) with KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with hexane. The compound was obtained as a white solid (76 mg, 87%).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 7.55- 7.52 (m, 2H), 7.47 (d, 2H, *J* = 8 Hz), 7.40-7.33 (m, 6H), 7.10 (d, 1H, *J* = 16 Hz), 6.44 (d, 1H, *J* = 16 Hz).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 141.2, 136.3, 131.5, 128.7, 128.6, 128.3, 128.1, 126.3, 123.4, 108.1, 91.7, 88.9.

(*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(methylbenzene) (2bb):[1]

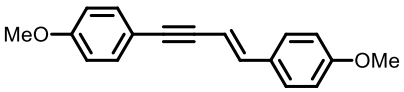


Prepared according to general procedure described above by reacting 4-ethynyltoluene (108 µL) with KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with hexane. The compound was obtained as a light yellowish solid (76 mg, 77%).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 7.37 (d, 2H, *J* = 8Hz), 7.33 (d, 2H, *J* = 8Hz), 7.15 (t, 4H, *J* = 7.2 Hz), 7.01 (d, 1H, *J* = 16.4 Hz), 6.34 (d, 1H, *J* = 16Hz), 2.36 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 140.9, 138.6, 138.2, 133.7, 131.3, 129.4, 129.1, 126.2, 120.4, 107.1, 91.6, 88.4, 21.5, 21.3.

(*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(methoxybenzene) (2cc):[1]

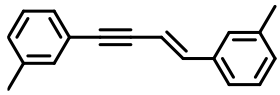


Prepared according to general procedure described above by reacting 4-ethynylanisole (110 µL) with KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 1% ethyl acetate in hexane. The compound was obtained as a white solid (73mg, 65%).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ 7.38 (ppm) (dd, 4H, J_1 = 20 Hz, J_2 = 8 Hz), 6.96 (d, 1H, *J* = 16 Hz), 6.89- 6.85 (m, 4H), 6.24 (d, 1H, *J* = 16 Hz), 3.82 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 160.0, 159.5, 140.0, 132.9, 129.4, 127.5, 115.8, 114.2, 114.0, 106.0, 91.0, 87.9, 55.3, 55.2.

(*E*)-3,3'-(but-1-en-3-yne-1,4-diyl)bis(methylbenzene) (2dd):[2]

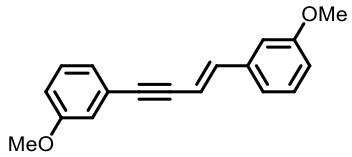


Prepared according to general procedure described above by reacting 3-ethynyltoluene (109 µL) with KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with hexane. The compound was obtained as a pale yellowish solid (74 mg, 75%).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 7.37- 7.34 (m, 2H), 7.30- 7.28 (m, 4H), 7.20- 7.17 (m, 2H), 7.06 (d, 1H, *J* = 16 Hz), 6.43 (d, 1H, *J* = 16 Hz), 2.42 (s, 3H), 2.40 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 141.3, 138.3, 138.0, 136.3, 132.1, 129.4, 129.0, 128.6, 128.6, 128.2, 127.0, 123.4, 123.2, 108.0, 91.8, 88.7, 21.4, 21.2.

(*E*)-3,3'-(but-1-en-3-yne-1,4-diyl)bis(methoxybenzene) (2ee):[1]

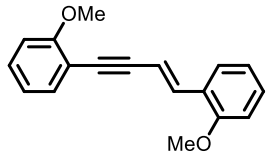


Prepared according to general procedure described above by reacting 3-ethynylanisole (108 µL) with KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with hexane. The compound was obtained as a yellowish solid (95 mg, 85%).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 7.23- 7.17 (m, 2H), 7.05- 6.95 (m, 4H), 6.90 (s, 1H), 6.84- 6.79 (m, 2H), 6.32 (d, 1H, *J* = 16 Hz), 3.77 (s, 3H), 3.76 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 159.8, 159.3, 141.3, 137.7, 129.7, 129.4, 124.3, 124.1, 119.0, 116.2, 114.9, 114.3, 111.5, 108.4, 91.8, 88.6, 55.2, 55.2.

(*E*)-2,2'-(but-1-en-3-yne-1,4-diyl)bis(methoxybenzene) (2ff):[1]

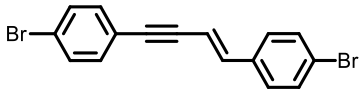


Prepared according to general procedure described above by reacting 2-ethynylanisole (111 µL) with KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with hexane. The compound was obtained as a pale yellowish solid (92 mg, 82%).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 7.49- 7.47 (m, 2H), 7.40 (d, 1H, *J* = 16 Hz), 7.32- 7.28 (m, 2H), 6.98- 6.90 (m, 4H), 6.57 (d, 1H, *J* = 16 Hz), 3.93 (s, 3H), 3.88 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 159.7, 156.9, 136.3, 133.4, 129.5, 126.8, 125.4, 120.6, 120.4, 112.7, 111.0, 110.5, 109.0, 93.8, 87.5, 55.7, 55.4.

(*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(bromobenzene) (2gg):[1]

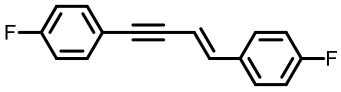


Prepared according to general procedure described above by reacting 1-bromo-4-ethynylbenzene (154 mg) with KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 2% ethylacetate in hexane. The compound was obtained as a white solid (51 mg, 33%).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 7.48- 7.45 (m,4H), 7.33-7.27 (m,4H), 6.97 (d, 1H, *J* = 16Hz), 6.34 (d, 1H, *J* = 16Hz).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 140.3, 135.1, 132.9, 131.9, 131.7, 127.8, 122.7, 122.6, 122.2, 108.6, 91.2, 89.7.

(*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(fluorobenzene) (2hh):[1]



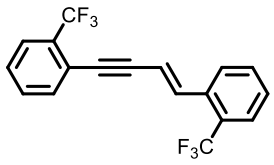
Prepared according to general procedure described above by reacting 1-ehynyl-4-fluorobenzene (99 µL) with KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 1% ethylacetate with hexane. The compound was obtained as a white solid (70 mg, 68%).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 7.46- 7.43 (m, 2H), 7.41- 7.37 (m, 2H), 7.06- 6.97 (m, 5H), 6.27 (d, 1H, *J* = 20Hz).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 164.2, 163.7, 161.7, 161.2, 140.0, 137.4, 133.4, 132.5, 132.4, 130.5, 130.4, 128.0, 127.9, 119.4, 119.4, 115.9, 115.8, 115.7, 115.6, 115.4, 115.2, 107.7, 106.8, 90.6, 88.3.

^{19}F NMR (376 MHz, $CDCl_3$, 298K) δ (ppm) -110.8, -112.3.

(*E*)-2,2'-(but-1-en-3-yne-1,4-diyl)bis((trifluoromethyl)benzene) (2ii):[2]



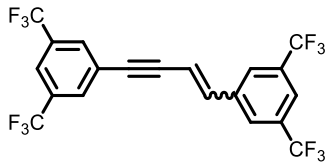
Prepared according to general procedure described above by reacting 1-ethynyl-2-(trifluoromethyl)benzene (119 µL) with KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 1% ethyl acetate in hexane. The compound was obtained as a light yellowish solid (123 mg, 85 %).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 7.71- 7.64 (m, 4H), 7.56- 7.50 (m, 2H), 7.47-7.39 (m, 3H), 6.42 (d, 1H, *J* = 16Hz).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 137.8, 134.9, 133.9, 132.0, 131.4, 128.4, 128.1, 127.7, 127.4, 126.7, 126.1, 126.0, 125.9, 125.9, 122.7, 122.1, 121.3 111.8, 93.7, 88.4.

^{19}F NMR (376 MHz, $CDCl_3$, 298K) δ (ppm) -59.24, -62.31.

(*E*)-5,5'-(but-1-en-3-yne-1,4-diyl)bis(1,3-bis(trifluoromethyl)benzene) (2jj):[3]



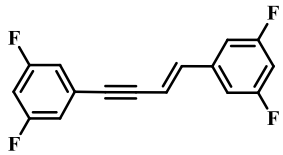
Prepared according to general procedure described above by reacting 1-ethynyl-3,5-bis(trifluoromethyl)benzene (151 µL) with KO^{t}Bu (3.6 mg) and 18-crown-6 (9 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 3% ethyl acetate in hexane. The compound was obtained as a colorless solid (63 mg, 31 %).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 8.36 (s, 2H), 7.91- 7.82 (m, 8H), 6.89 (d, 1H, *J* = 12 Hz), 6.15 (d, 1H, *J* = 12 Hz).

E isomer: 7.15 (d, *J* = 16 Hz), 6.52 (d, *J* = 16 Hz)

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 139.8, 137.8, 137.3, 132.5, 132.2, 132.1, 131.9, 131.7, 131.3, 128.4, 126.2, 125.1, 124.7, 124.4, 124.1, 122.3, 122.0, 121.4, 111.2, 110.4, 94.4, 90.7, 89.6.

(*E*)-5,5'-(but-1-en-3-yne-1,4-diyl)bis(1,3-difluorobenzene) (2kk):[1]

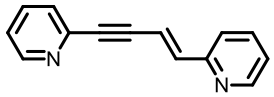


Prepared according to general procedure described above by reacting 1-ethynyl-3,5-difluorobenzene (101 µL) with KO^{t}Bu (3.6 mg) and 18-crown-6 (9 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 3% ethyl acetate in hexane. The compound was obtained as a yellowish solid product (41mg, 35%).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 6.99- 6.92 (m, 5H), 6.83- 6.73 (m, 2H), 6.35 (d, 1H, *J* = 4Hz).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 164.6, 164.4, 164.0, 163.9, 162.1, 161.9, 161.5, 161.4, 140.1, 125.6, 114.6, 110.2, 109.2, 109.0, 90.8, 89.7.

(*E*)-2,2'-(but-1-en-3-yne-1,4-diyl)dipyridine (2ll):[4]

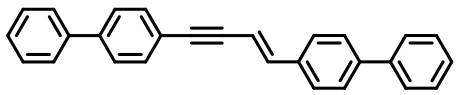


Prepared according to general procedure described above by reacting 2-ethynylpyridine (86 µL) with KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with ethylacetate only. The compound was obtained as deep green oily product (56 mg, 63%).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 8.60 (t, 2H), 7.67-7.64 (m, 2H), 7.49 (d, 1H, J = 4 Hz), 7.28- 7.15 (m, 4H), 6.97 (d, 1H, J = 16 Hz).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 153.8, 150.1, 149.9, 143.3, 141.8, 136.7, 136.1, 127.2, 123.3, 122.8, 122.7, 111.8, 92.4, 88.5.

(*E*)-4,4''-(but-1-en-3-yne-1,4-diyl)di-1,1'-biphenyl (2mm):[5]

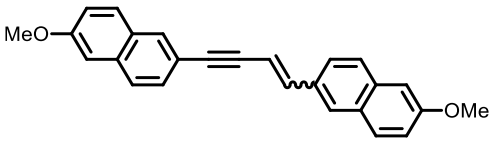


Prepared according to general procedure described above by reacting 4-ethynylbiphenyl (152 mg) with KO^{t}Bu (3.6 mg) and 18-crown-6 (9 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 4% ethylacetate in hexane. The compound was obtained as a yellowish white (69 mg, 46 %).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 8.04 (d), 7.66-7.32 (m), 7.13-7.08 (m, 1H), 6.77 (d), 6.50-6.44 (m, 1H), 6.06-5.96 (m).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 142.4, 141.1, 140.5, 140.3, 138.2, 135.7, 131.9, 129.3, 128.8, 128.5, 127.7, 127.5, 127.4, 127.2, 127.1, 127.0, 126.9, 126.8, 126.8, 125.4, 122.3, 109.0, 108.1, 107.4, 105.3, 96.1, 92.0, 89.8, 89.1.

6,6'-(but-1-en-3-yne-1,4-diyl)bis(2-methoxynaphthalene) (2nn):[1]



Prepared according to general procedure described above by reacting 2-ethynyl-6-methoxynaphthalene (156 mg) with KO^{t}Bu (3.6 mg) and 18-crown-6 (9 mg). The crude

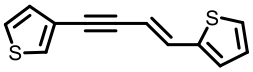
product was purified by column chromatography using silica gel (100-200 mesh) with 3% ethyl acetate in hexane. The compound was obtained in 40% yield (62 mg).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 7.93 (s, 1H), 7.74-7.68 (m, 5H), 7.60 (d, 1H, *J* = 8 Hz), 7.51 (d, 1H, *J* = 8Hz), 7.17 -7.12 (m, 5H), 6.49 (d, 1H, *J* = 16Hz), 3.93 (s, 6H).

Z isomer: 8.35, 8.14 (d), 7.97 (s), 7.76 (m), 7.55 (d), 6.845 (d), 5.985 (d), 3.94 (s)

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 158.4, 158.3, 158.2, 158.1, 141.2, 138.5, 134.7, 134.6, 134.2, 134.1, 131.9, 131.1, 129.9, 129.8, 129.4, 129.3, 129.1, 129.0, 128.9, 128.7, 128.6, 128.6, 128.4, 128.0, 127.8, 127.6, 127.3, 127.0, 126.9, 126.8, 126.7, 126.6, 123.7, 123.4, 119.5, 119.2, 118.5, 118.4, 107.4, 106.8, 106.1, 106.0, 105.9, 105.8, 105.7, 105.6, 96.5, 92.4, 89.0, 88.6, 55.5, 55.4 (both *E* and *Z* isomer present).

(*E*)-2-(4-(thiophen-3-yl)but-1-en-3-yn-1-yl)thiophene (2pp):[6]



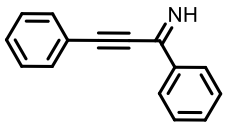
Prepared according to general procedure described above by reacting 3-ethynylthiophene (84 µL) with KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 2% ethylacetate in hexane. The compound was obtained as a colorless solid (66 mg, 72%).

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 7.48 (d, 1H, *J* = 4Hz), 7.35-7.27 (m, 4H), 7.17 (d, 1H, *J* = 4Hz), 7.05 (d, 1H, *J* = 16Hz), 6.22 (d, 1H, *J* = 16Hz).

Z isomer peaks 5.82 (d, 1H, *J* = 12 Hz), 6.76 (d, 1H, *J* = 12 Hz), 7.21 (d, *J* = 4Hz), 7.53-7.52 (d, *J* = 4Hz)

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 139.2, 135.0, 129.7, 128.3, 126.5, 125.3, 124.4, 123.5, 122.5, 107.7, 88.3, 86.7.

1,3-diphenylprop-2-yn-1-imine (4aa):[7]



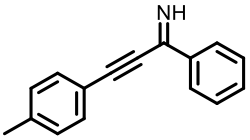
Prepared according to general procedure described above by reacting phenylacetylene (71 µL) with benzonitrile (44 µL) in presence of KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 4 % ethyl acetate in hexane along with triethylamine. The compound was obtained as a reddish orange oil (58 mg, 67%).

HRMS m/z calcd for $C_{15}H_{11}N$ = 206.09 found = 206.0950.

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 8.13 (d, 2H, *J* = 8Hz), 7.60 (d, 2H, *J* = 8Hz), 7.51-7.46 (m, 3H), 7.42-7.38 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 160.2, 136.5, 132.2, 131.5, 129.8, 128.6, 128.4, 127.6, 121.2, 92.6, 85.5.

1-phenyl-3-(p-tolyl)prop-2-yn-1-imine (4ab):



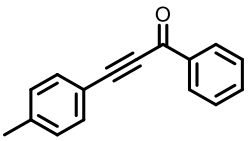
Prepared according to general procedure described above by reacting 4-ethynyltoluene (81 µL) with benzonitrile (44 µL) in presence of KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 5 % ethyl acetate in hexane along with triethylamine. The compound was obtained as a yellowish red oil (69 mg, 74%).

HRMS m/z calcd for $C_{16}H_{13}N$ = 220.11 found = 220.1111.

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 8.13 (d, 2H, *J* = 8Hz), 7.51- 7.48 (m, 4H), 7.46-7.44 (m, 1H), 7.21 (d, 2H, *J* = 8Hz), 2.40 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 160.3, 140.3, 136.6, 132.1, 131.4, 129.3, 128.4, 127.6, 118.1, 93.0, 85.1, 21.6.

1-phenyl-3-(p-tolyl)prop-2-yn-1-one (4abO):



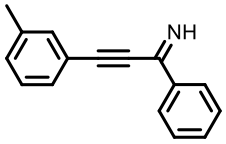
The compound was obtained as yellowish red oily. This was formed during purification of **4ab** by column chromatography using silica gel (100-200 mesh).

HRMS m/z calcd for $C_{16}H_{12}O$ = 221.09 found = 221.0961.

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 8.23 (d, 2H, *J* = 8 Hz), 7.63-7.58 (m, 3H), 7.54-7.50 (m, 2H), 7.23 (d, 2H, *J* = 8 Hz), 2.41 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 178.1, 141.6, 137.0, 134.0, 133.1, 129.5, 129.4, 128.6, 117.0 93.8, 86.5, 21.8.

1-phenyl-3-(m-tolyl)prop-2-yn-1-imine (4ad):



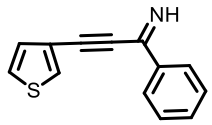
Prepared according to general procedure described above by reacting 3-ethynyltoluene (81 µL) with benzonitrile (44 µL) in presence of KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 3 % ethyl acetate in hexane. The compound was obtained as yellowish orange oily (50 mg, 53 %).

HRMS m/z calcd for $C_{16}H_{13}N$ = 220.1121 found = 220.1110.

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 10.33 (broad, 1H), 8.16 (d, 2H, J = 8 Hz), 7.53-7.47 (m, 3H), 7.45-7.42 (m, 2H), 7.33-7.28 (m, 2H), 2.41(s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 160.2, 138.4, 136.6, 132.7, 131.4, 130.7, 129.3, 128.5, 128.4, 127.6, 121.0, 92.8, 85.2, 21.2.

1-phenyl-3-(thiophen-3-yl)prop-2-yn-1-imine (4ap):



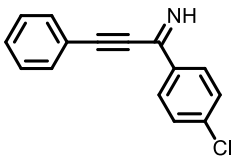
Prepared according to general procedure described above by reacting 3-ethynylthiophene (63 µL) with benzonitrile (44 µL) in presence of KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 4% ethylacetate in hexane. The compound was obtained as a yellowish red colour oil (48 mg, 53 %).

HRMS m/z calcd for $C_{13}H_9NS$ = 212.0528 found = 212.0523.

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 8.06 (d, 2H, J = 8 Hz), 7.69 (d, 1H, J = 4 Hz), 7.44-7.42 (m, 2H), 7.37- 7.35 (m, 1H), 7.25- 7.24 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 158.9, 137.7, 135.0, 131.5, 129.8, 129.0, 128.6, 126.1, 120.1, 88.3, 84.8.

1-(4-chlorophenyl)-3-phenylprop-2-yn-1-imine (4qa):[7]



Prepared according to general procedure described above by reacting phenylacetylene (71 µL) with 4-cholorobenzonitrile (59 mg) in presence of KO^{t}Bu (3.6 mg). The crude product was

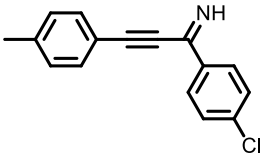
purified by column chromatography using silica gel (100-200 mesh) with 4 % ethyl acetate in hexane. The compound was obtained as a deep red oil (58 mg, 57%).

HRMS m/z calcd for $C_{15}H_{10}ClN$ = 240.0575 found = 240.0585.

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 10.36 (broad, 1H), 8.09-8.08 (d, 2H, *J* = 4 Hz), 7.59 (d, 2H, *J* = 8 Hz), 7.45-7.41 (m, 5H).

^{13}C NMR (125 MHz, $CDCl_3$, 298K) δ (ppm) 158.9, 137.7, 135.1, 132.2, 130.0, 129.0, 128.7, 128.6, 121.0, 93.0, 85.0.

1-(4-chlorophenyl)-3-(p-tolyl)prop-2-yn-1-imine (4qb):



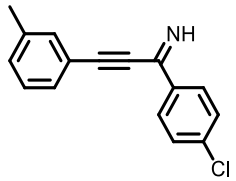
Prepared according to general procedure described above by reacting 4-ethynyltoluene (81 µL) with 4-cholorobenzonitrile (59 mg) in presence of KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 6 % ethylacetate in hexane. The compound was obtained as a yellowish red oil (59 mg, 55%).

HRMS m/z calcd for $C_{16}H_{12}ClN$ = 254.07 found = 254.0744.

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 10.29(broad, 1H), 8.08 (d, 2H, *J* = 8Hz), 7.49-7.42 (m, 4H), 7.21 (d, 2H, *J* = 8Hz), 2.40 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ (ppm) 159.0, 140.5, 137.6, 135.1, 132.1, 129.4, 129.0, 128.6, 117.8, 93.4 84.6, 21.6.

1-(4-chlorophenyl)-3-(m-tolyl)prop-2-yn-1-imine (4qd):



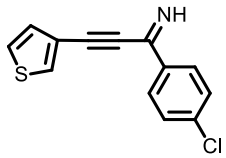
Prepared according to general procedure described above by reacting 3-ethynyltoluene (81 µL) with 4-cholorobenzonitrile (59 mg) in presence of KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 5 % ethylacetate in hexane. The compound was obtained as reddish orange oily (56 mg, 52%).

HRMS m/z calcd for $C_{16}H_{12}ClN$ = 254.07 found = 254.0713.

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 10.35 (broad, 1H), 8.10 (d, 2H, *J* = 8 Hz), 7.46 - 7.40 (m, 4H), 7.32 -7.28 (m, 2H), 2.40 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$, 298K) δ (ppm) 159.0, 138.4, 137.7, 135.1, 132.7, 130.9, 129.3, 129.0, 128.6, 128.5, 120.8, 93.3, 84.7, 21.2.

1-(4-chlorophenyl)-3-(thiophen-3-yl)prop-2-yn-1-imine (4qp):



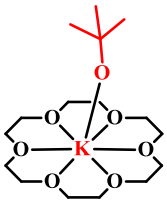
Prepared according to general procedure described above by reacting 3-ethynylthiophene (63 µL) with 4-cholorobenzonitrile (59 mg) in presence of KO^{t}Bu (3.6 mg). The crude product was purified by column chromatography using silica gel (100-200 mesh) with 5 % ethyl acetate in hexane. The compound was obtained as a yellowish orange oil (53 mg, 51%).

HRMS m/z calcd for $C_{13}H_{18}ClNS$ = 246.01 found = 246.0115.

^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ (ppm) 8.06 (d, 2H, J = 8 Hz), 7.69 (d, 1H, J = 4 Hz), 7.44- 7.42 (m, 2H), 7.37 -7.35 (m, 1H), 7.25- 7.24 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$, 298K) δ (ppm) 158.9, 137.7, 135.0, 131.5, 129.8, 129.0, 128.6, 126.1, 120.0, 88.3, 84.9.

Intermediate A:[8]



A

The crystals of **A** were first washed with dry hexane and dried over low pressure. NMR spectroscopic measurements were carried out in THF-d_8 solvent.

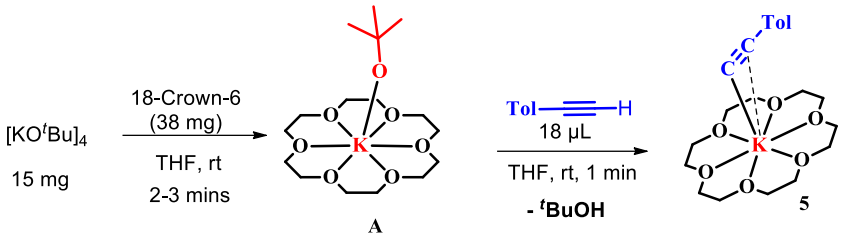
^{1}H NMR (500 MHz, THF-d_8, 298K) δ (ppm) 1.10 (s, 3H), 3.61 (s, 24H).

^{13}C NMR (125 MHz, THF-d_8, 298K) δ (ppm) 36.0, 66.9, 71.3.

Synthesis of intermediate 5:

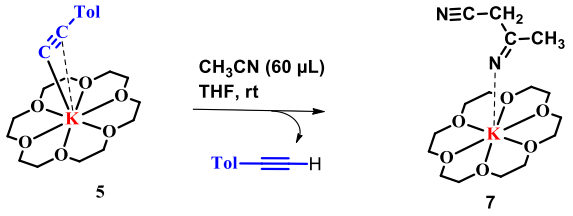
Inside a nitrogen filled glovebox, 15 mg (0.133 mmol) of KO^{t}Bu and 38 mg (0.147 mmol) of 18-crown-6 were taken in a 5 ml vial with 1.2 mL THF. The reaction mixture was stirred for 2-3 mins which offered a clear solution. 18 µL (0.133 mmol) of 4-ethynyltoluene was added which resulted a brownish solution. Within 1 min, that brown solution was kept at -36 °C for

crystallization inside the glovebox. Colorless crystal was obtained on overnight standing. The crystal was characterized by solid state structure and NMR spectroscopy.



Synthesis of complex 7:

Inside a nitrogen filled glovebox, 20 mg crystalline material of **5** was treated with 60 µL of dry acetonitrile in a 5 mL vial. The reaction mixture was diluted with 1.2 mL of THF which offered a clear reddish yellow solution. 600 µL of hexane was added to this clear solution and the clear solution was kept at -36 °C for crystallization inside the glovebox. Yellow colored crystal was obtained on overnight standing. The crystal was characterized by solid state structure and NMR spectroscopy.



III. ^{1}H NMR and ^{13}C NMR spectra of the products

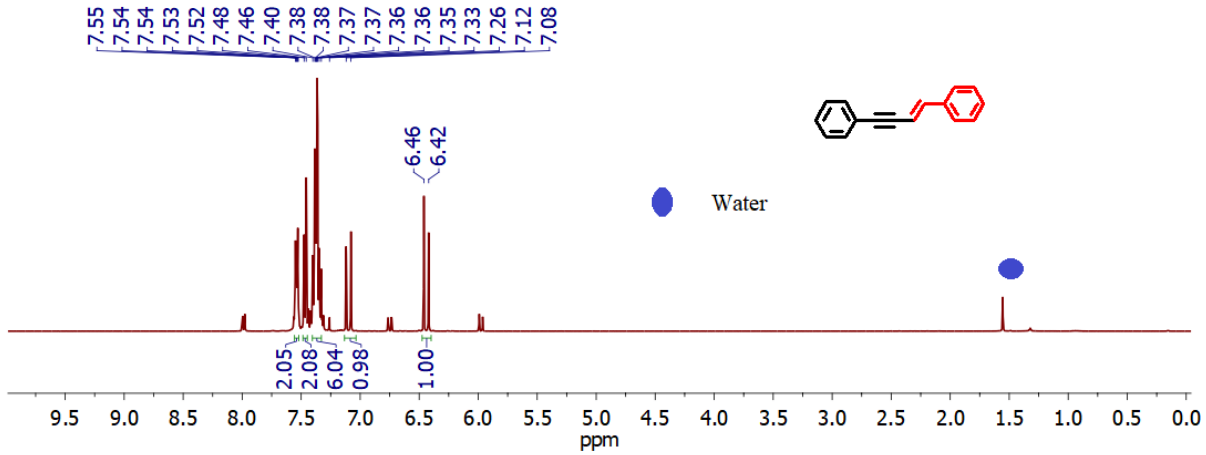


Figure S3. ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-but-1-en-3-yne-1,4-diyldibenzene (**2aa**). The minor peaks are assigned to the *Z*- isomer.

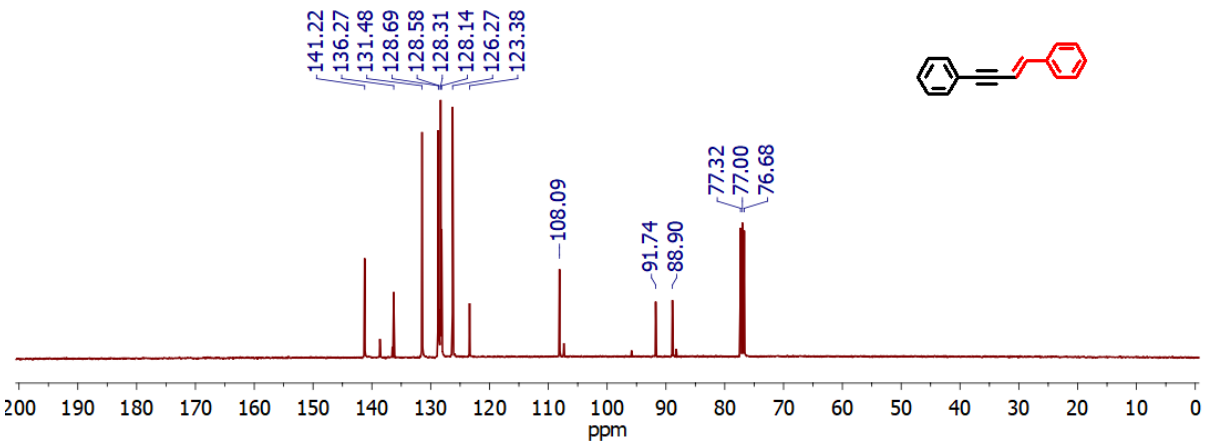


Figure S4. ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-but-1-en-3-yne-1,4-diyldibenzene (**2aa**). The minor peaks are assigned to the *Z*- isomer.

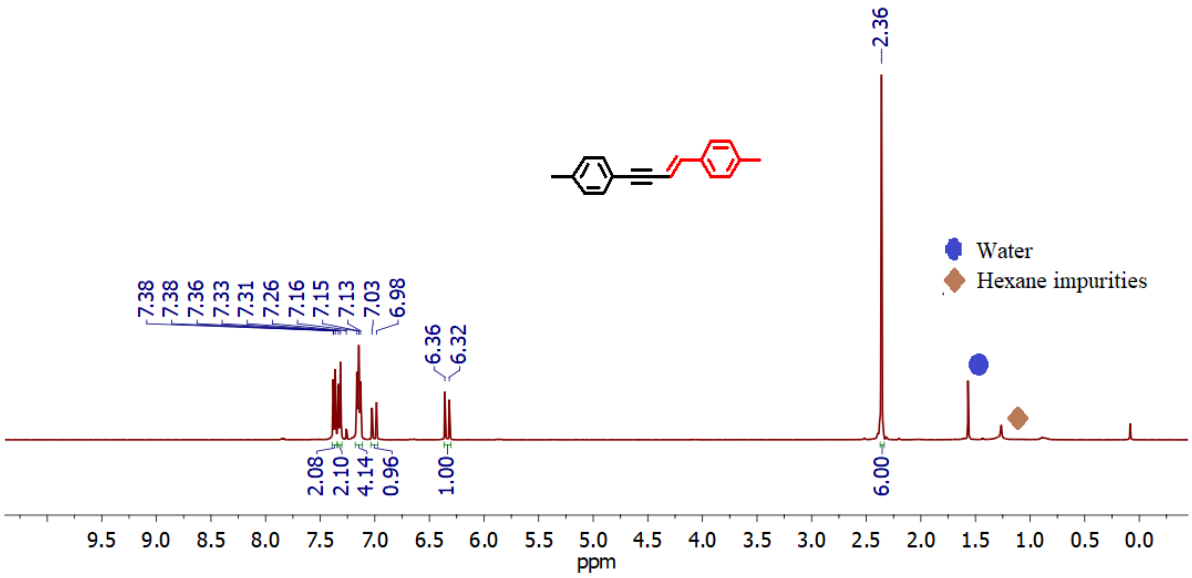


Figure S5. ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(methylbenzene) (**2bb**).

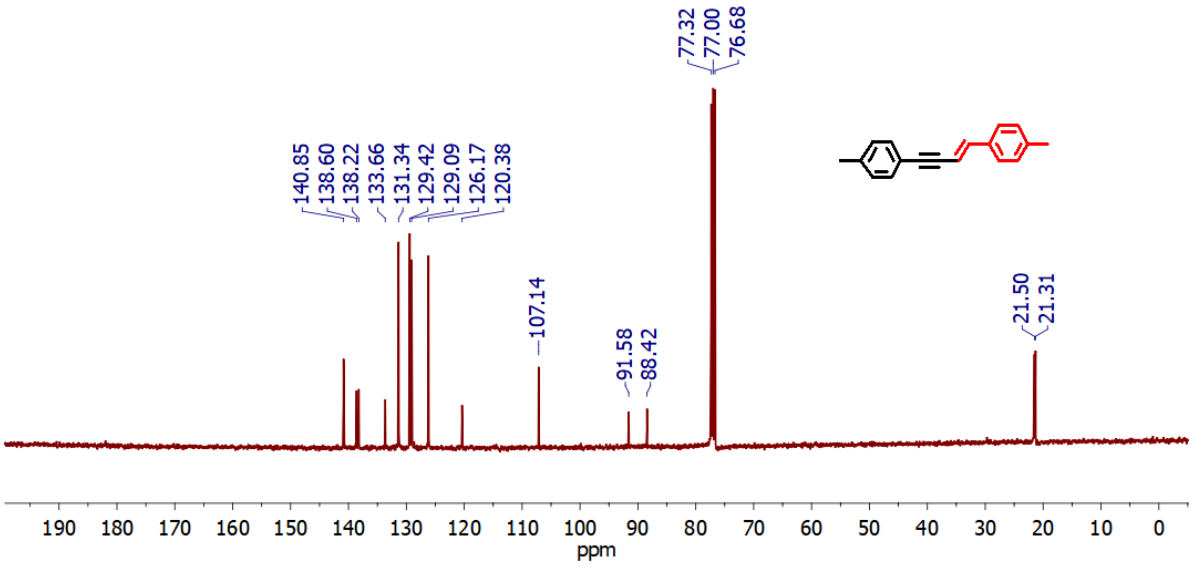


Figure S6. ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(methylbenzene) (**2bb**).

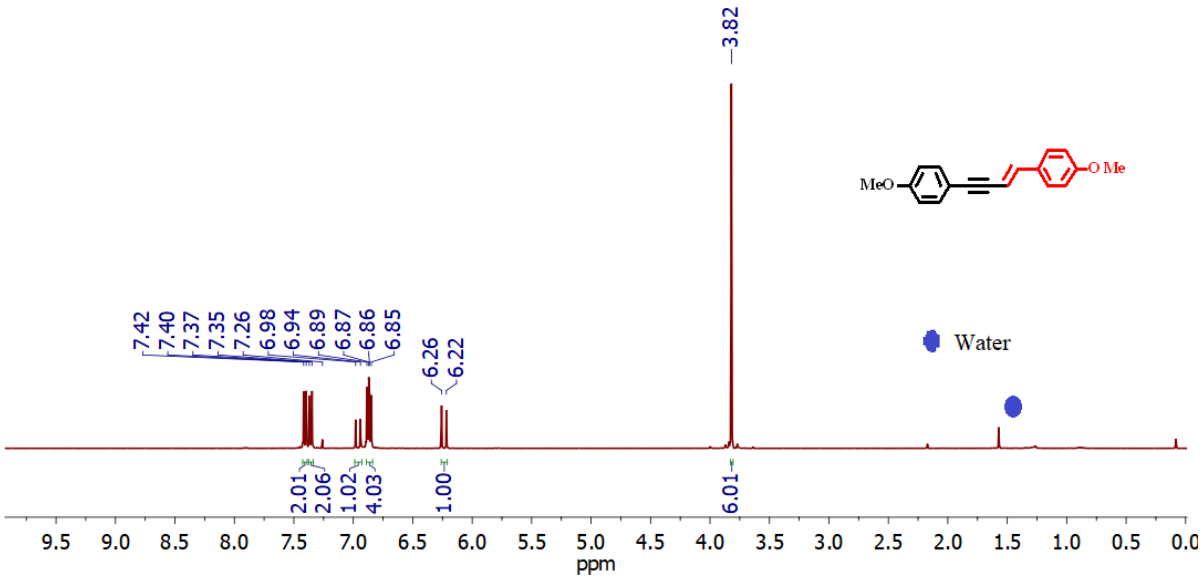


Figure S7. ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(methoxybenzene) (**2cc**).

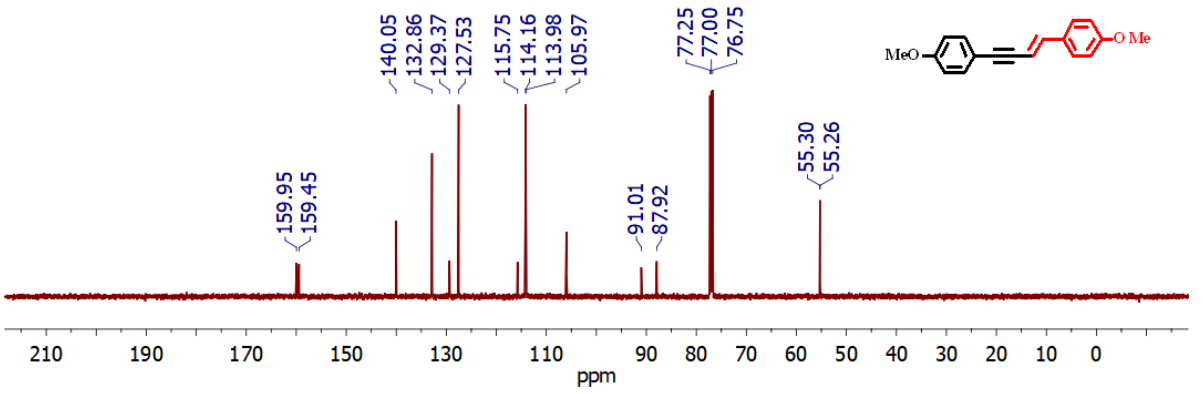


Figure S8. ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(methoxybenzene) (**2cc**).

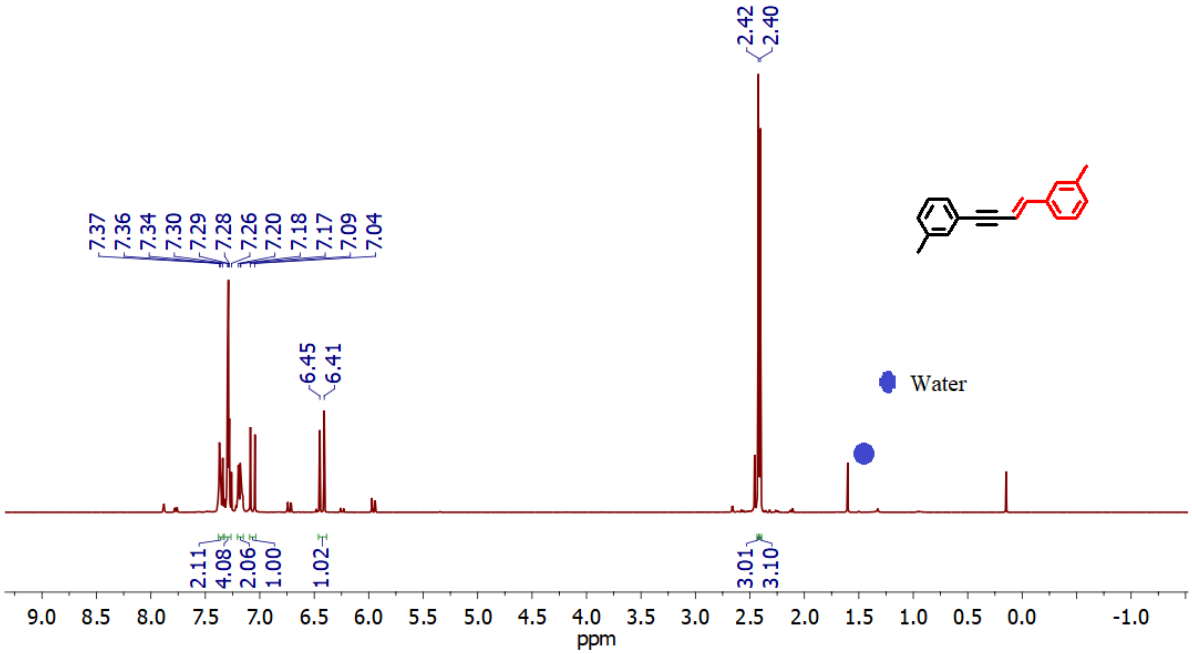


Figure S9. ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-3,3'-(but-1-en-3-yne-1,4-diyl)bis(methylbenzene) (**2dd**). The minor peaks are assigned to the *Z*- isomer.

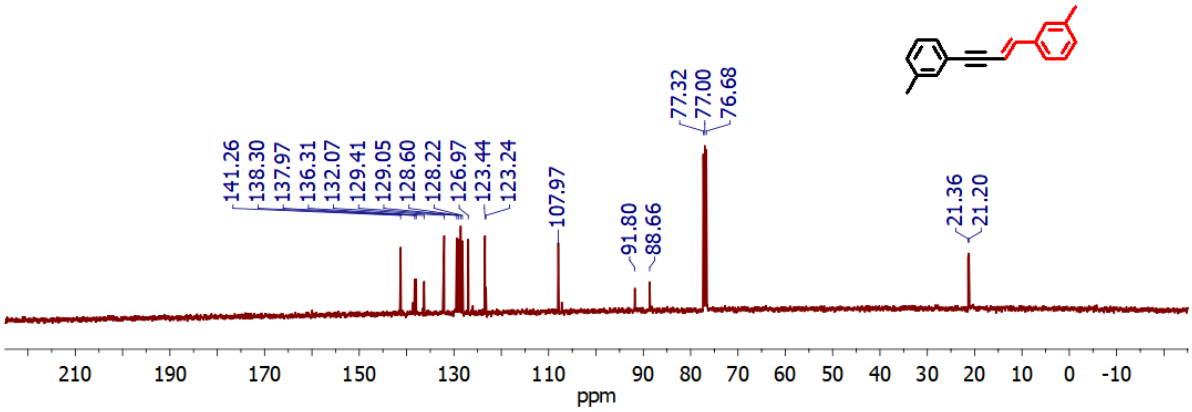


Figure S10. ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-3,3'-(but-1-en-3-yne-1,4-diyl)bis(methylbenzene) (**2dd**). The minor peaks are assigned to the *Z*- isomer.

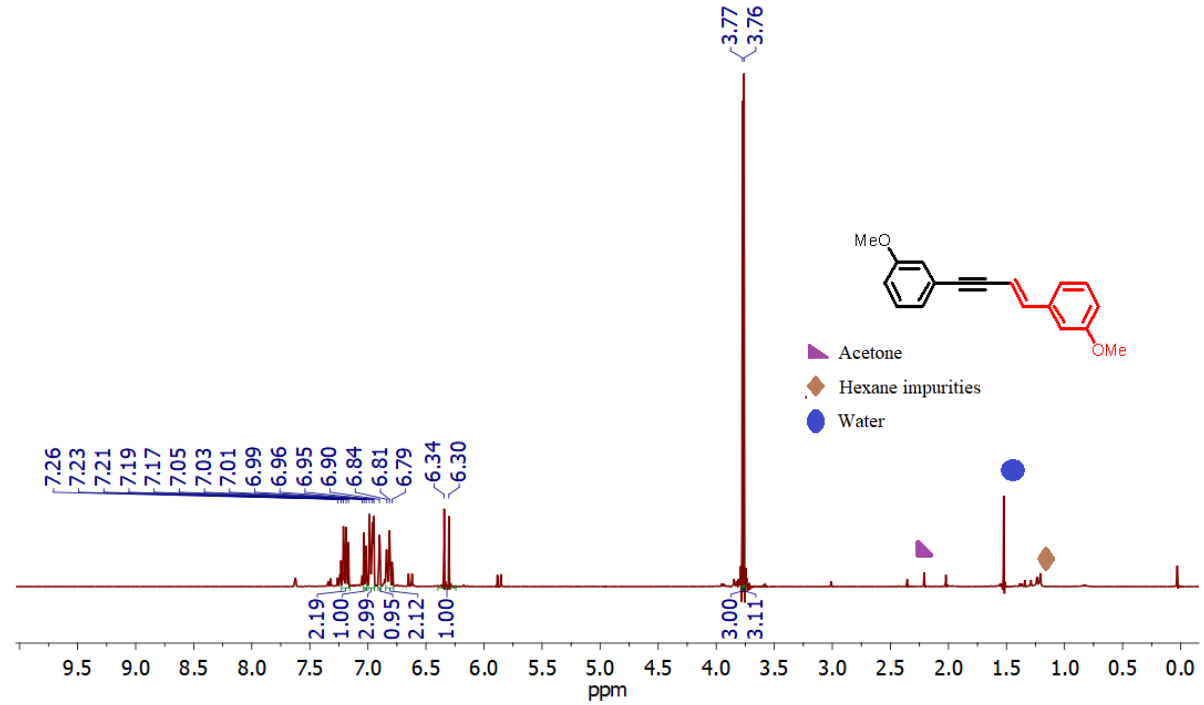


Figure S11. ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-3,3'-(but-1-en-3-yne-1,4-diyl)bis(methoxybenzene) (**2ee**). The minor peaks are assigned to the *Z*- isomer.

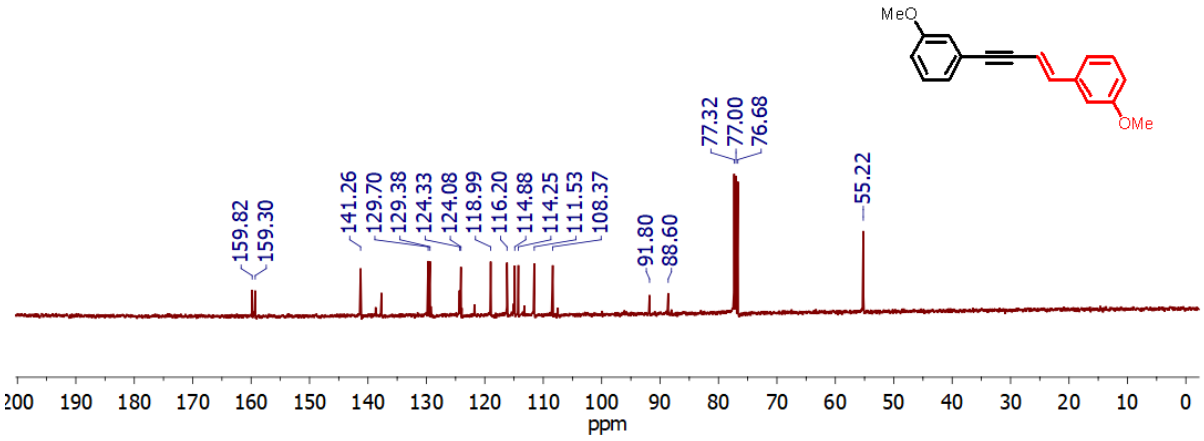


Figure S12. ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-3,3'-(but-1-en-3-yne-1,4-diyl)bis(methoxybenzene) (**2ee**). The minor peaks are assigned to the *Z*- isomer.

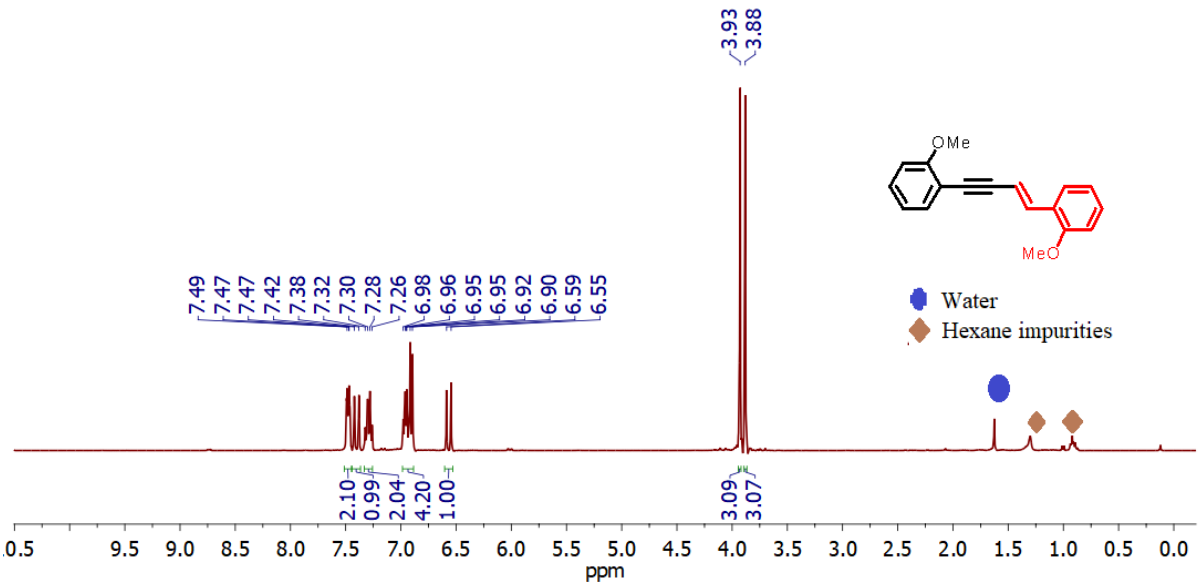


Figure S13. ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-2,2'-(but-1-en-3-yne-1,4-diyl)bis(methoxybenzene) (**2ff**).

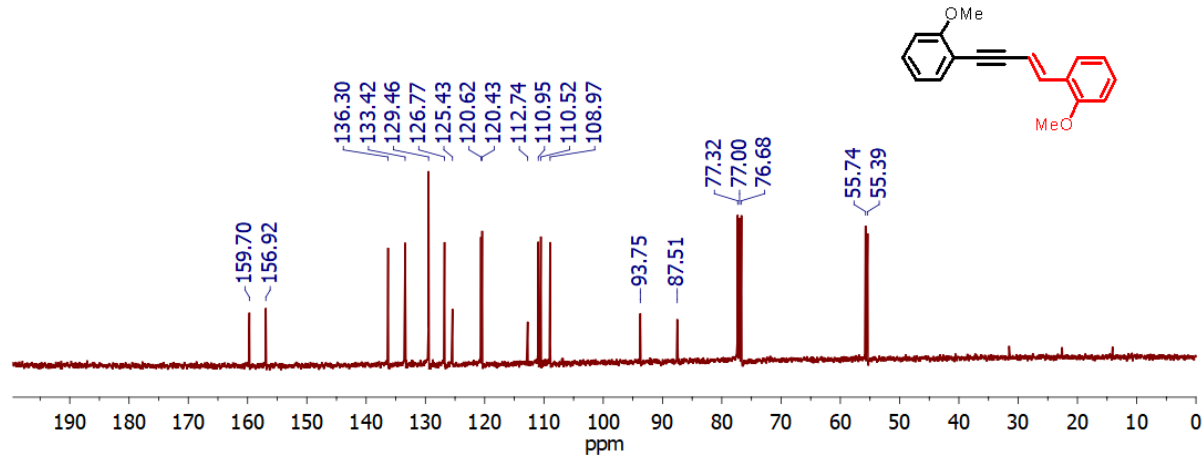


Figure S14. ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-2,2'-(but-1-en-3-yne-1,4-diyl)bis(methoxybenzene) (**2ff**).

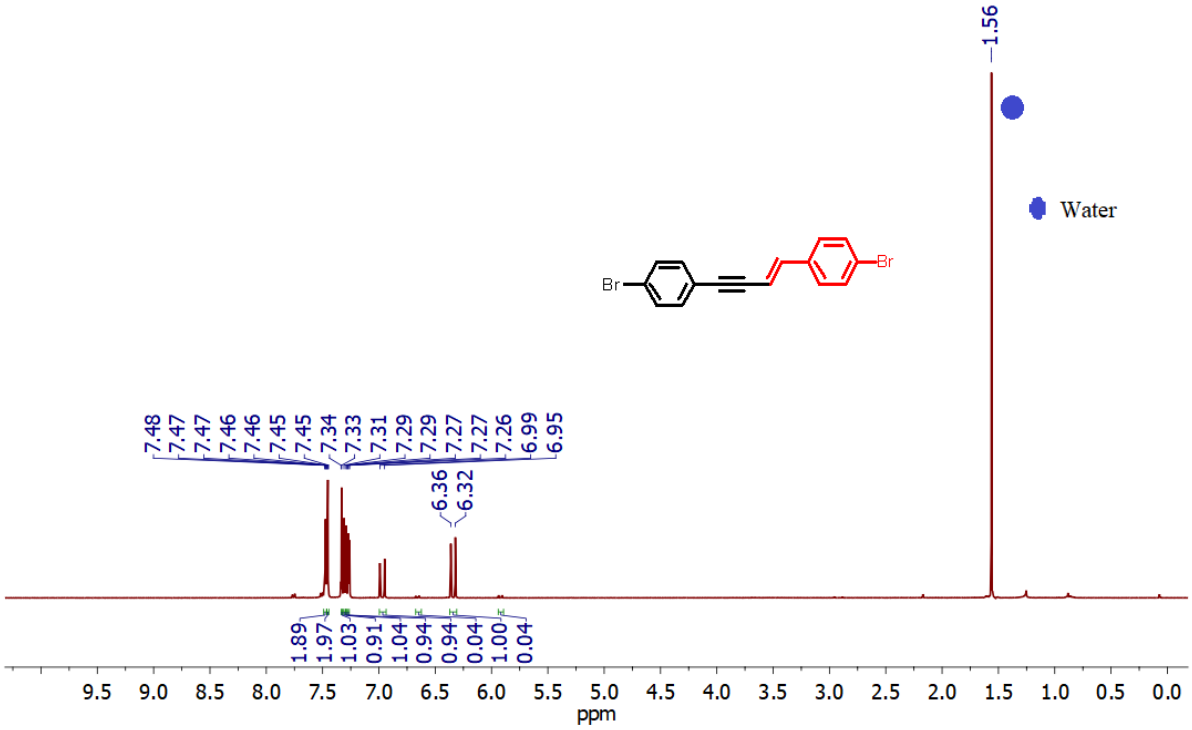


Figure S15. ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(bromobenzene) (**2gg**). The minor peaks are assigned to the *Z*- isomer.

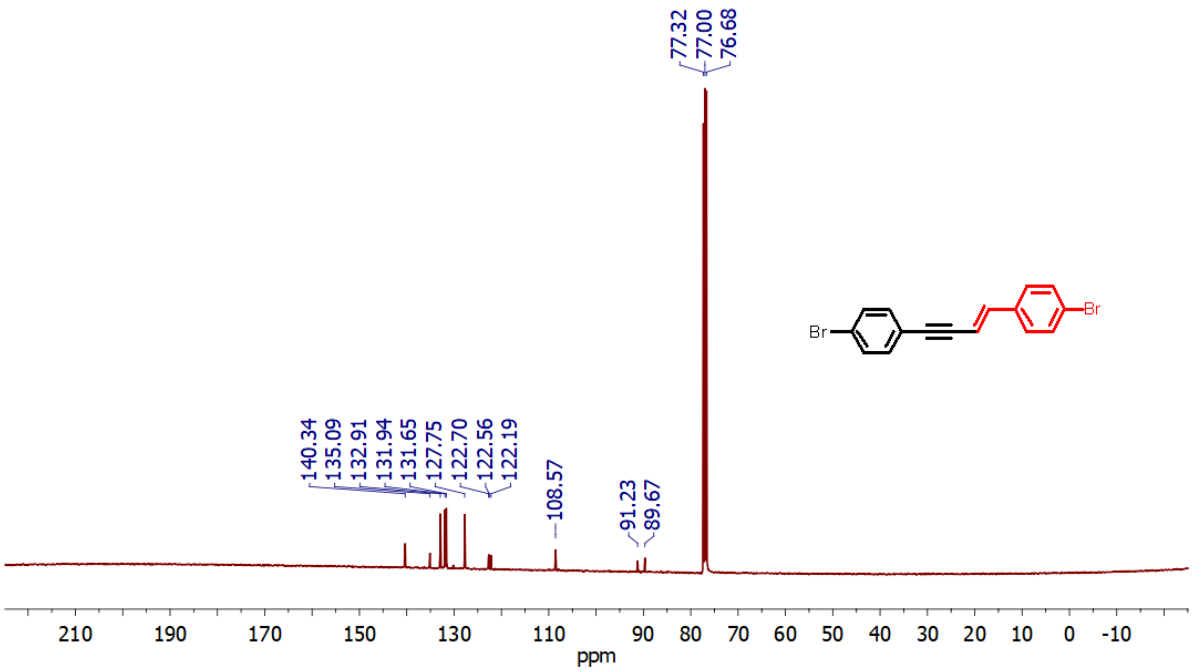


Figure S16. ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(bromobenzene) (**2gg**).

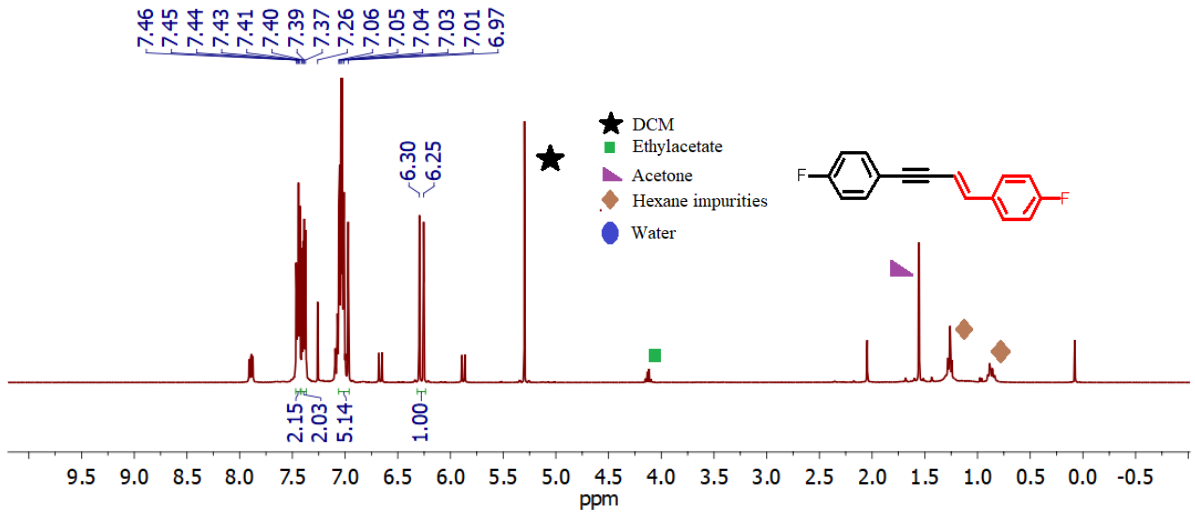


Figure S17. ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(fluorobenzene) (**2hh**). The minor peaks are assigned to the *Z*- isomer.

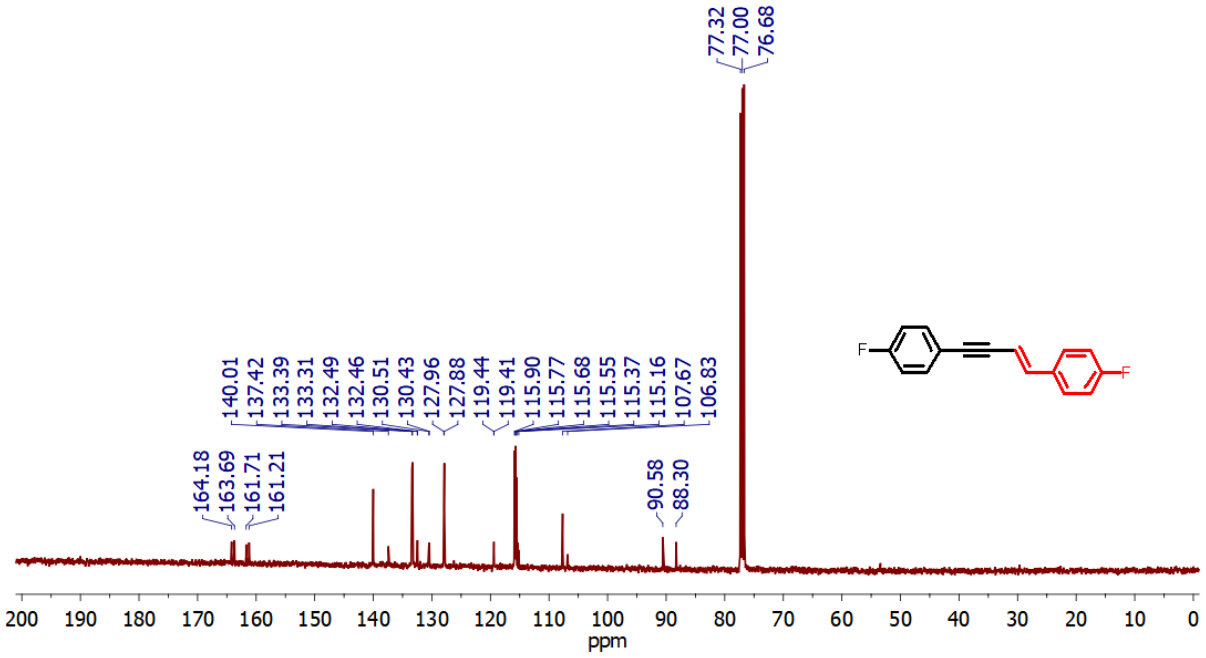


Figure S18. ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(fluorobenzene) (**2hh**). The minor peaks are assigned to the *Z*- isomer.

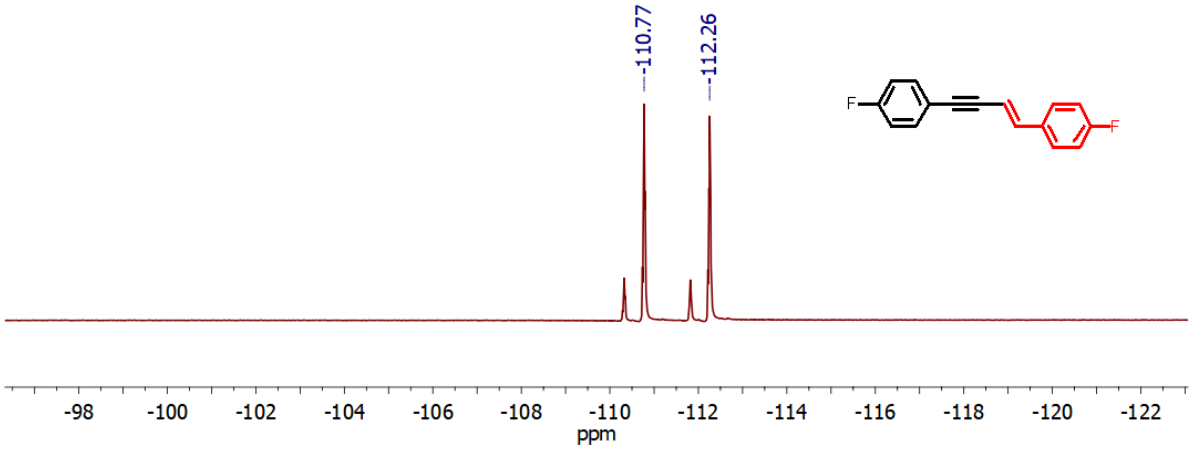


Figure S19. ^{19}F NMR ($CDCl_3$) spectrum of (E)-4,4'-(but-1-en-3-yne-1,4-diyl)bis(fluorobenzene) (**2hh**). The minor peaks are assigned to the *Z*- isomer.

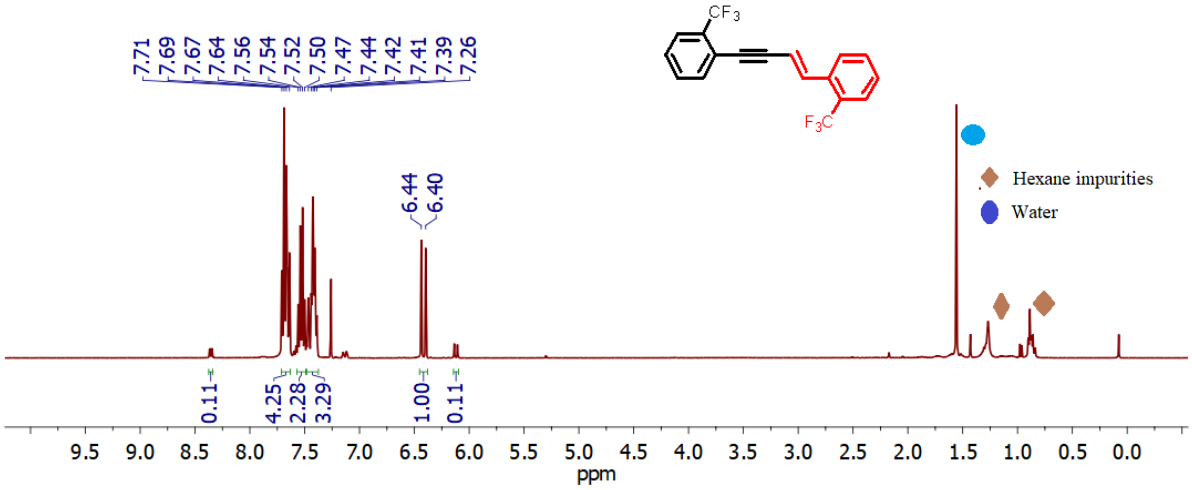


Figure S20. ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-2,2'-(but-1-en-3-yne-1,4-diyl)bis((trifluoromethyl) benzene) (**2ii**). The minor peaks are assigned to the *Z*- isomer.

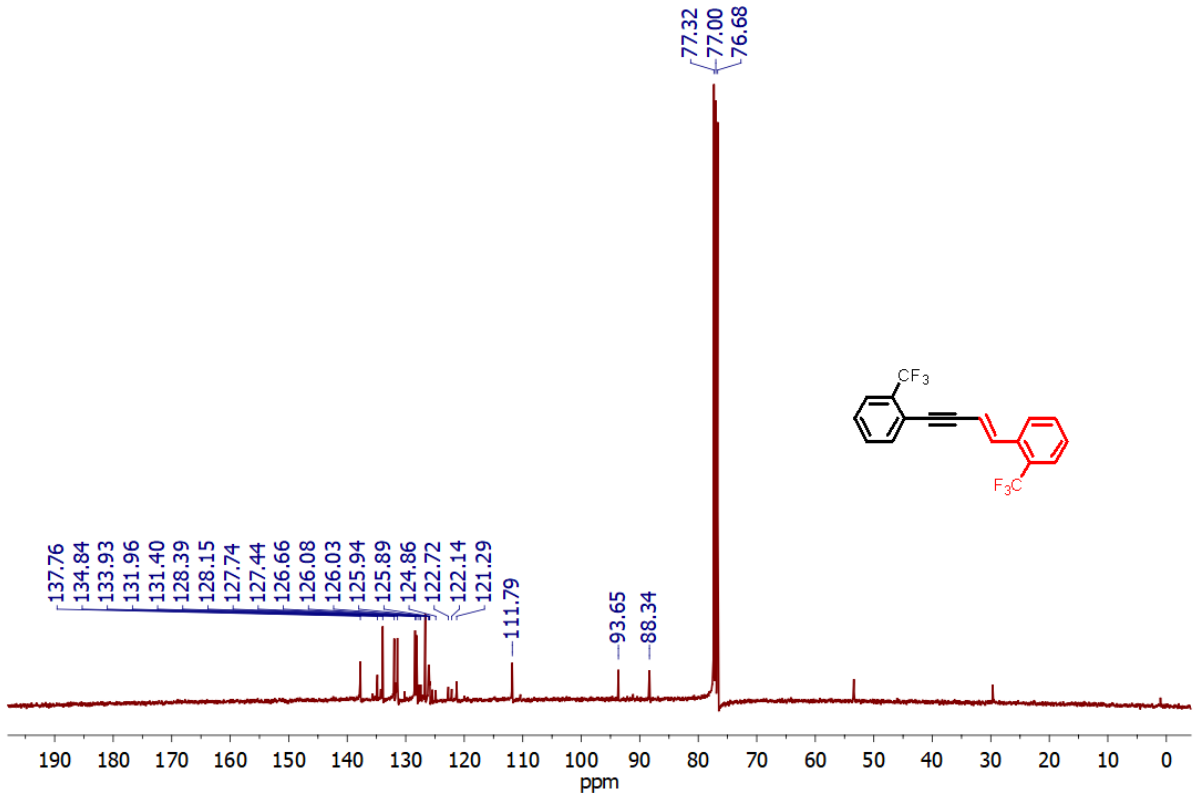


Figure S21. ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-2,2'-(but-1-en-3-yne-1,4-diyl)bis((trifluoromethyl) benzene) (**2ii**). The minor peaks are assigned to the *Z*- isomer.

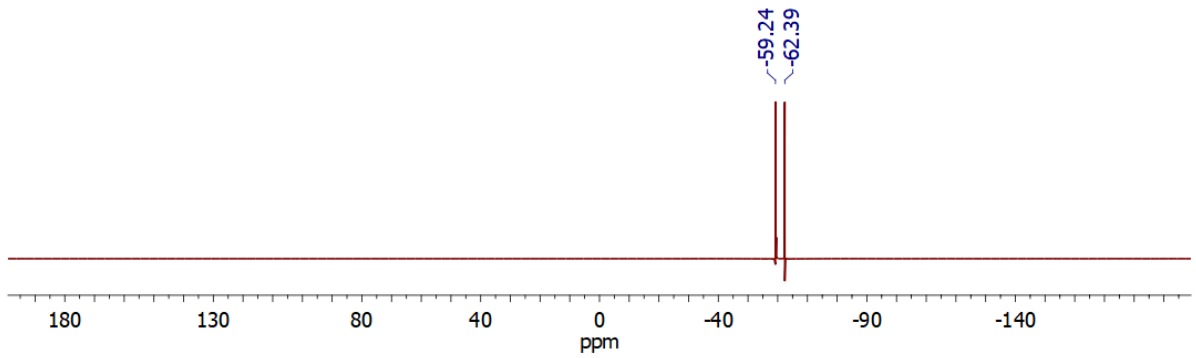


Figure S22. ^{19}F NMR ($CDCl_3$) spectrum of (*E*)-2,2'-(but-1-en-3-yne-1,4-diyl)bis((trifluoromethyl) benzene) (**2ii**).

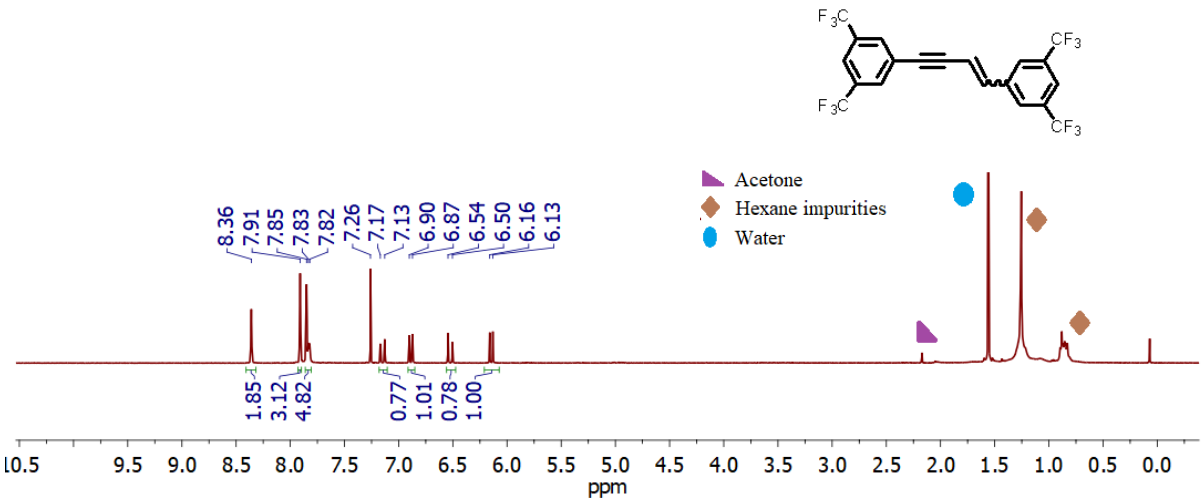


Figure S23. ^{1}H NMR ($CDCl_3$) spectrum *E/Z* mixture of 5,5'-(But-1-en-3-yne-1,4-diyl)bis(1,3-bis(trifluoromethyl)benzene) (**2jj**).

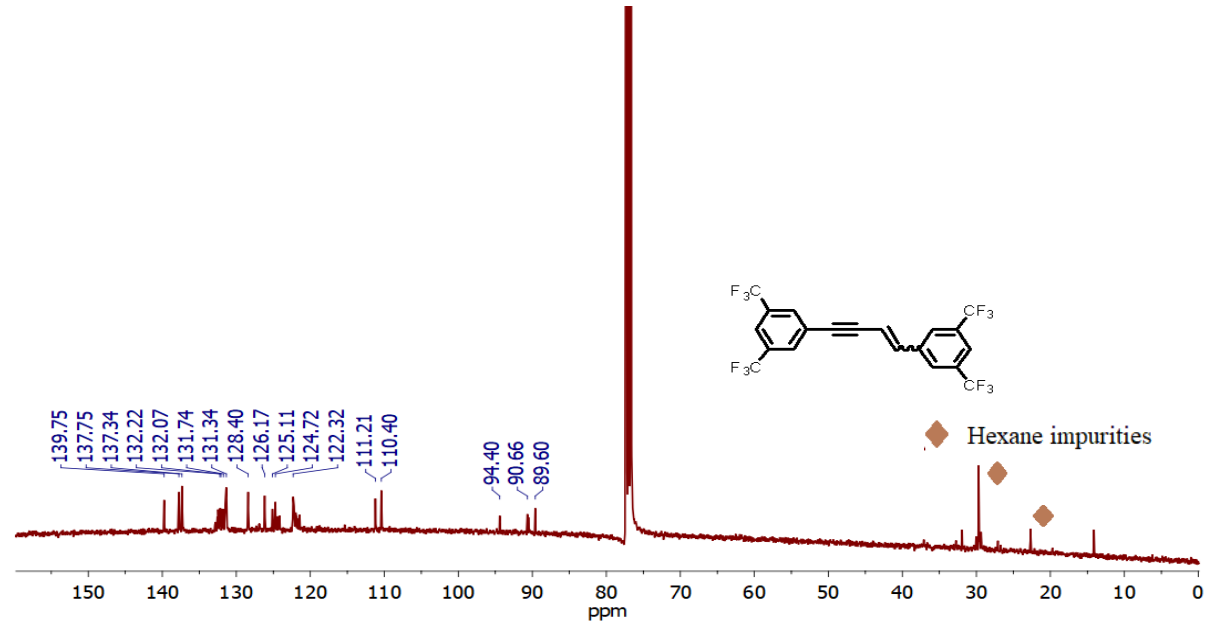


Figure S24. ^{13}C NMR ($CDCl_3$) spectrum *E/Z* mixture of 5,5'-(But-1-en-3-yne-1,4-diyl)bis(1,3-bis(trifluoromethyl)benzene) (**2jj**).

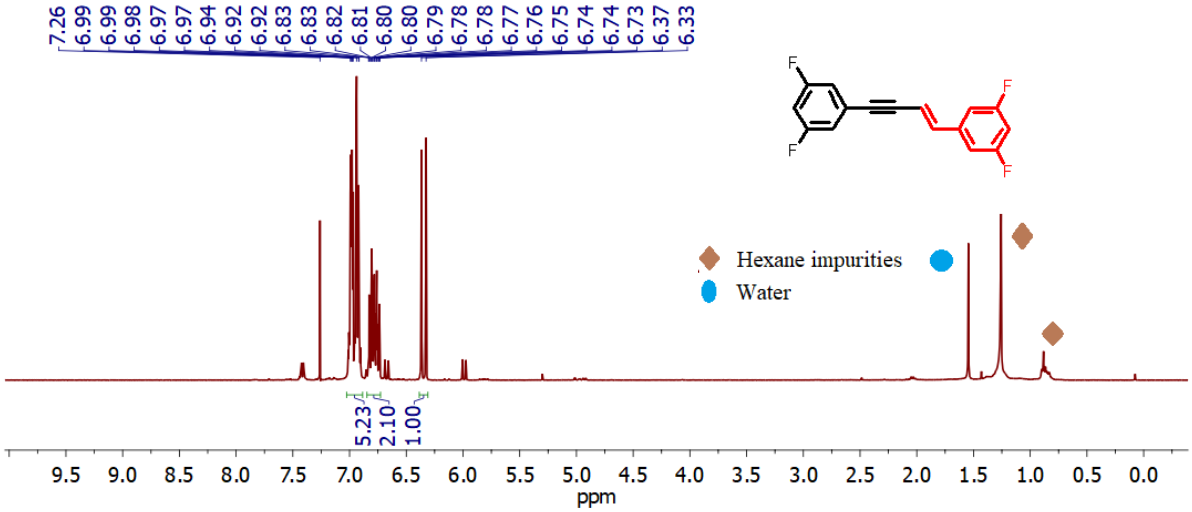


Figure S25. ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-5,5'-(but-1-en-3-yne-1,4-diyl)bis(1,3-difluorobenzene) (**2kk**). The minor peaks are assigned to the *Z*- isomer.

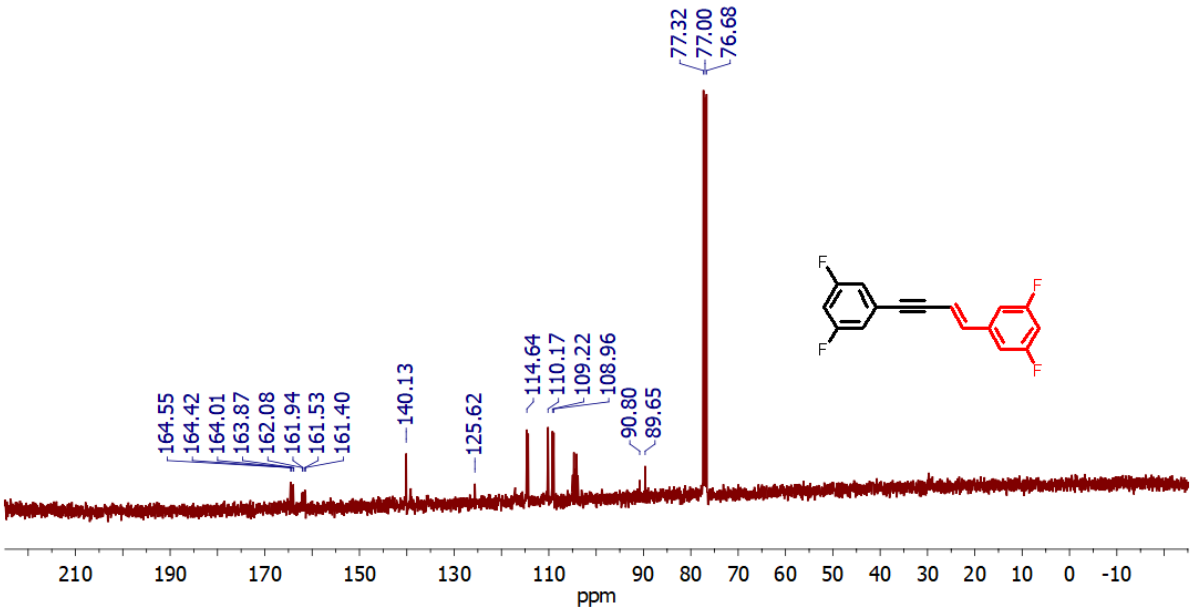


Figure S26. ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-5,5'-(but-1-en-3-yne-1,4-diyl)bis(1,3-difluorobenzene) (**2kk**). The minor peaks are assigned to the *Z*- isomer.

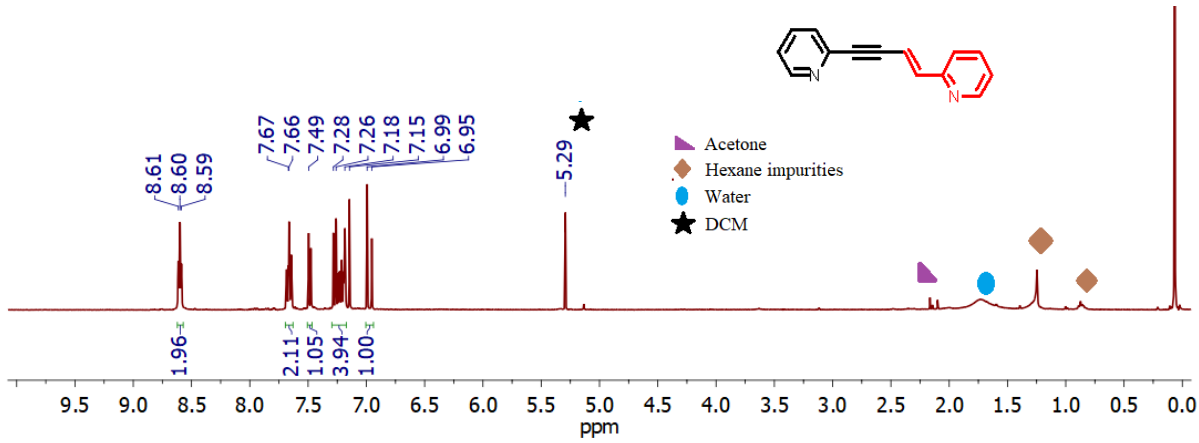


Figure S27. ^{1}H NMR ($CDCl_3$) spectrum of (*E*)-2,2'-(but-1-en-3-yne-1,4-diyl)dipyridine (**2ll**).

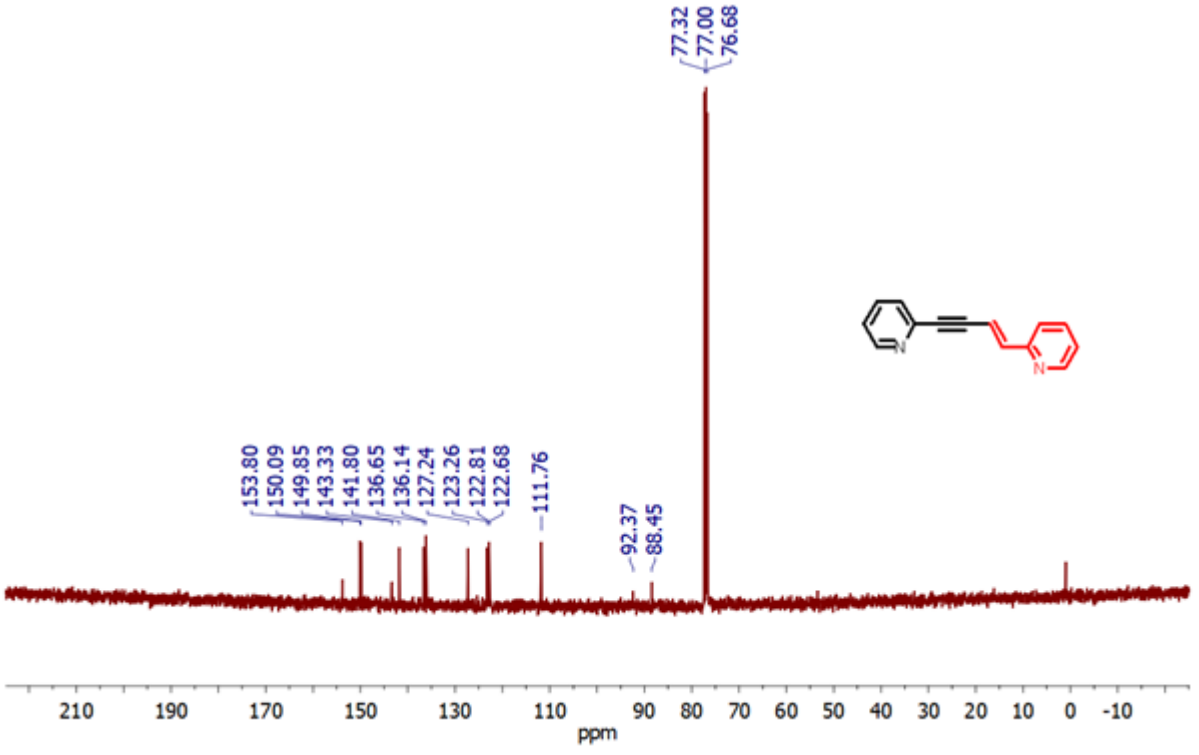


Figure S28. ^{13}C NMR ($CDCl_3$) spectrum of (*E*)-2,2'-(but-1-en-3-yne-1,4-diyl)dipyridine (**2ll**).

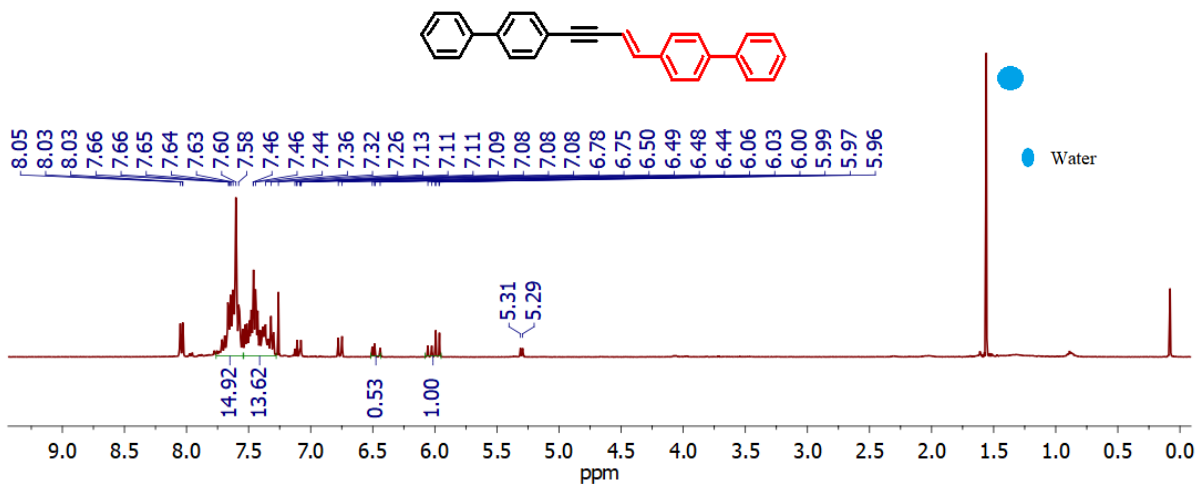


Figure S29. ^{1}H NMR ($CDCl_3$) spectrum of *E/Z* mixture of 4,4"-(But-1-en-3-yne-1,4-diyl)di-1,1'-biphenyl (THF) (**2mm**).

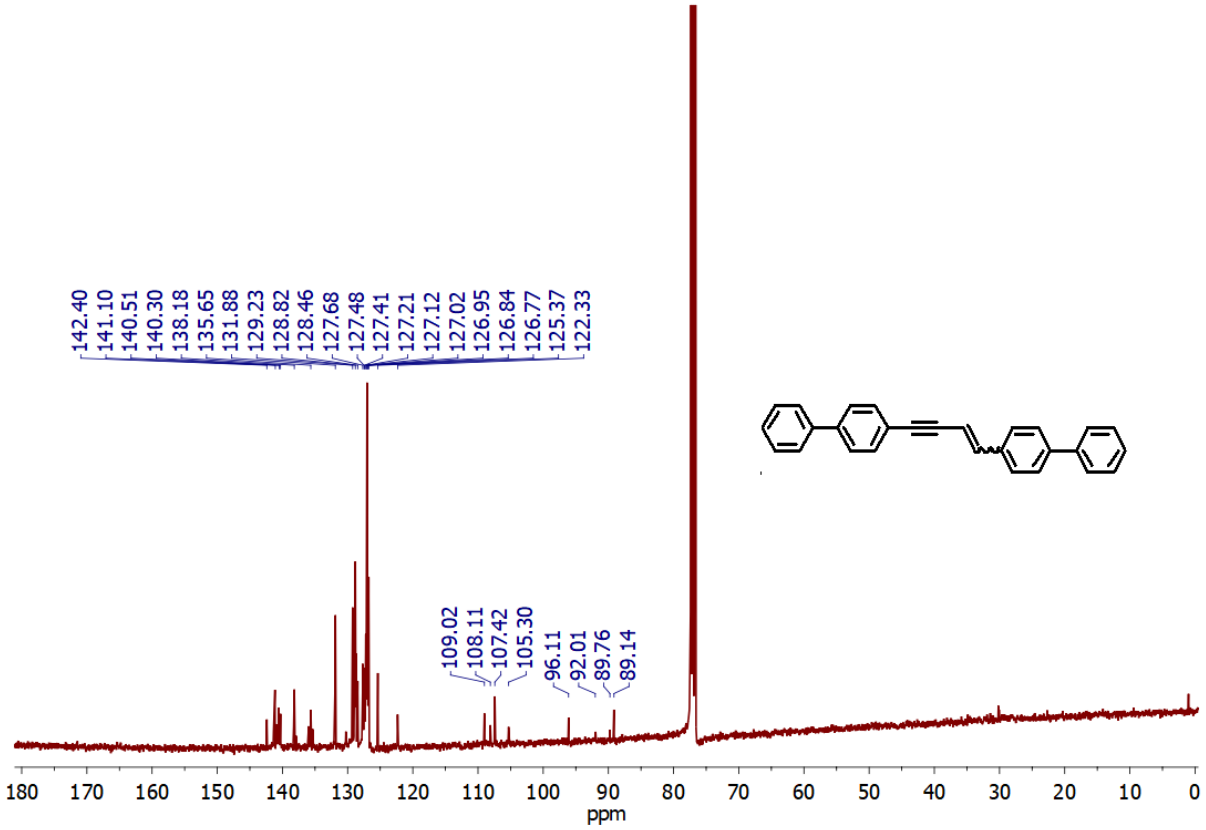


Figure S30. ^{13}C NMR ($CDCl_3$) spectrum of *E/Z* mixture of 4,4"-(But-1-en-3-yne-1,4-diyl)di-1,1'-biphenyl (THF) (**2mm**).

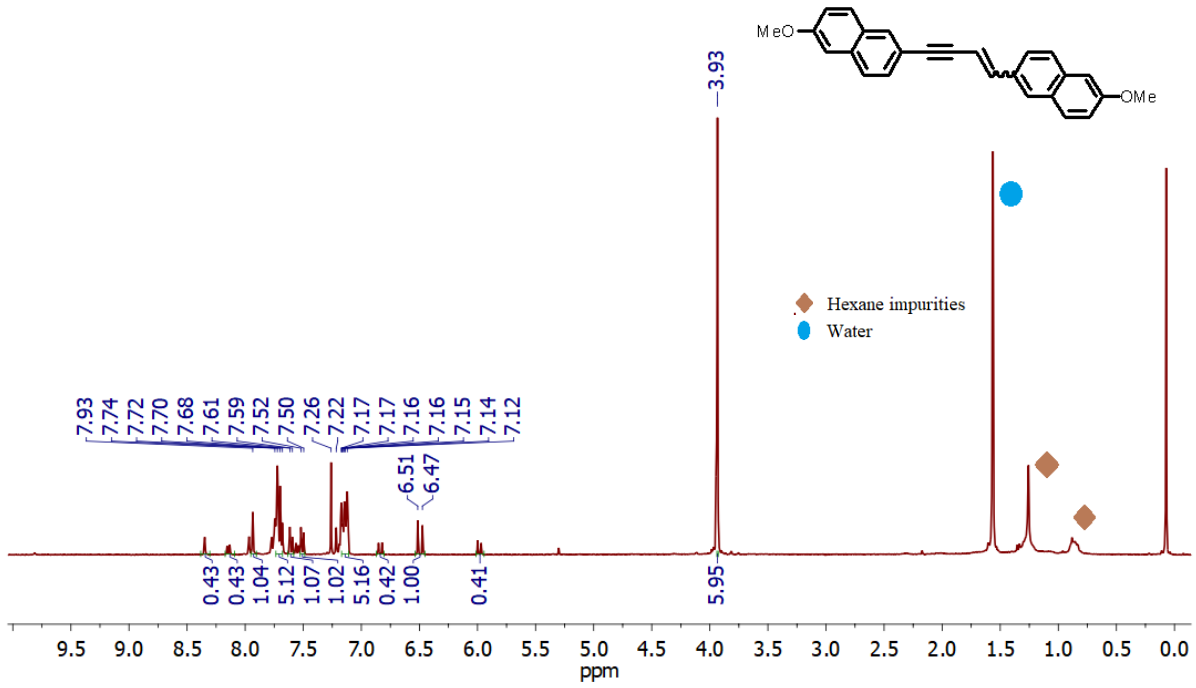


Figure S31. ^{1}H NMR ($CDCl_3$) spectrum of *E/Z* mixture of 6,6'-(But-1-en-3-yne-1,4-diyl)bis(2-methoxynaphthalene) (**2nn**). The small signals are corresponding to *Z*- isomer.

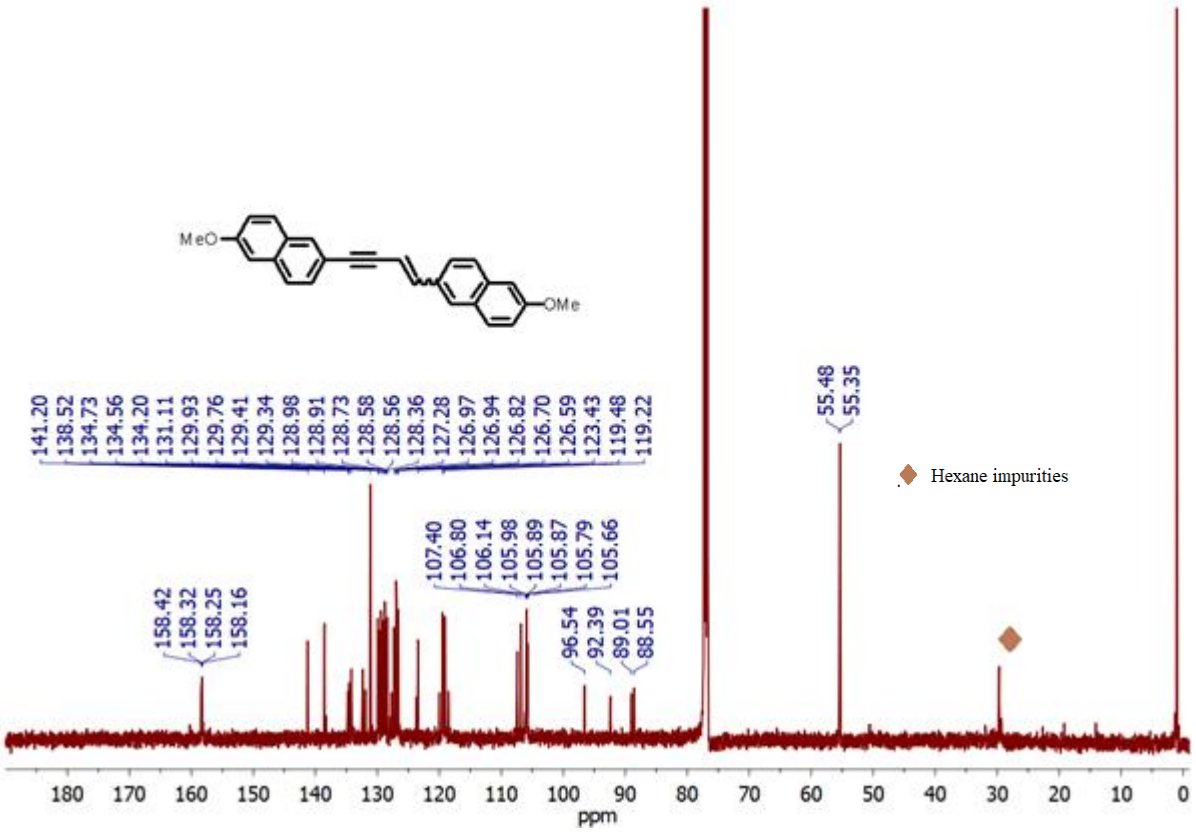


Figure S32. ^{13}C NMR ($CDCl_3$) spectrum *E/Z* mixture of of 6,6'-(But-1-en-3-yne-1,4-diyl)bis(2-methoxynaphthalene) (**2nn**).

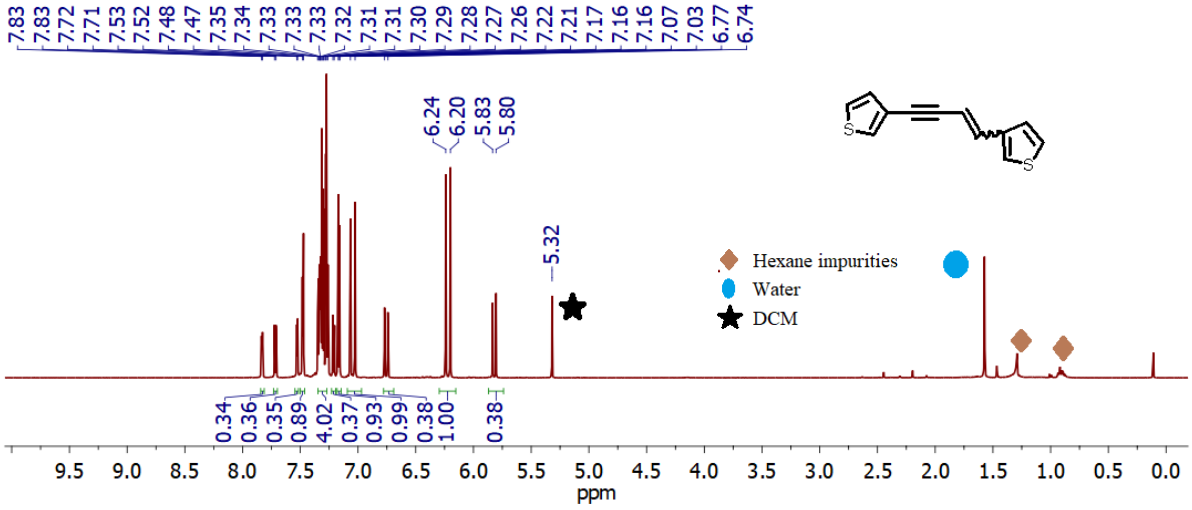


Figure S33. ^{1}H NMR ($CDCl_3$) spectrum of *E/Z* mixture of 2-(4-(thiophen-3-yl)but-1-en-3-yn-1-yl)thiophene (**2pp**). The minor peaks are assigned to the *Z*- isomer.

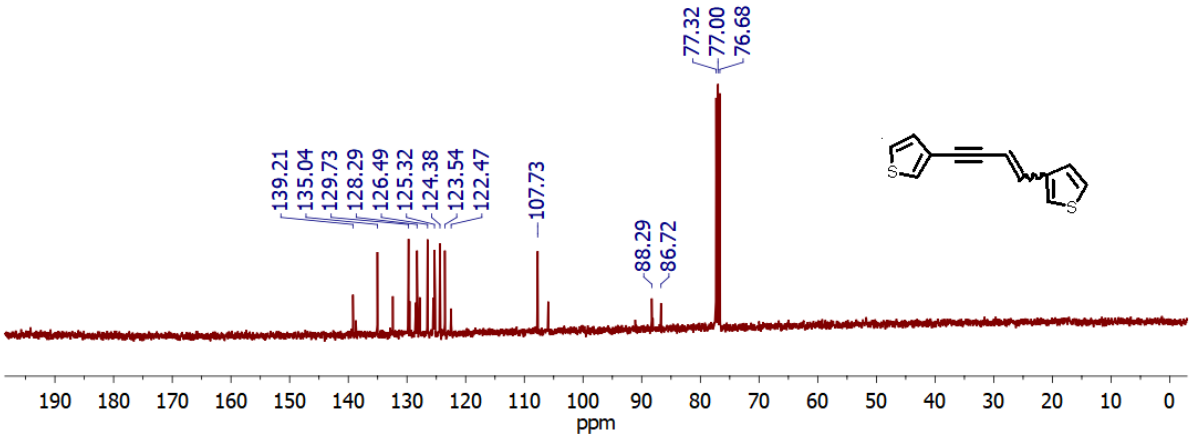


Figure S34 .^{13}C NMR ($CDCl_3$) spectrum of *E/Z* mixture of 2-(4-(thiophen-3-yl)but-1-en-3-yn-1-yl)thiophene (**2pp**). The minor peaks are assigned to the *Z*- isomer.

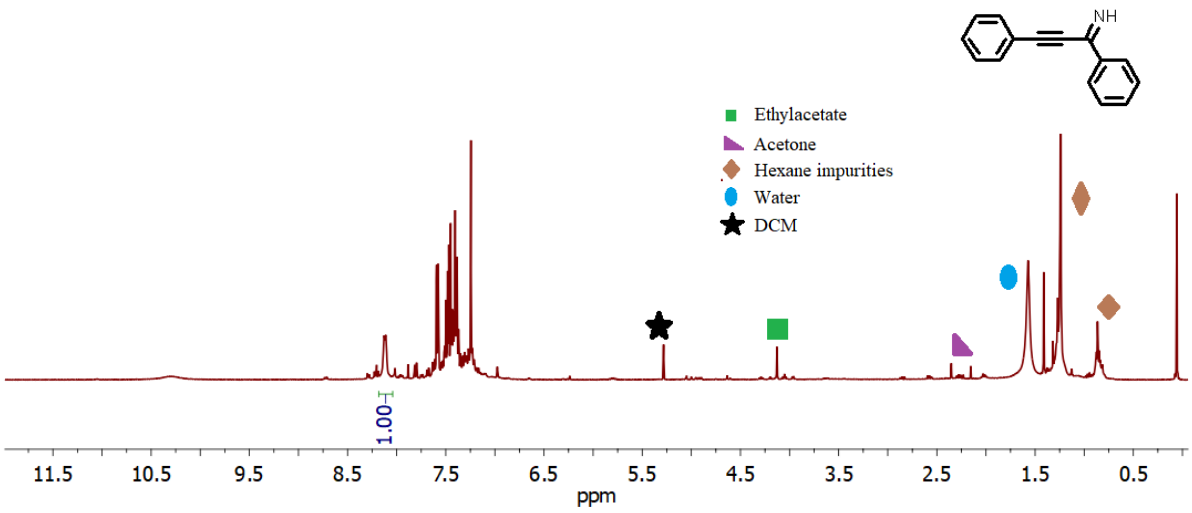


Figure S35. ^{1}H NMR ($CDCl_3$) spectrum of reaction mixture of 1,3-diphenylprop-2-yn-1-imine (**4aa**) which indicates full product formation.

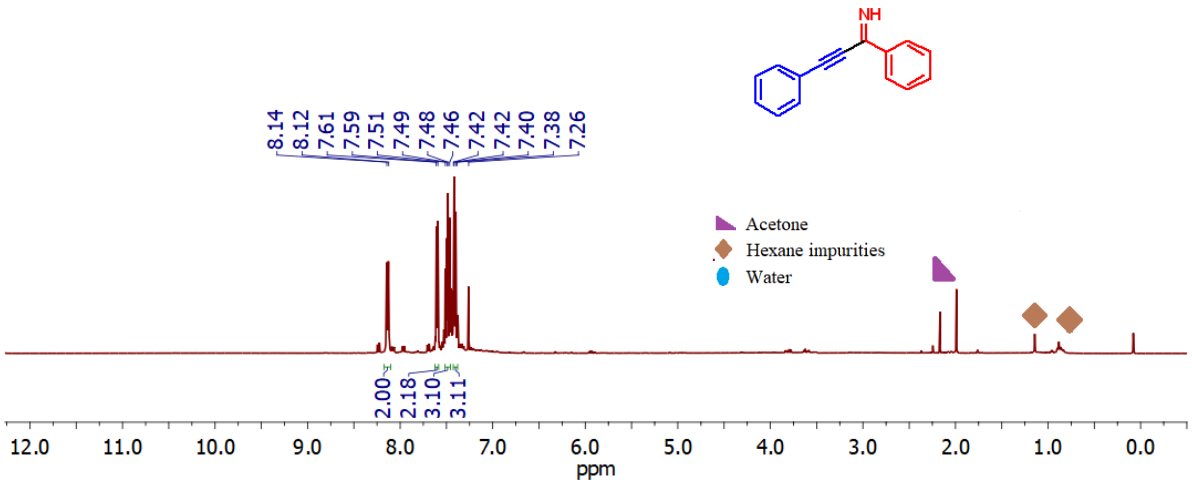


Figure S36. ^{1}H NMR ($CDCl_3$) spectrum of 1,3-diphenylprop-2-yn-1-imine (**4aa**).

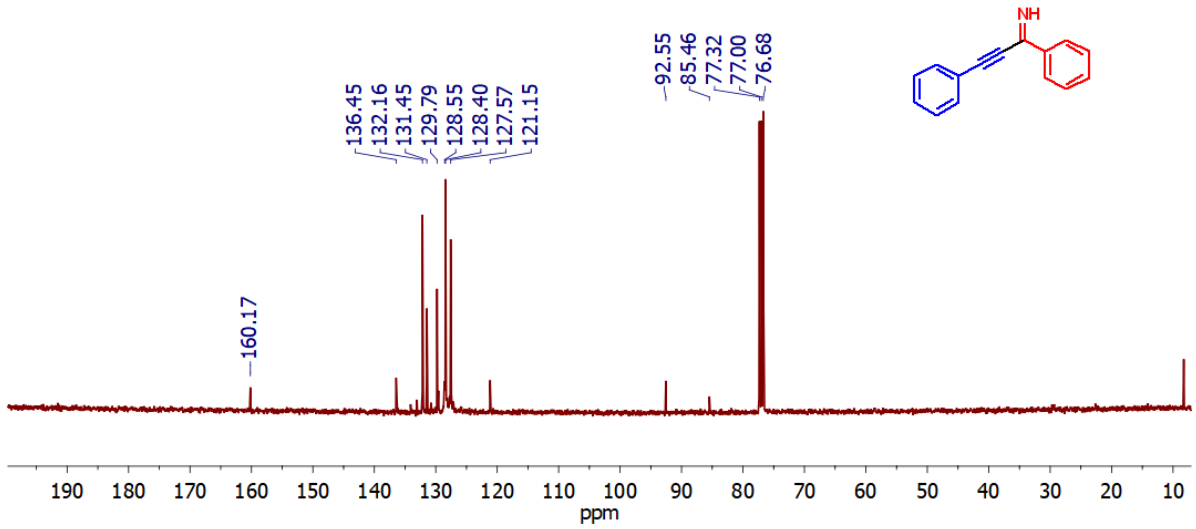


Figure S37. ^{13}C NMR ($CDCl_3$) spectrum of 1,3-diphenylprop-2-yn-1-imine (**4aa**).

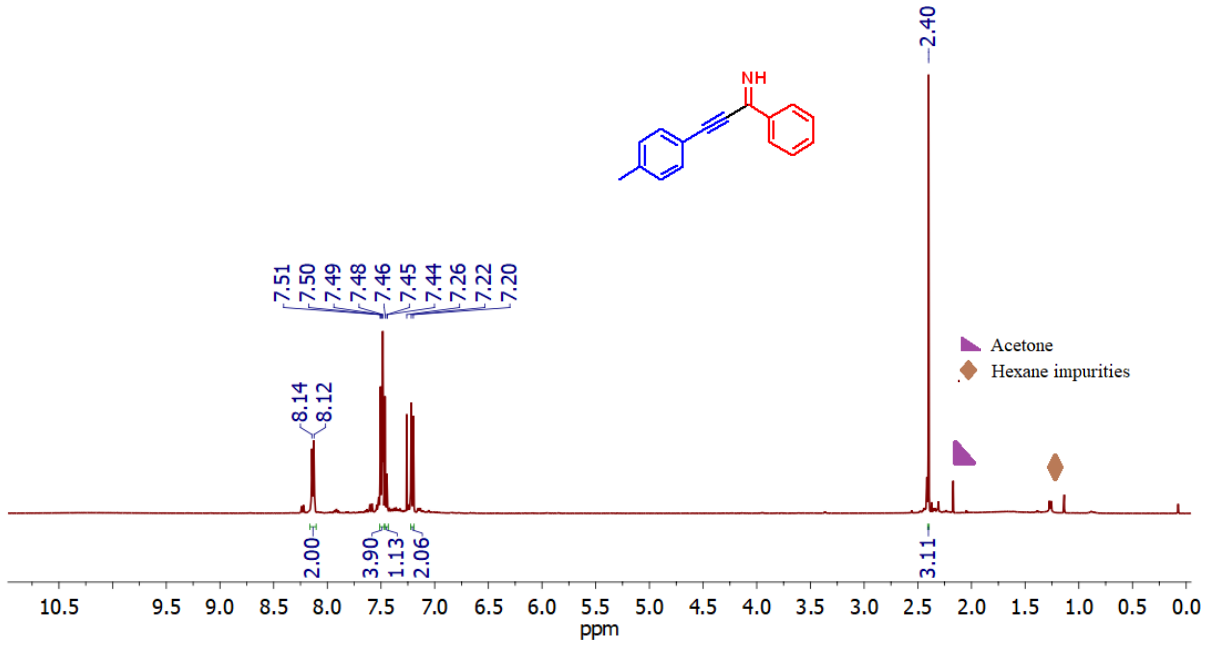


Figure S38. ^{1}H NMR ($CDCl_3$) spectrum of 1-phenyl-3-(p-tolyl)prop-2-yn-1-imine (**4ab**).

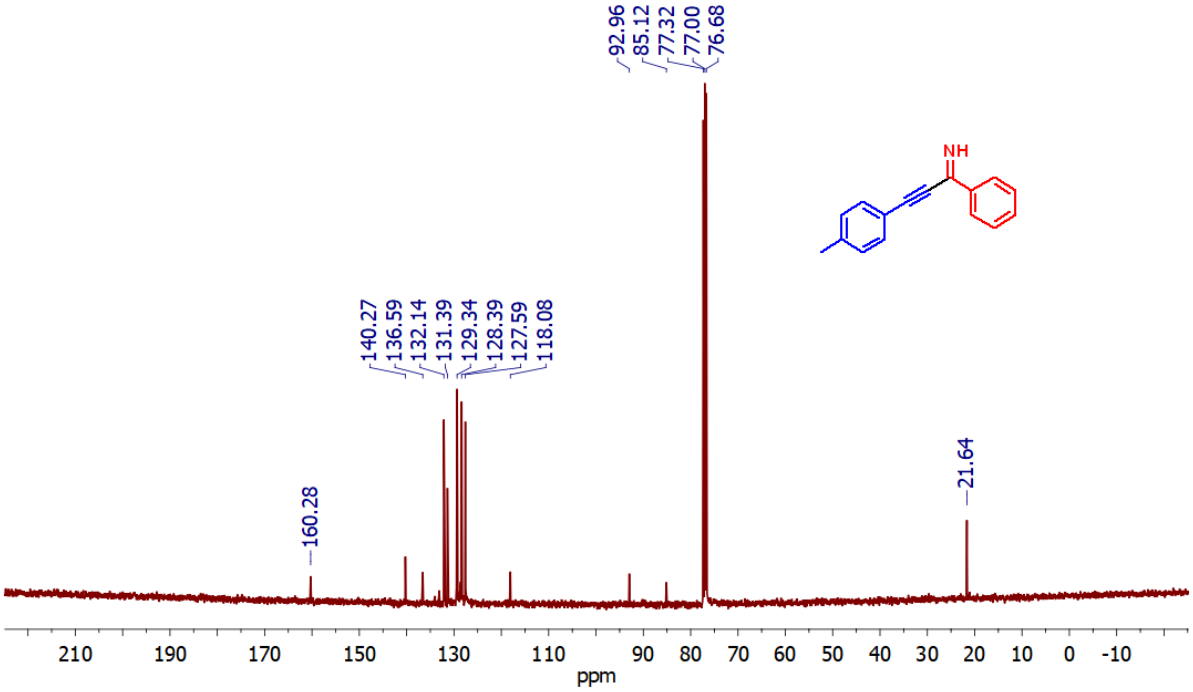


Figure S39. ^{13}C NMR ($CDCl_3$) spectrum of 1-phenyl-3-(p-tolyl)prop-2-yn-1-imine (**4ab**).

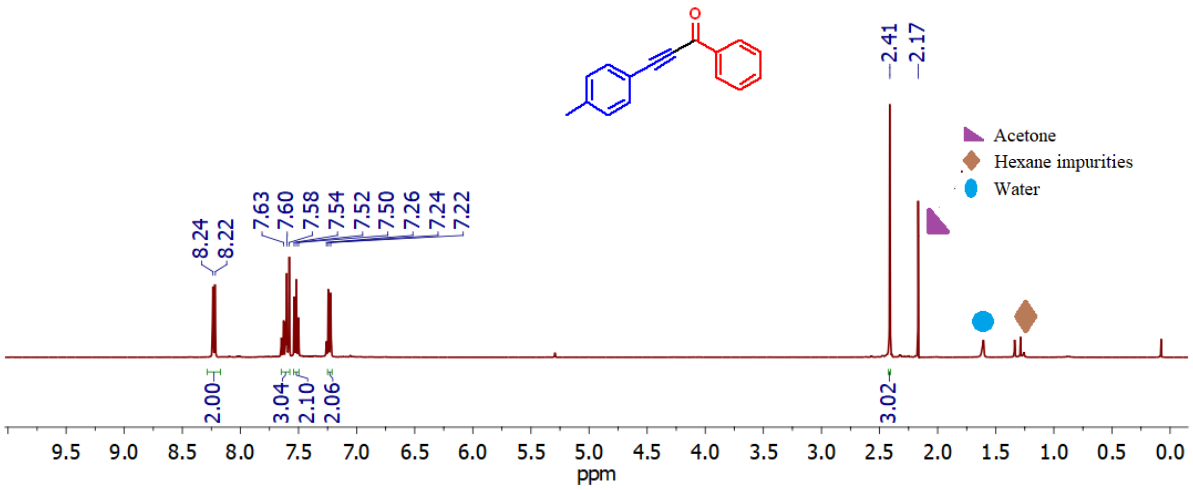


Figure S40. ^{1}H NMR ($CDCl_3$) spectrum of 1-phenyl-3-(p-tolyl)prop-2-yn-1-one (**4abO**).

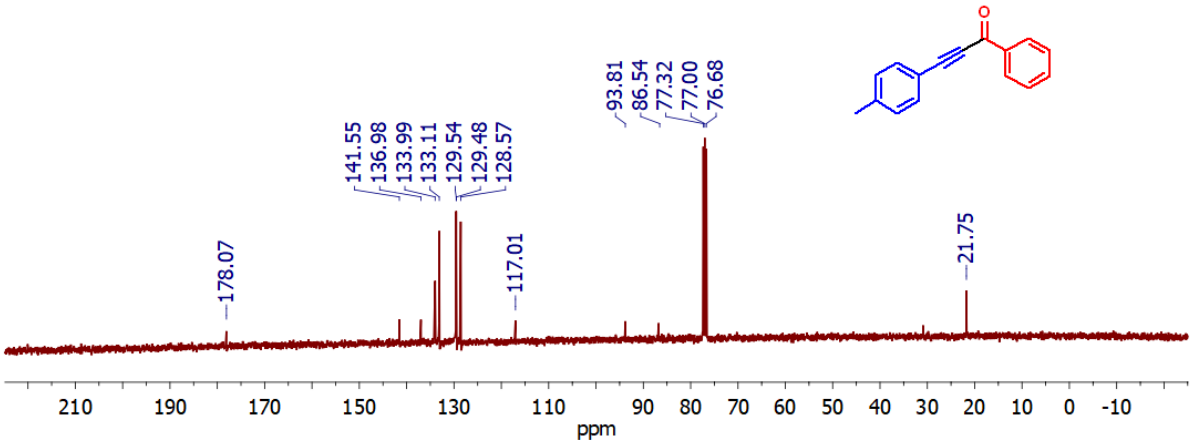


Figure S41. ^{13}C NMR ($CDCl_3$) spectrum of 1-phenyl-3-(p-tolyl)prop-2-yn-1-one (**4abO**).

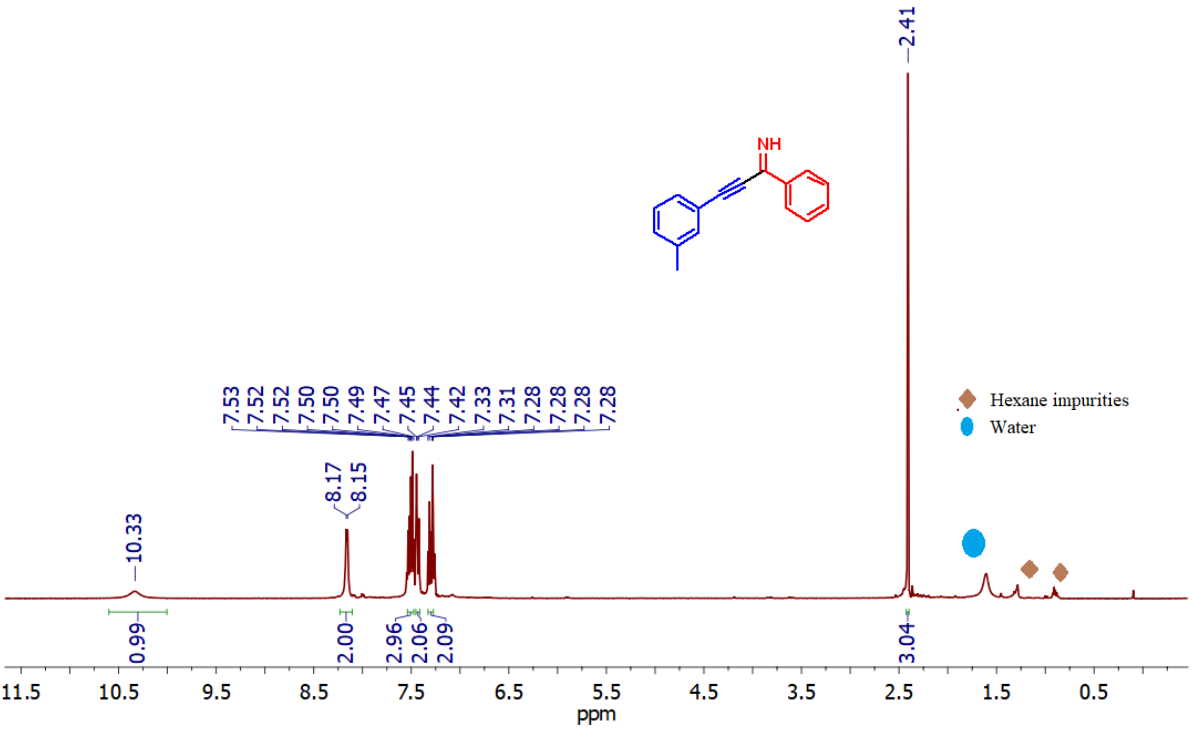


Figure S42. ^{1}H NMR ($CDCl_3$) spectrum of 1-phenyl-3-(m-tolyl)prop-2-yn-1-imine (**4ad**).

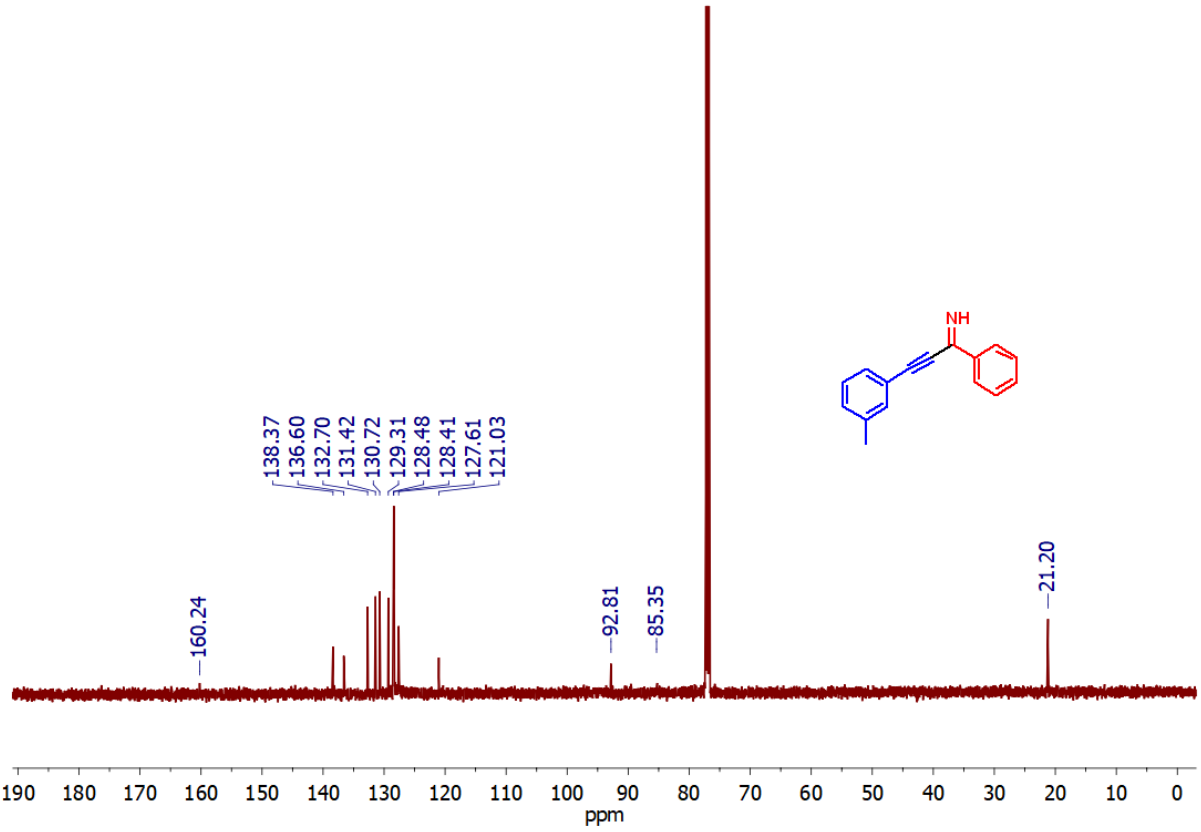


Figure S43. ^{13}C NMR ($CDCl_3$) spectrum of 1-phenyl-3-(m-tolyl)prop-2-yn-1-imine (**4ad**).

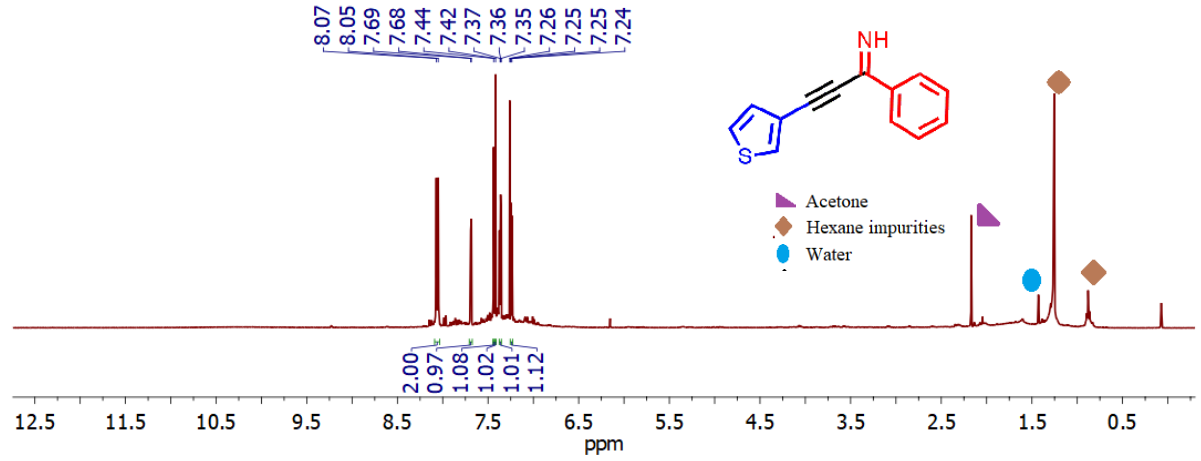


Figure S44. ^{1}H NMR ($CDCl_3$) spectrum of 1-phenyl-3-(thiophen-3-yl)prop-2-yn-1-imine (**4ap**).

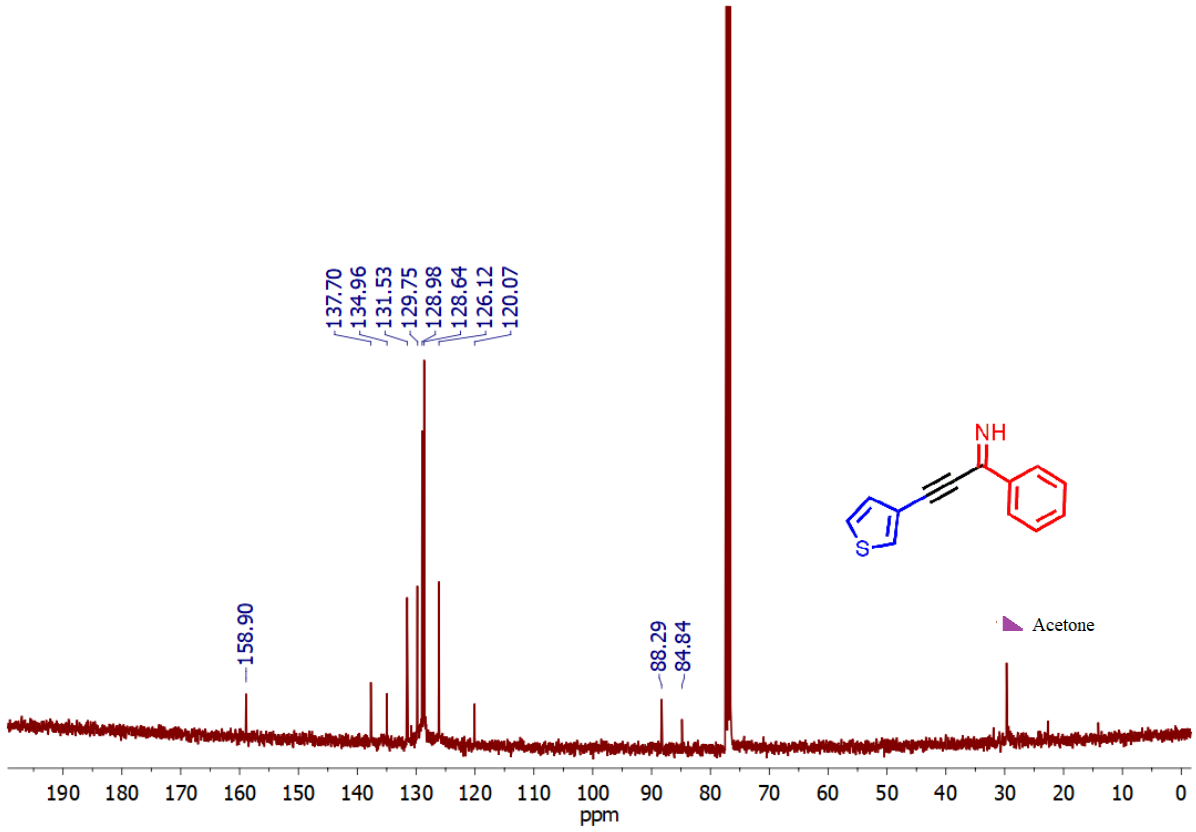


Figure S45. ^{13}C NMR ($CDCl_3$) spectrum of 1-phenyl-3-(thiophen-3-yl)prop-2-yn-1-imine (**4ap**).

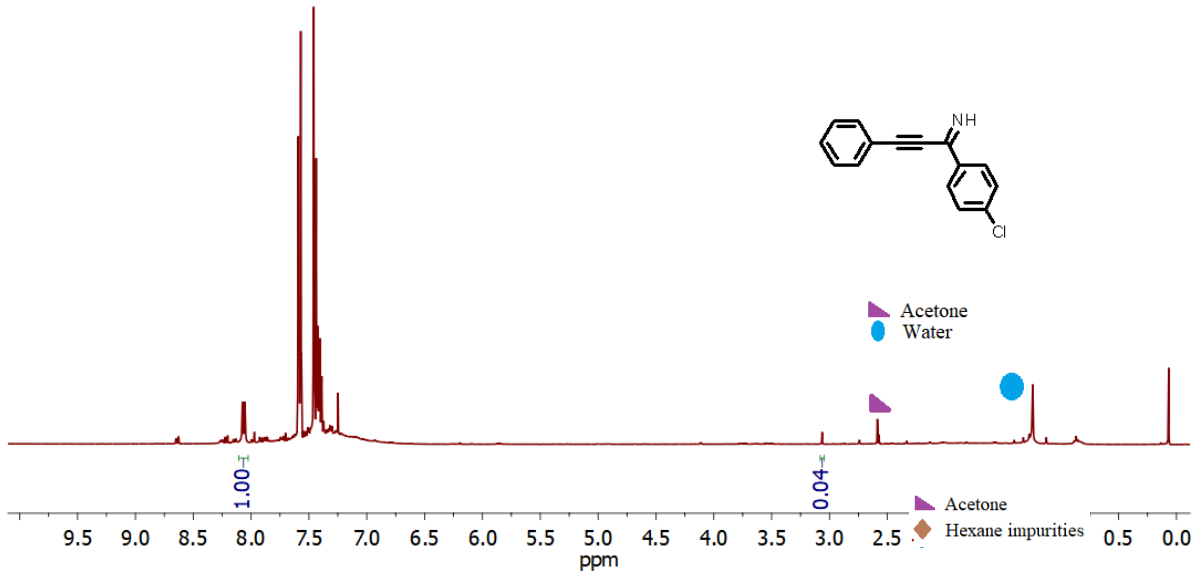


Figure S46. ^{1}H NMR ($CDCl_3$) spectrum of reaction mixture of 1-(4-chlorophenyl)-3-phenylprop-2-yn-1-imine (**4qa**).

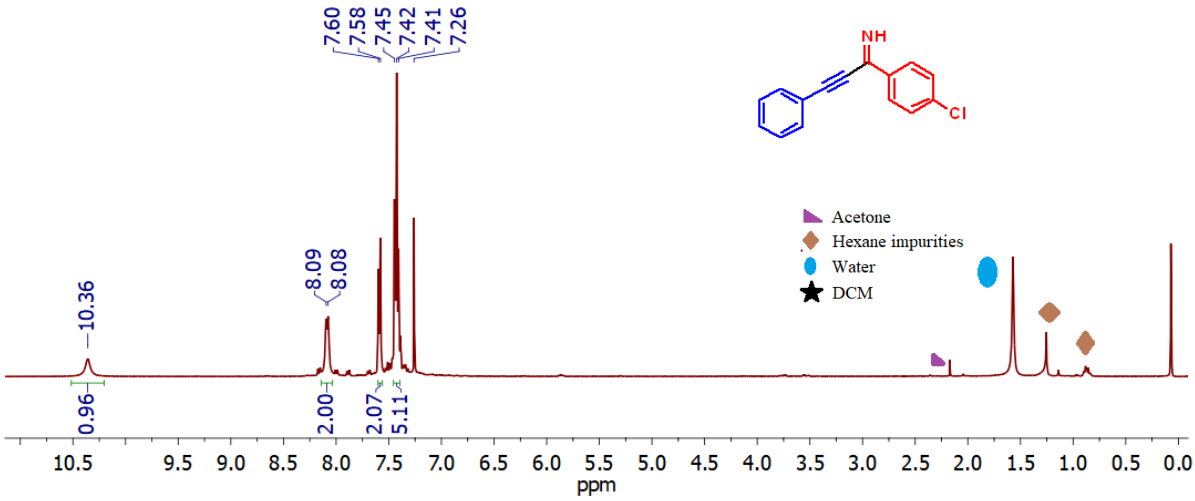


Figure S47. ^{1}H NMR ($CDCl_3$) spectrum of 1-(4-chlorophenyl)-3-phenylprop-2-yn-1-imine (**4qa**).

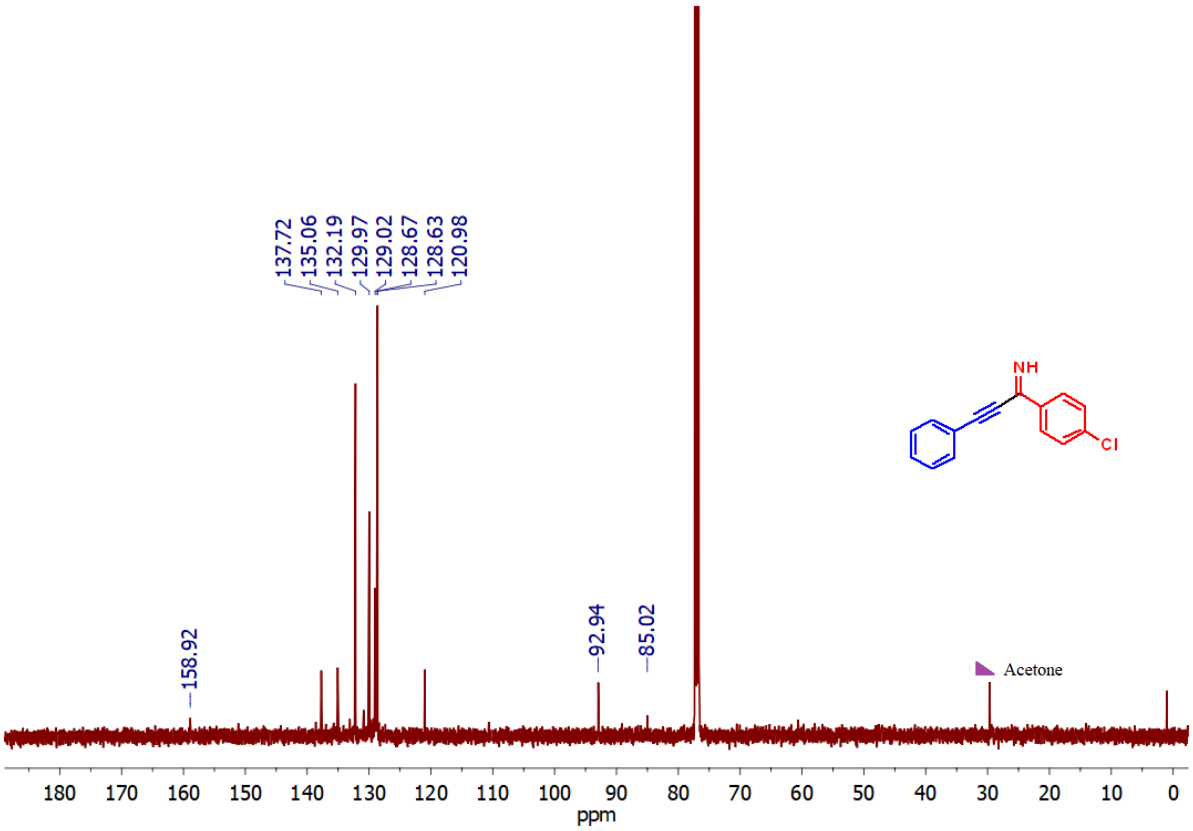


Figure S48. ^{13}C NMR ($CDCl_3$) spectrum of 1-(4-chlorophenyl)-3-phenylprop-2-yn-1-imine (**4qa**).

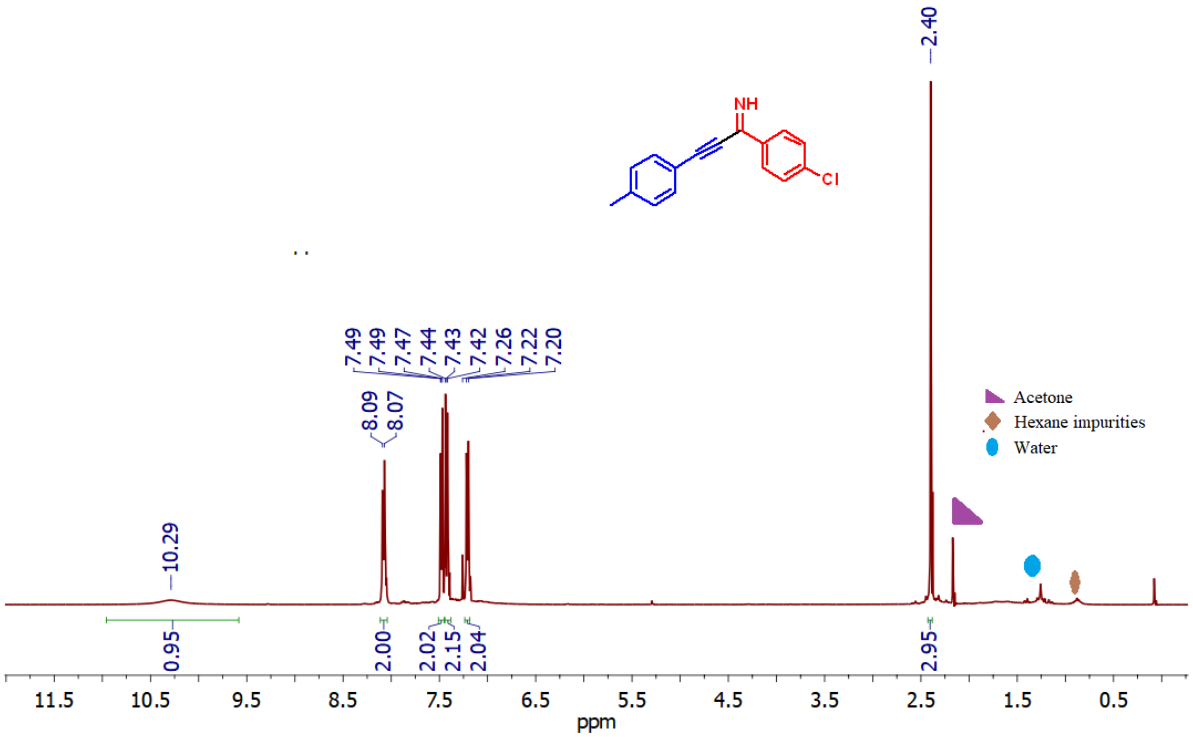


Figure S49. ^{1}H NMR ($CDCl_3$) spectrum of 1-(4-chlorophenyl)-3-(p-tolyl)prop-2-yn-1-imine (**4qb**).

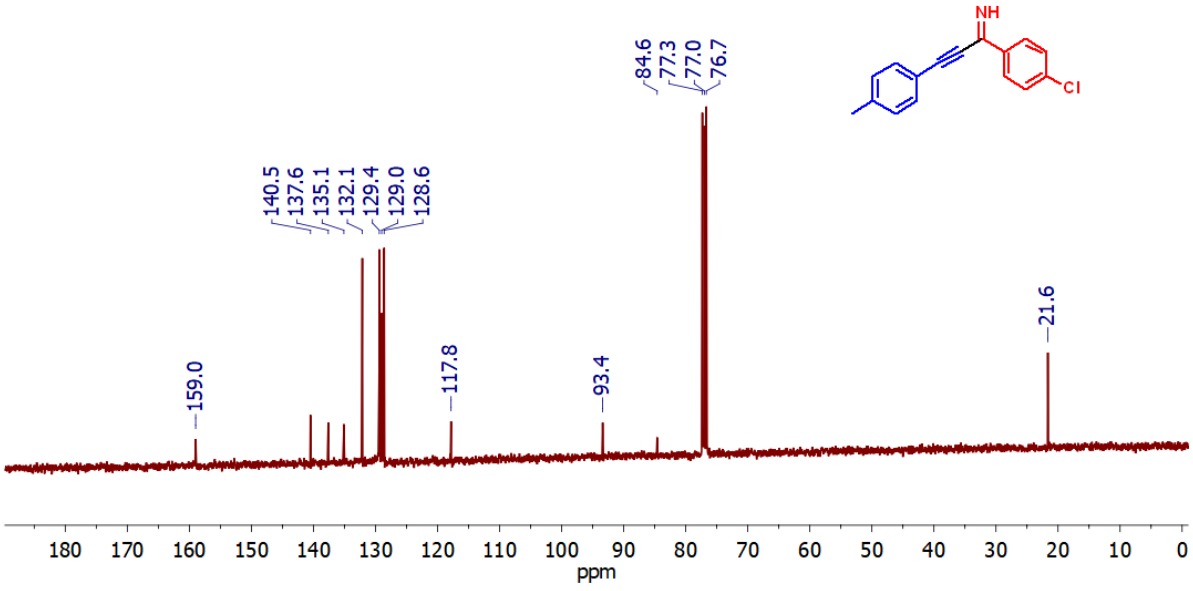


Figure S50. ^{13}C NMR ($CDCl_3$) spectrum of 1-(4-chlorophenyl)-3-(p-tolyl)prop-2-yn-1-imine (**4qb**).

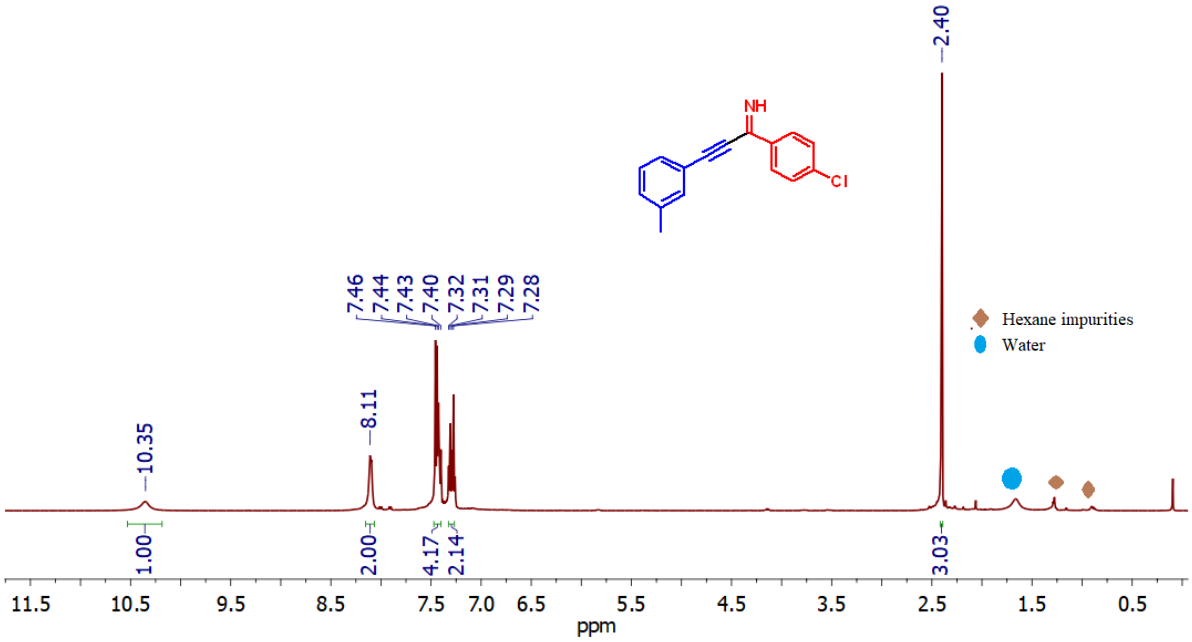


Figure S51. ^{1}H NMR ($CDCl_3$) spectrum of 1-(4-chlorophenyl)-3-(m-tolyl)prop-2-yn-1-imine (**4qd**).

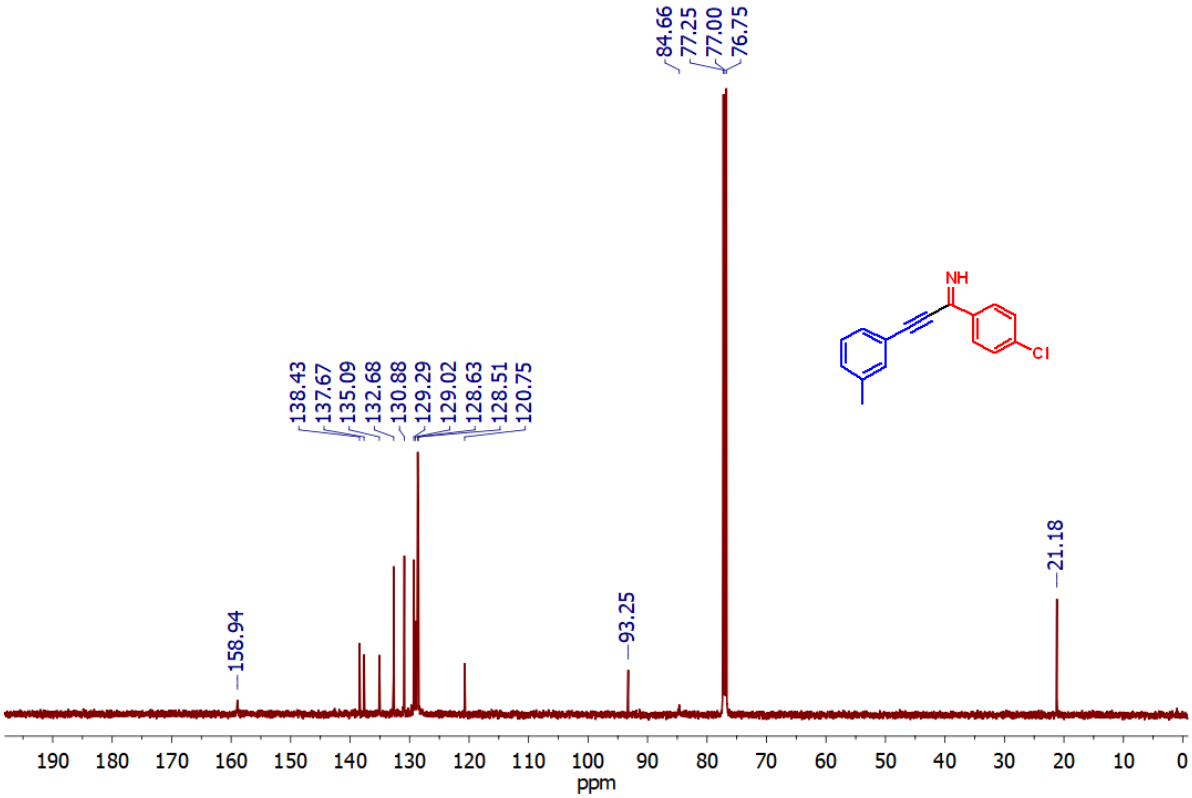


Figure S52. ^{13}C NMR ($CDCl_3$) spectrum of 1-(4-chlorophenyl)-3-(m-tolyl)prop-2-yn-1-imine (**4qd**).

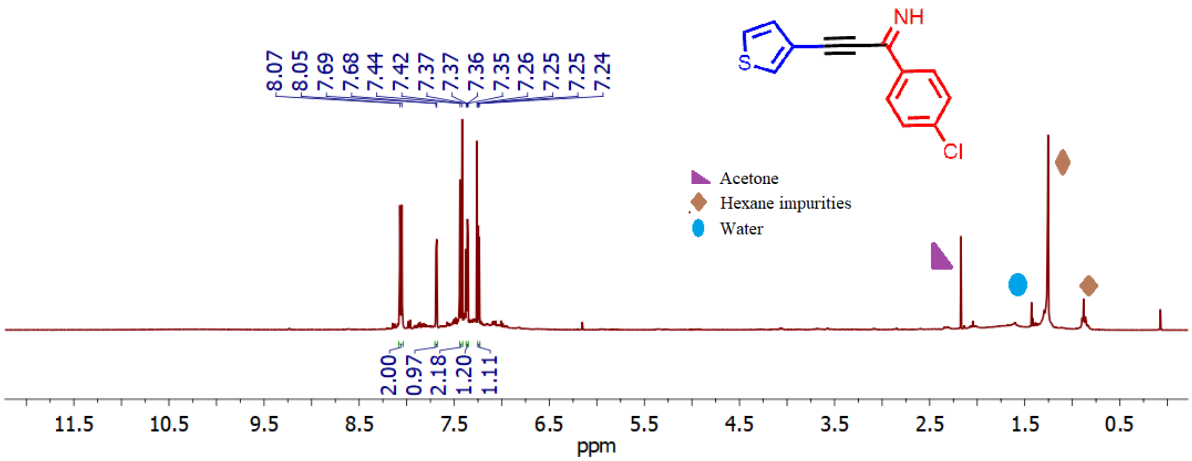


Figure S53. ^{1}H NMR ($CDCl_3$) spectrum of 1-(4-chlorophenyl)-3-(thiophen-3-yl)prop-2-yn-1-imine (**4qp**).

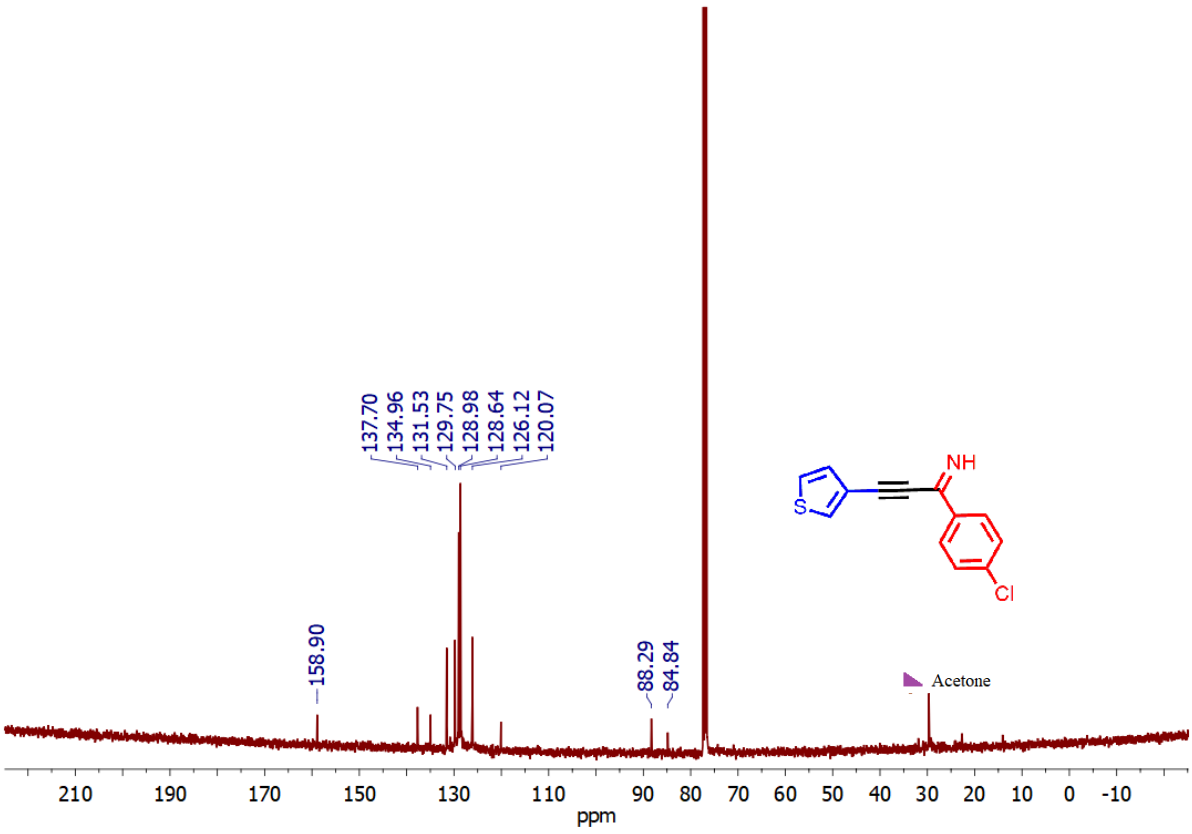


Figure S54. ^{13}C NMR ($CDCl_3$) spectrum of 1-(4-chlorophenyl)-3-(thiophen-3-yl)prop-2-yn-1-imine (**4qp**).

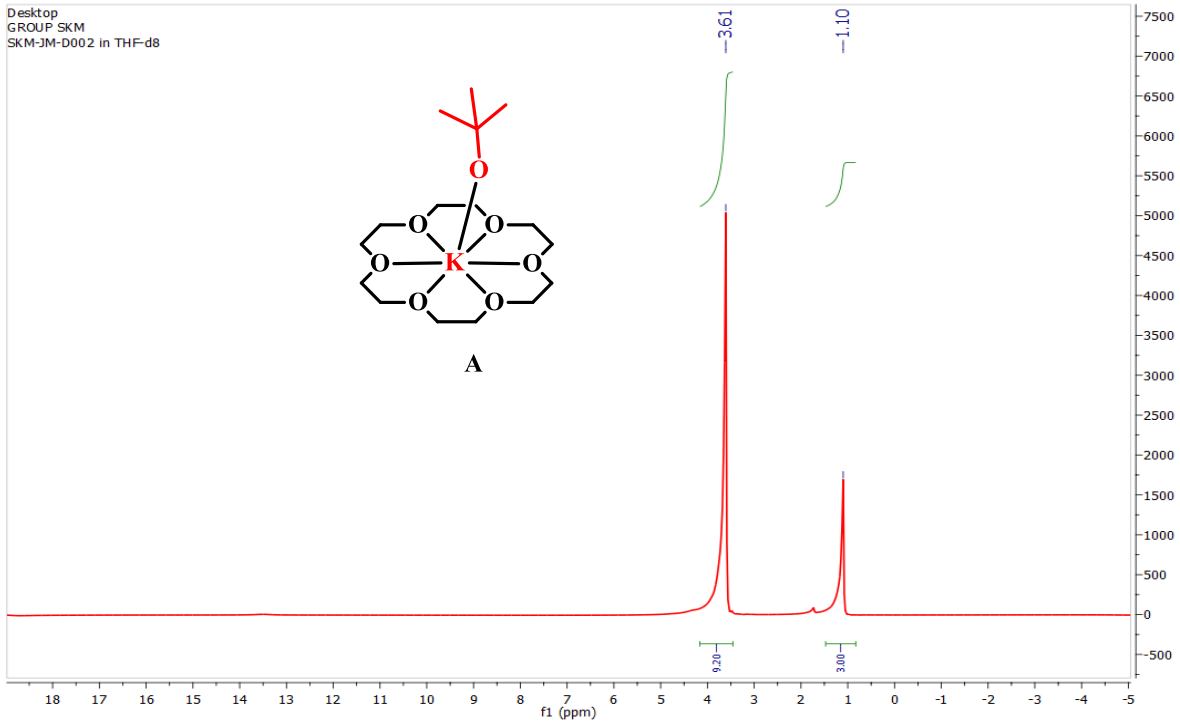


Figure S55. ^{1}H NMR (THF-d_8) spectrum of K-[18-Crown-6]-O^{t}Bu (**A**).

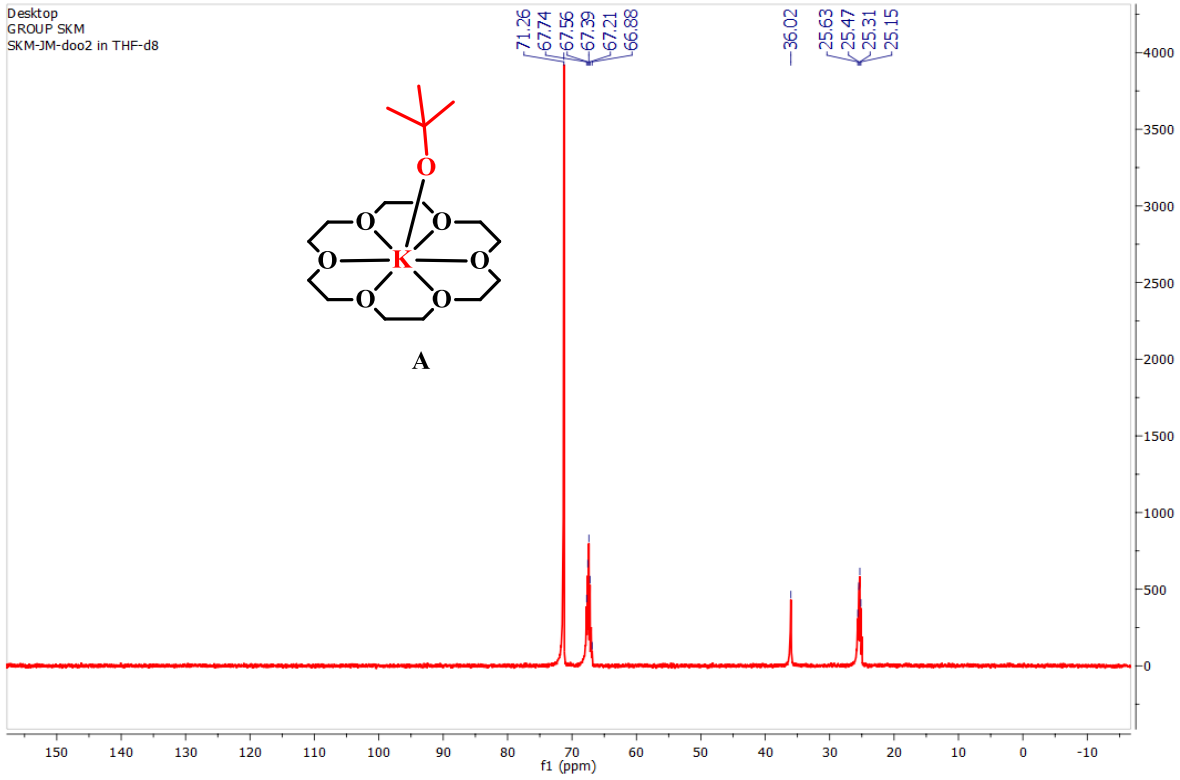


Figure S56. ^{13}C NMR (THF-d_8) spectrum of K-[18-Crown-6]-O^{t}Bu (**A**).

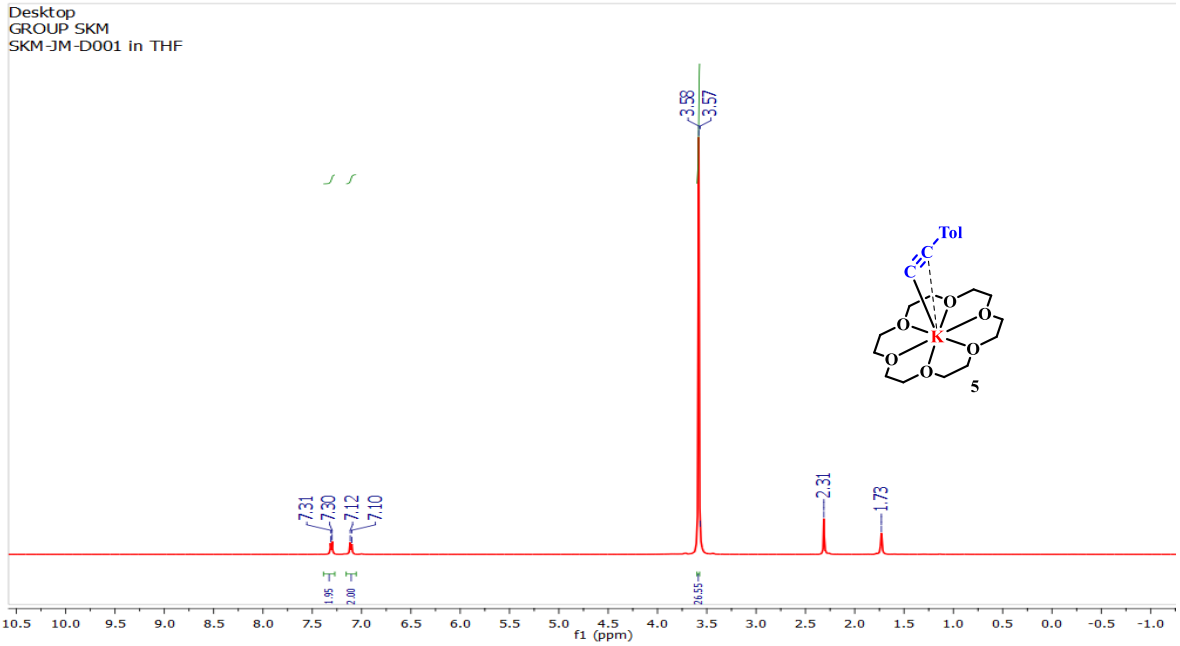


Figure S57. ^{1}H NMR (THF-d_8) spectrum of intermediate **5**.

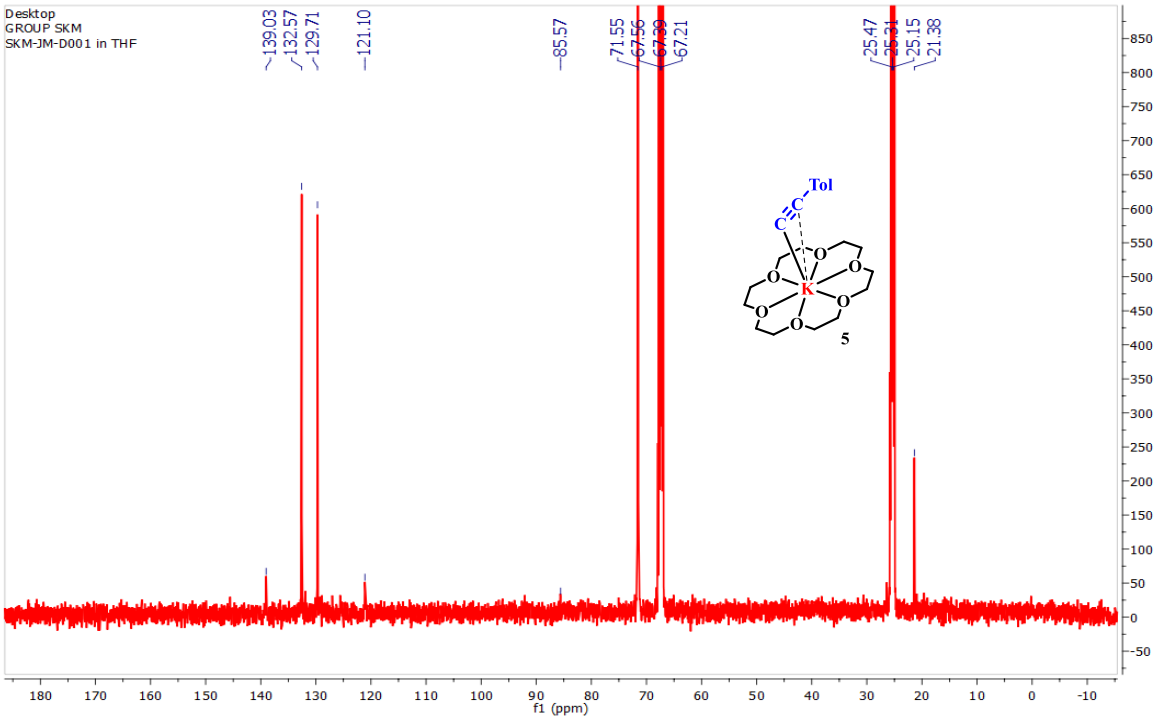


Figure S58. ^{13}C NMR (THF-d_8) spectrum of intermediate **5**.

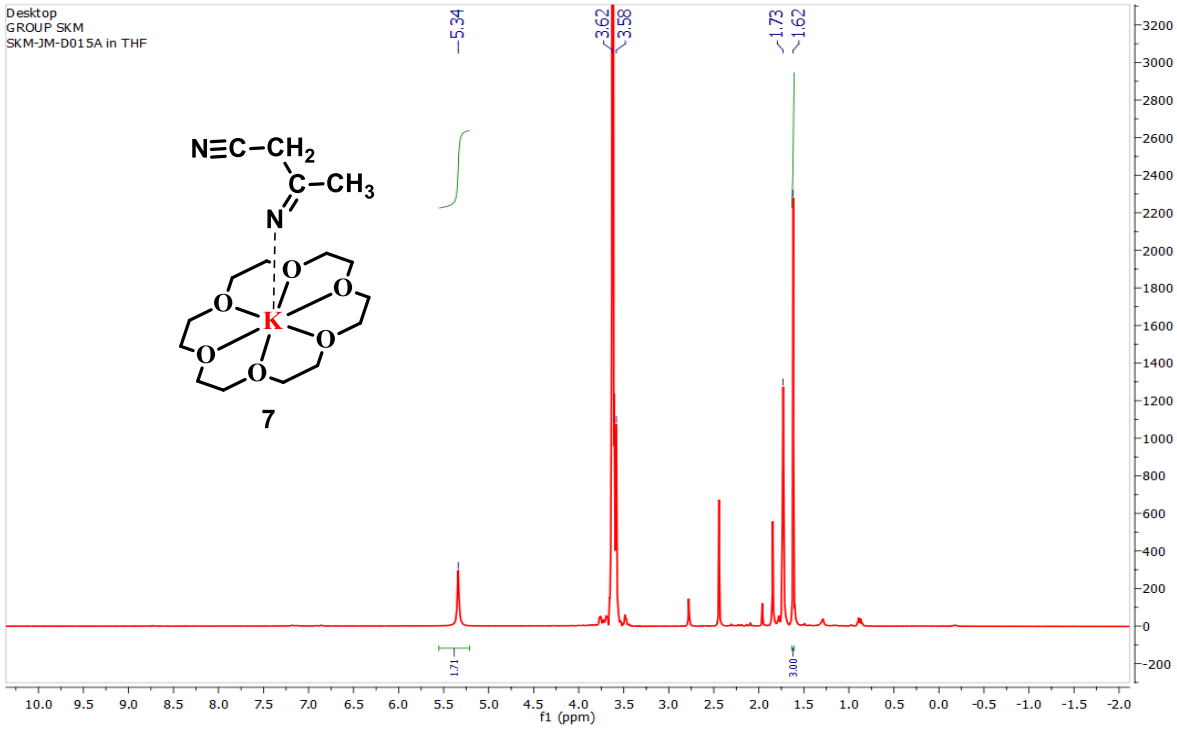


Figure S59. ^{1}H NMR (THF-d_8) spectrum of complex **7**

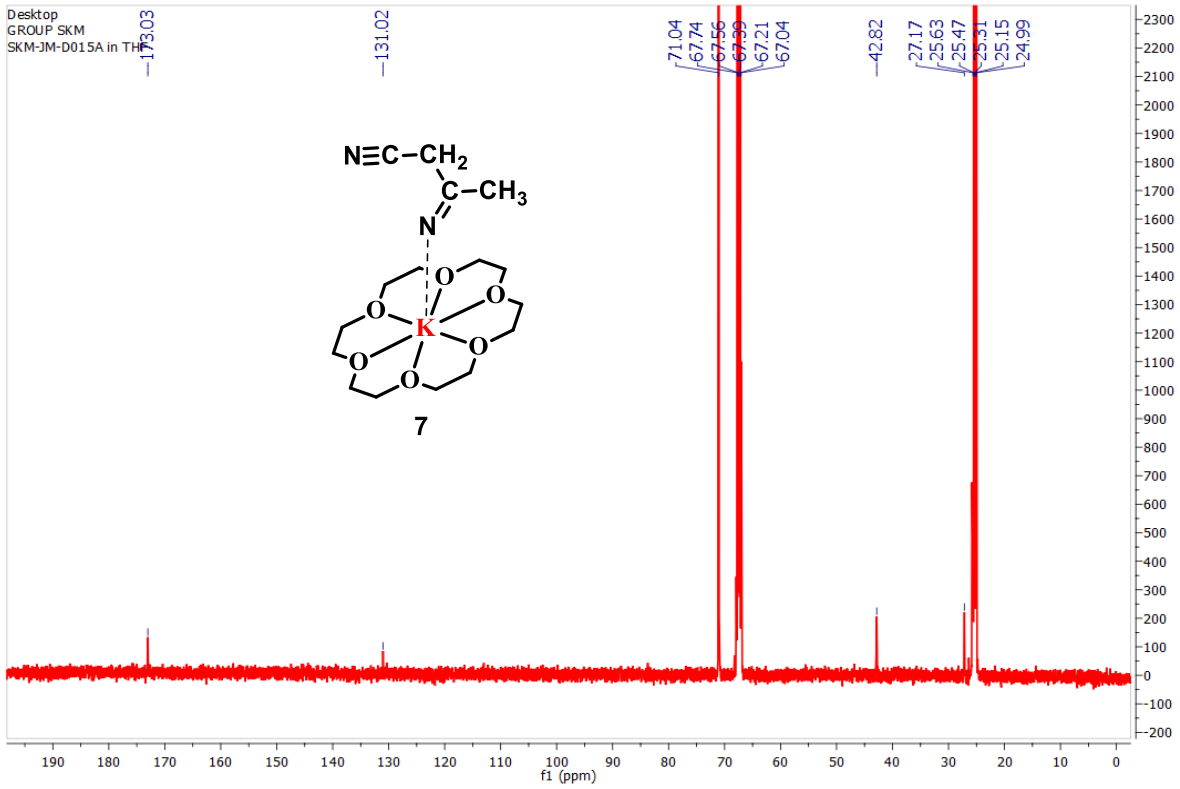


Figure S60. ^{13}C NMR (THF-d_8) spectrum of complex **7**.

IV. Mass spectra of the products

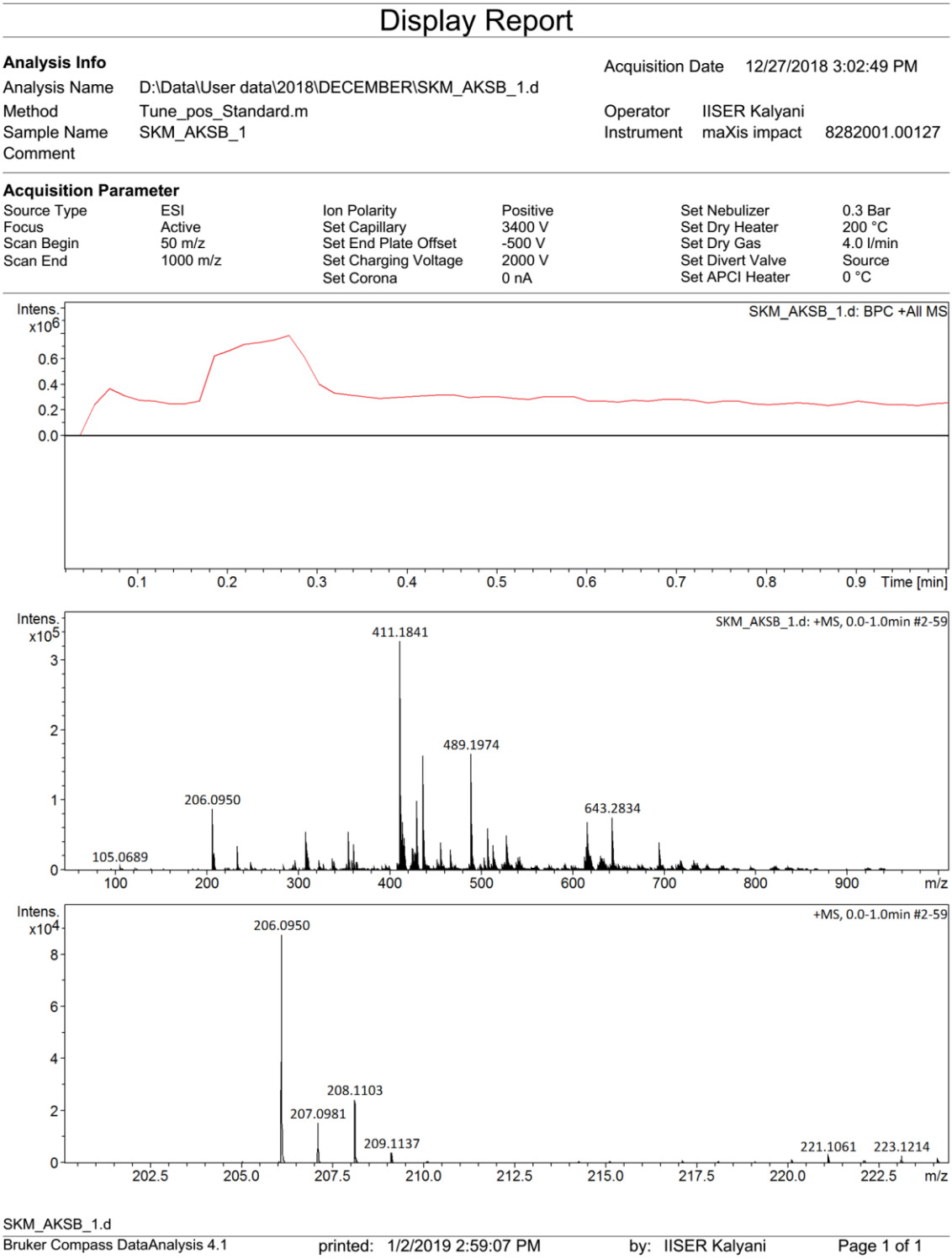


Figure S61. HRMS of 1,3-diphenylprop-2-yn-1-imine (**4aa**).

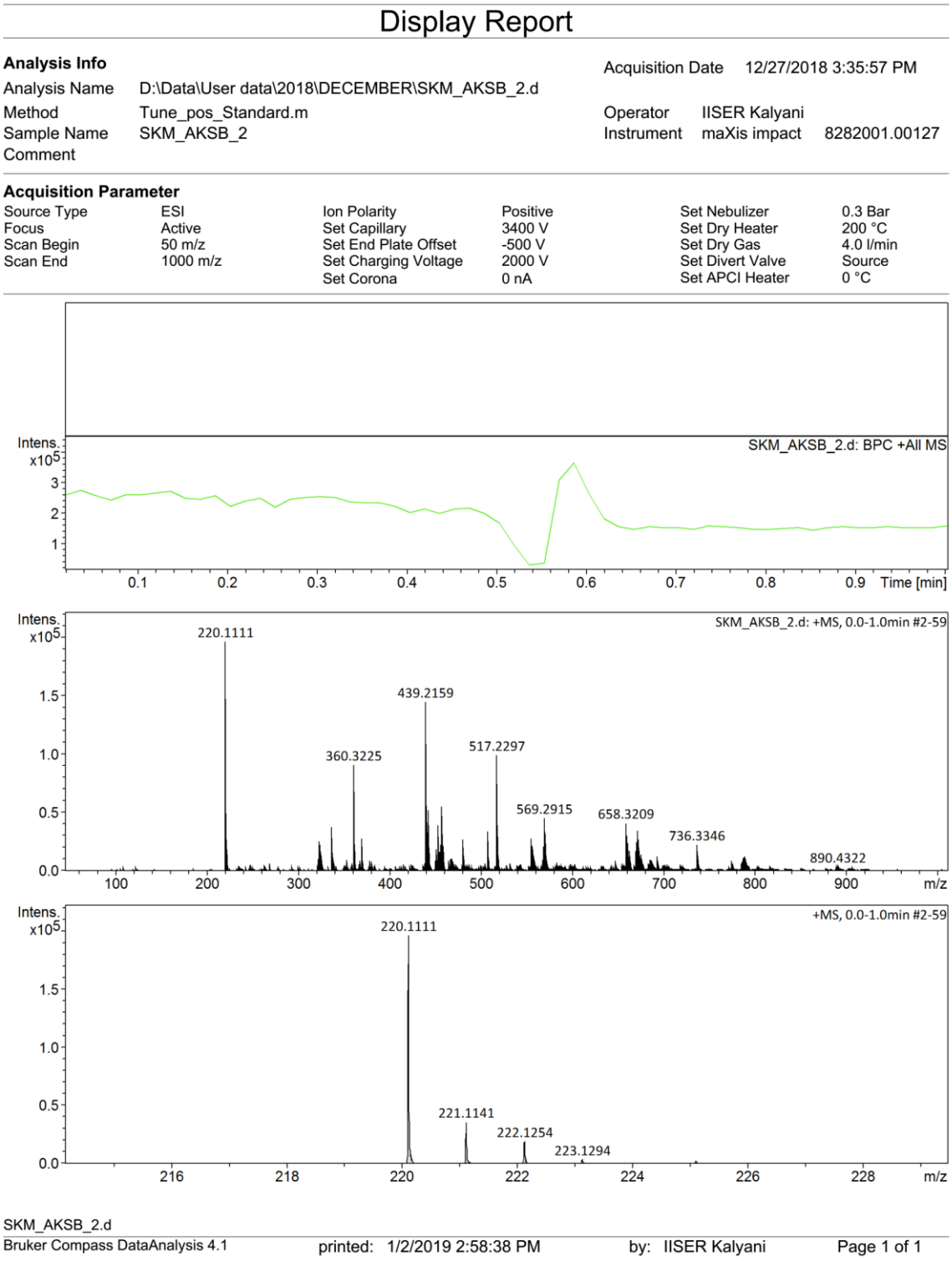


Figure S62. HRMS of 1-phenyl-3-(p-tolyl)prop-2-yn-1-imine (**4ab**).

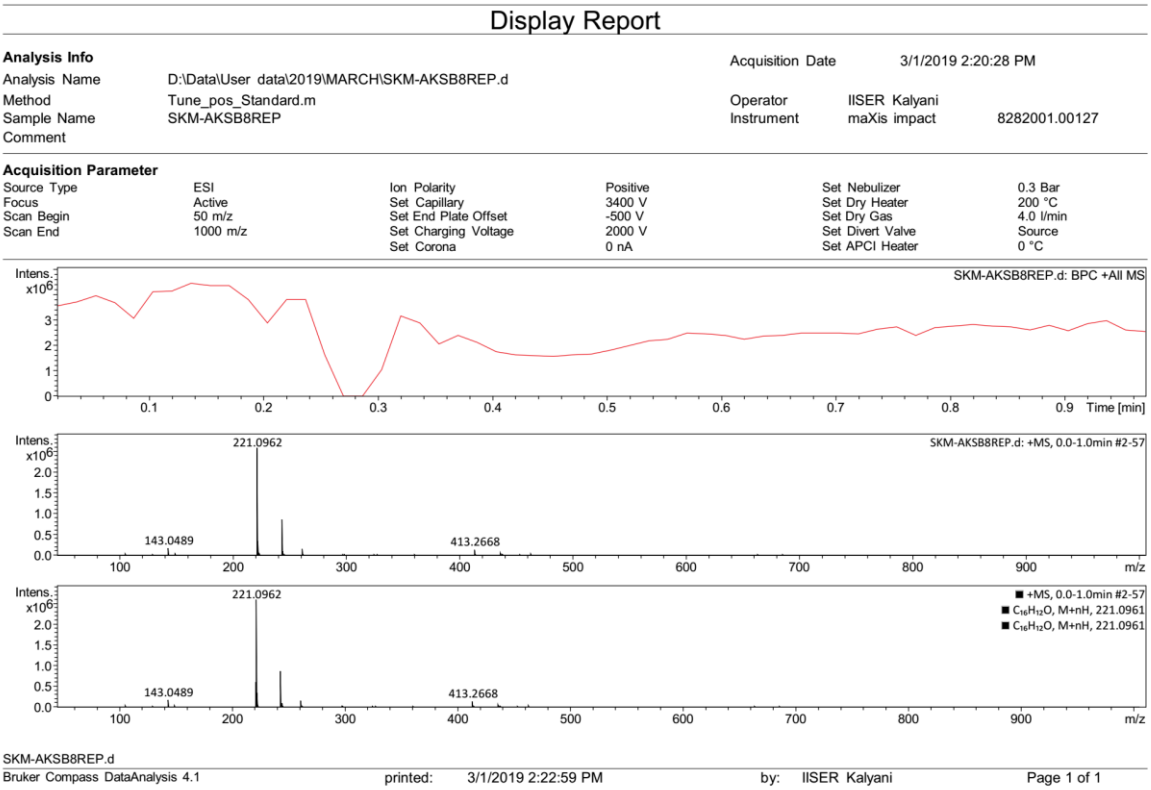


Figure S63. HRMS of 1-phenyl-3-(p-tolyl)prop-2-yn-1-one (**4abO**).

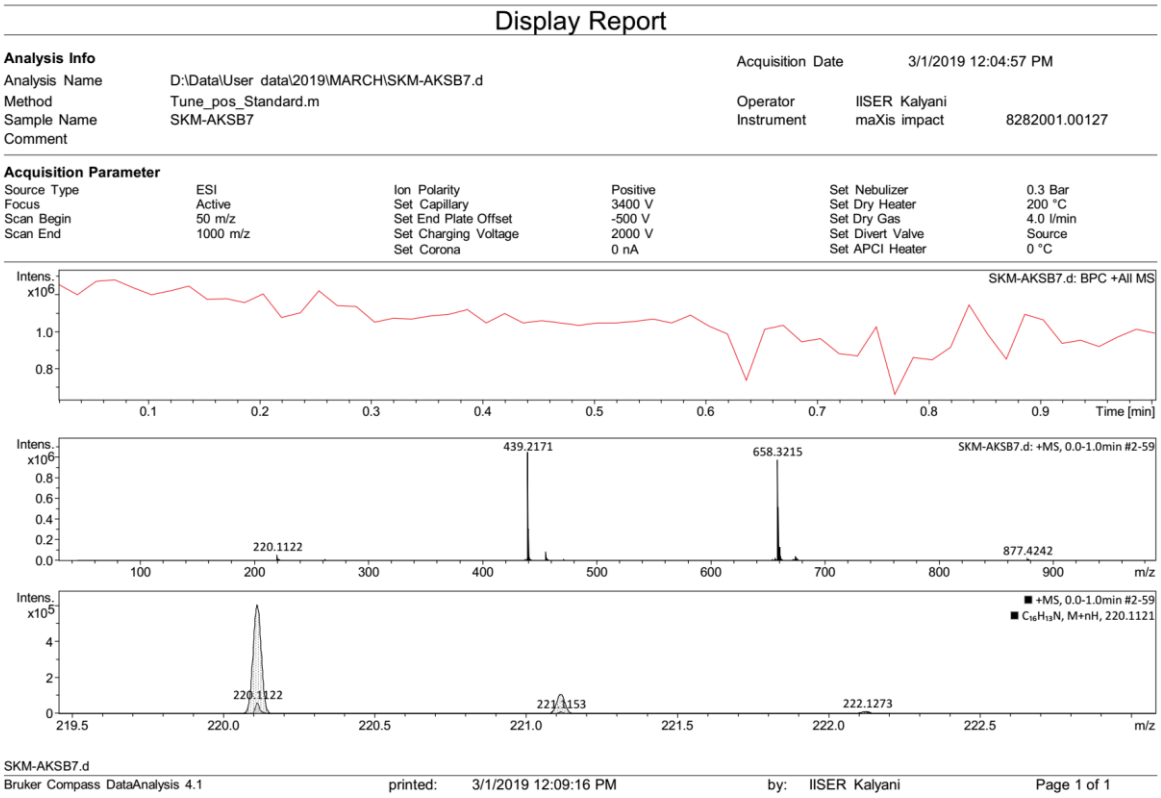


Figure S64. HRMS of 1-phenyl-3-(m-tolyl)prop-2-yn-1-imine (**4ad**).

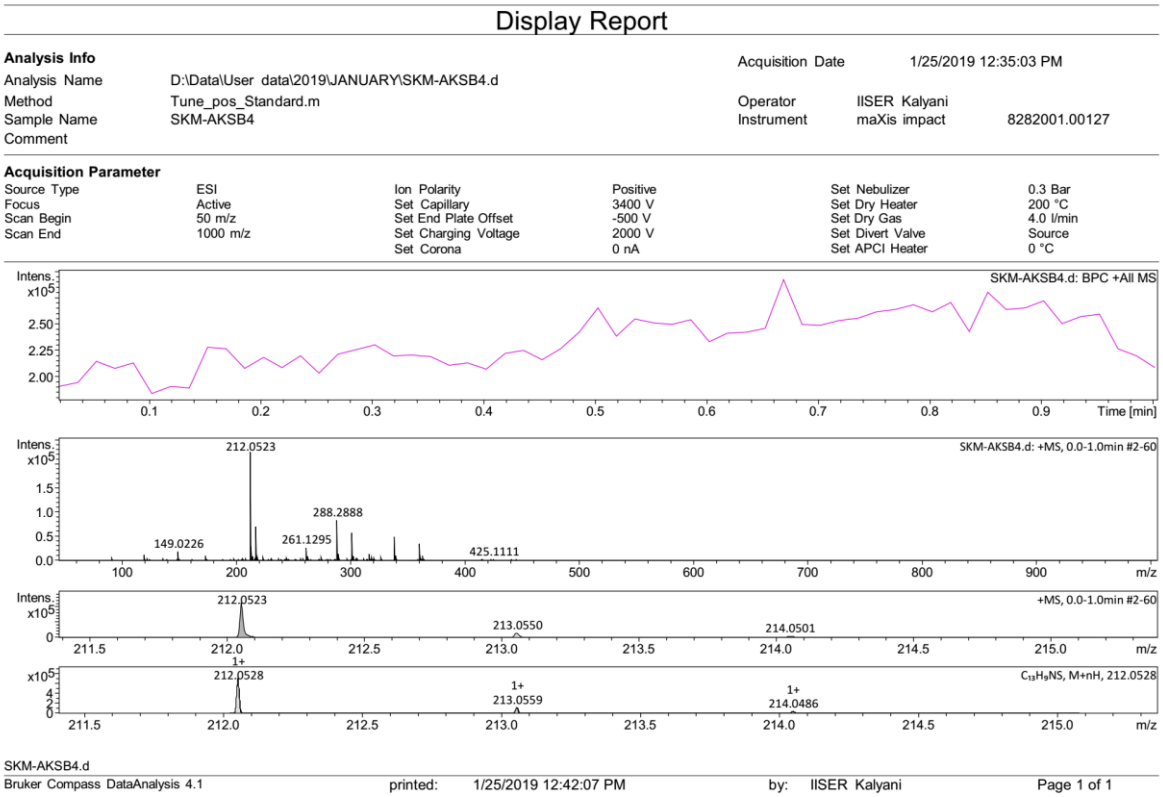


Figure S65. HRMS of 1-phenyl-3-(thiophen-3-yl)prop-2-yn-1-imine (**4ap**).

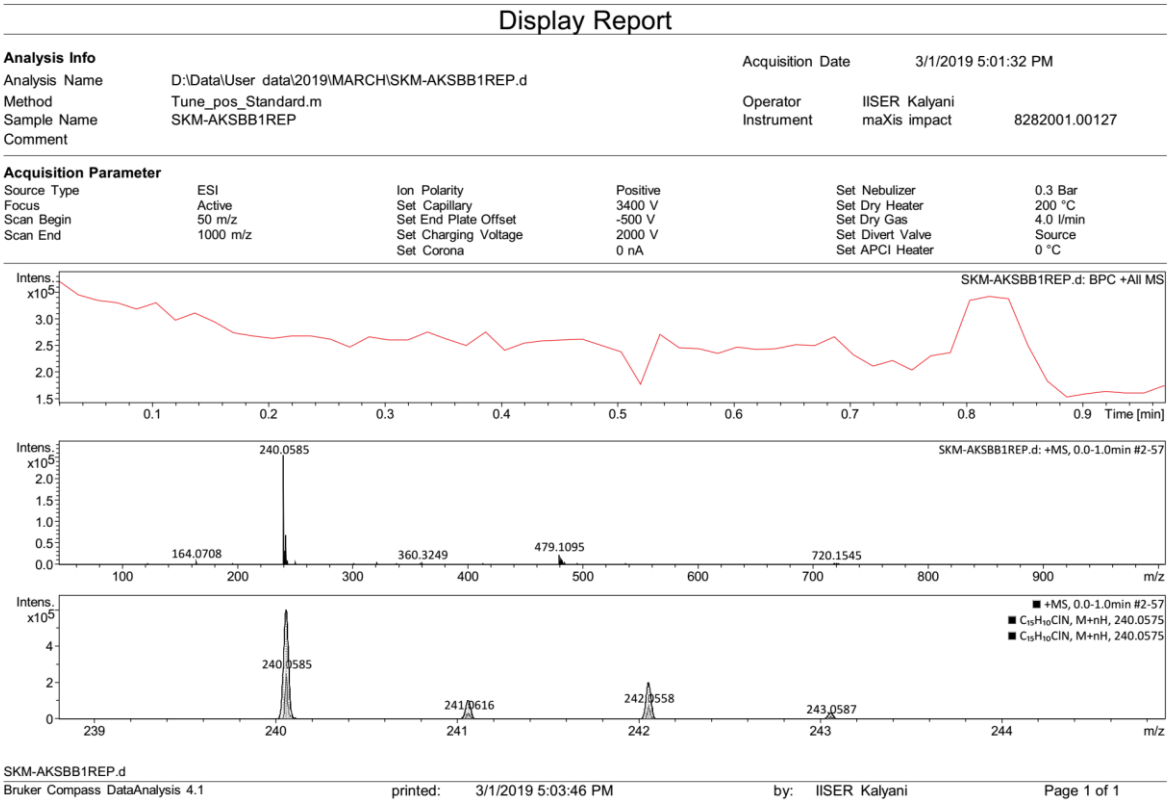


Figure S66. HRMS of 1-(4-chlorophenyl)-3-phenylprop-2-yn-1-imine (**4qa**).

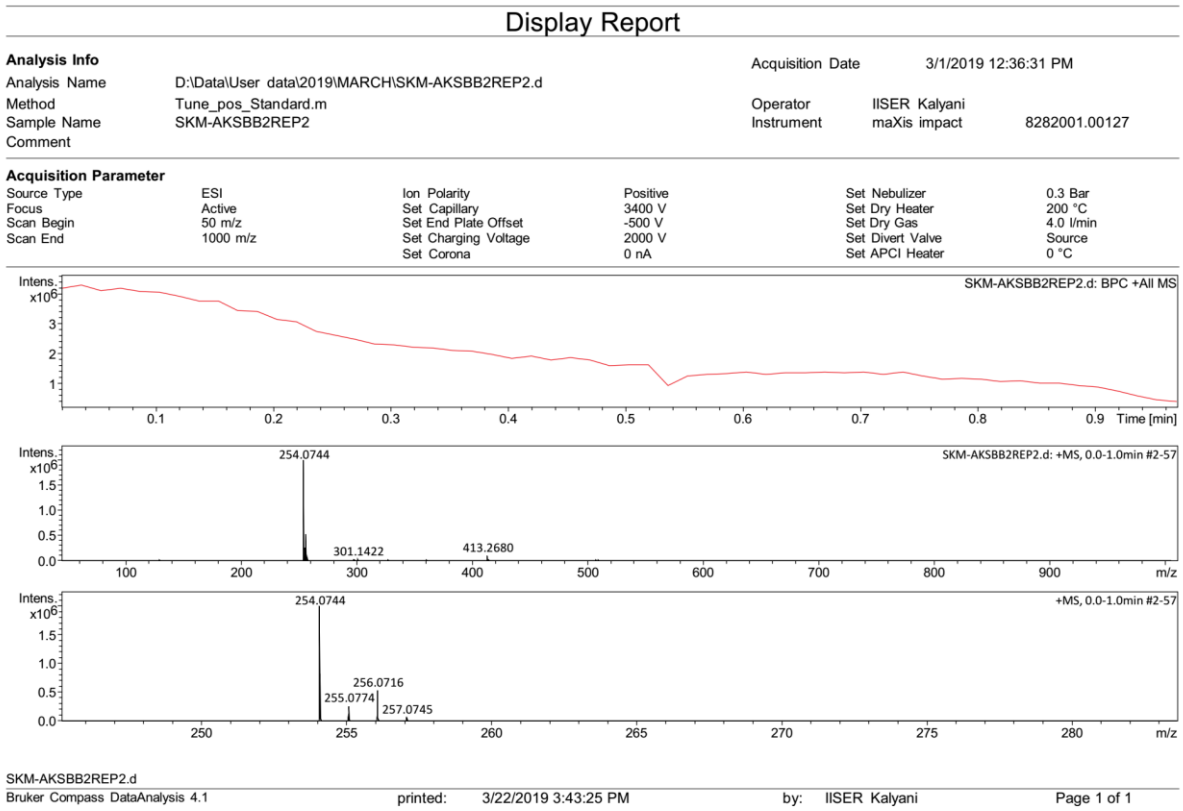


Figure S67. HRMS of 1-(4-chlorophenyl)-3-(p-tolyl)prop-2-yn-1-imine (**4qb**).

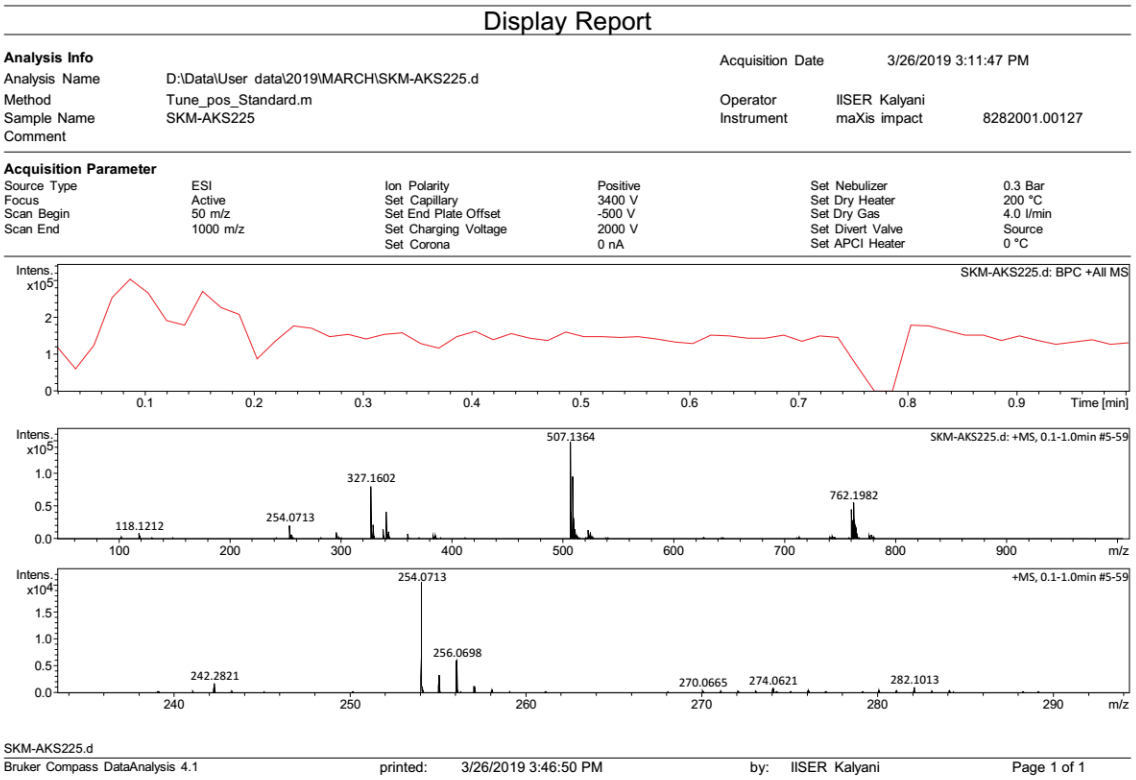


Figure S68. HRMS of 1-(4-chlorophenyl)-3-(m-tolyl)prop-2-yn-1-imine (**4qd**).

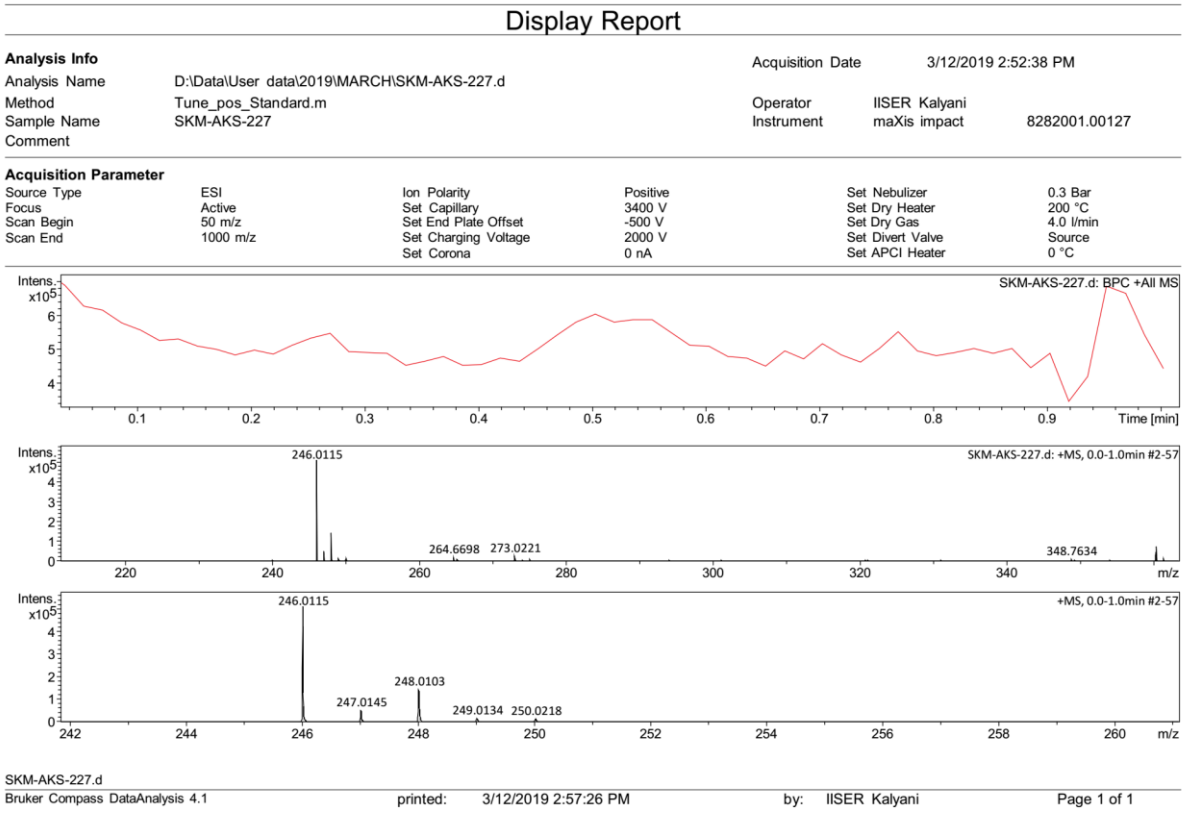


Figure S69. HRMS of 1-(4-chlorophenyl)-3-(thiophen-3-yl)prop-2-yn-1-imine (**4qp**).

V. Details of crystal measurement:

Suitable single crystal was selected and an intensity data were collected on a SuperNova, Dual, Cu at zero, Eos diffractometer. Using Olex2[9] the structure was solved with the Superflip[10] structure solution program using Charge Flipping and refined with the ShelXL[11] refinement package using Least Squares minimization.

X-ray structure and data of intermediate 5:

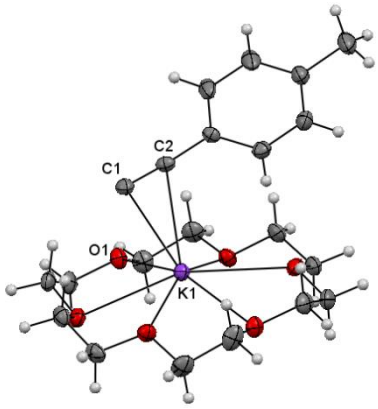


Figure S70. X-ray structure of intermediate **5**. Ellipsoids are shown at 50% probability. Selected bond lengths [Å] and bond angles [deg]: K1-C1 2.8899(16), K1-C2 3.1607(15), C1-C2 1.229(2), O1-K1-C1 86.60(4), O1-K1-C2 100.54(4).

Table S3. Crystallographic and data collection parameters for intermediate **5**.

	Compound
Empirical formula	$C_{21}H_{31}KO_6$
Formula weight	417.55
Temperature/K	100
Crystal system	Monoclinic
Space group	P21/n
a (Å)	8.1050(2)
b (Å)	19.2881(6)
c (Å)	14.1234(4)
α (°)	90
β (°)	92.977(3)
γ (°)	90
V(Å^3)	2204.93(11)
Z	4
D_{calc}(g/cm^3)	1.258
F (000)	892.0
μ (mm^{-1})	2.382
θ Range (°)	7.766 to 132.482
Goodness-of-fit	1.028
R, wR2	0.0321, 0.0815
R indexes [al l data]	0.0394 and 0.0857
Largest difference in peak and hole (e/ Å^3)	0.19/-0.30
CCDC Number	1940261

X-ray structure and data of complex 7:

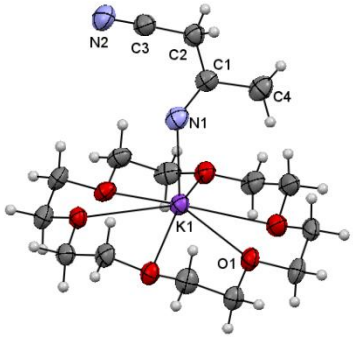


Figure S71. X-ray structure of **7**. Ellipsoids are shown at 50% probability. Selected bond lengths [Å] and bond angles [deg]: K1-N1 2.698(5), N1-C1 1.320(8), C1-C2 1.401(8), C2-C3 1.406(8), C3-N2 1.154(9), N1-C1-C2 128.0(6), C1-N1-K1 138.9(4).

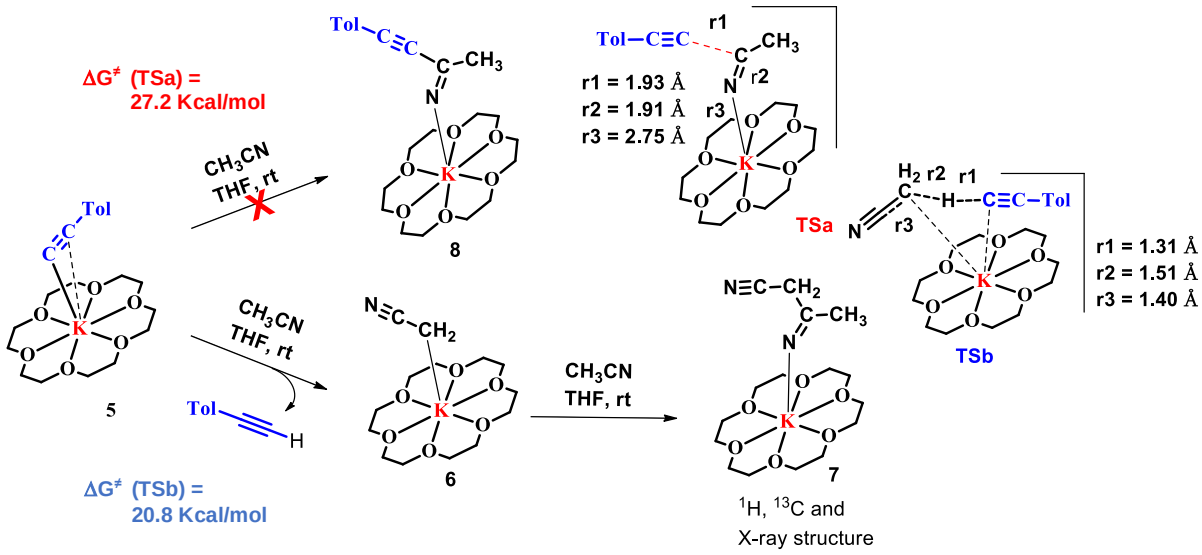
Table S4. Crystallographic and data collection parameters for complex **7**.

	Compound
Empirical formula	$C_{32}H_{57}K_2N_4O_{12}$
Formula weight	768.01
Temperature/K	99.73(16)
Crystal system	Monoclinic
Space group	P21/n
a (Å)	21.5229(14)
b (Å)	8.6696(3)
c (Å)	21.8344(19)
α (°)	90
β (°)	105.419(8)
γ (°)	90
V(Å^3)	3927.5(5)
Z	4
D_{calc}(g/cm^3)	1.299
F (000)	1644.0
μ (mm^{-1})	2.653
θ Range (°)	6.73 to 132.456
Goodness-of-fit	1.267
R, wR2	0.0993, 0.2896
R indexes [al l data]	0.1169 and 0.3165
Largest difference in peak and hole (e/ Å^3)	1.14/-1.16
CCDC Number	1944612

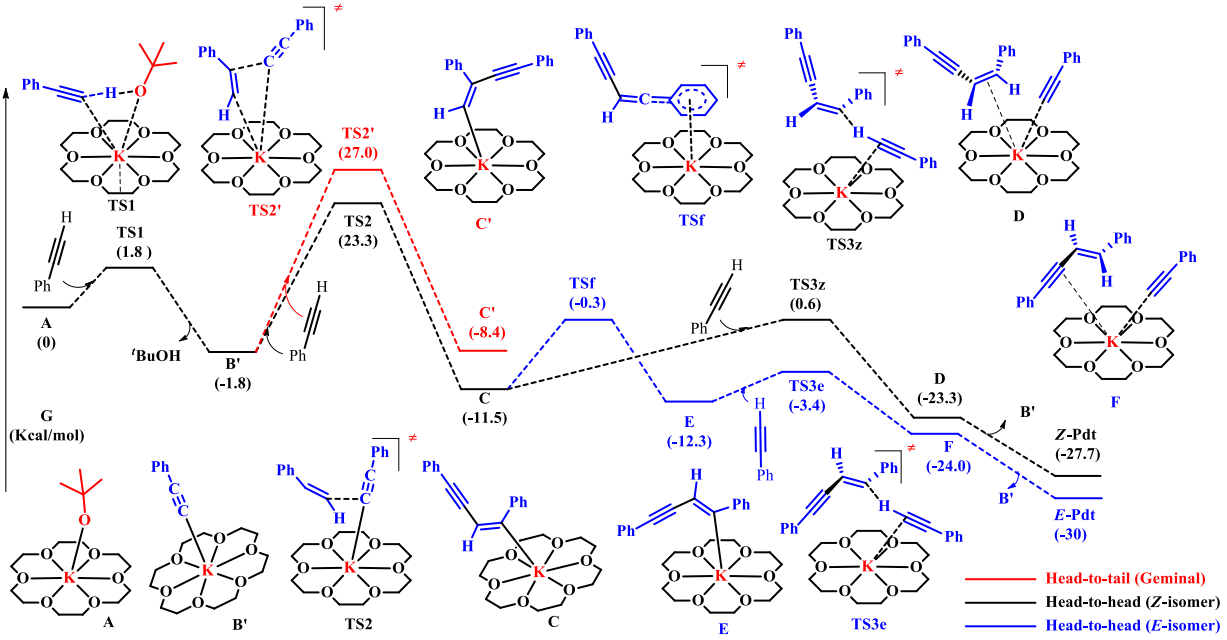
VI. Computational details

Theoretical calculation:

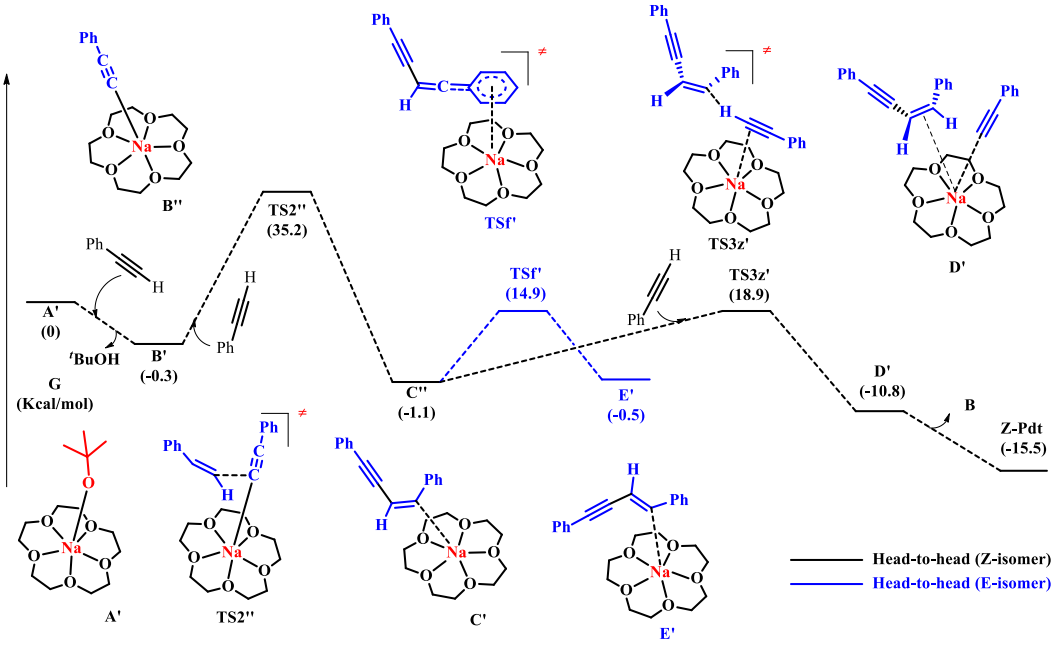
Theoretical calculation was carried out with the help of Gaussian16[12] at M062X/UM062X level of theory by using 6-311+g(d,p)[13] considering CPCM solvent model.[14]



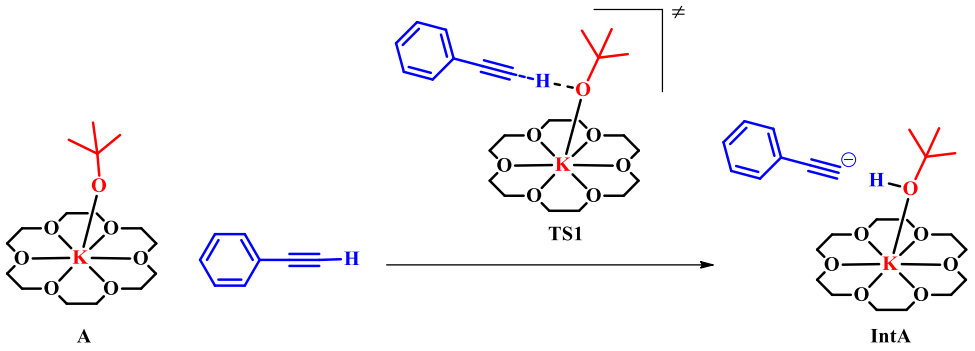
Scheme S1. Mechanistic proposal for formation of complex **7** by support of DFT calculations.



Scheme S2. Calculated energy profile diagram for terminal alkyne dimerzation by KO^{t}Bu in THF.



Scheme S3. Energy profile digram for NaO^{t}Bu catalyzed terminal alkyne dimerization.



Scheme S4. Proton abstraction of phenyl acetylene by K-Crown-O^{t}Bu complex.

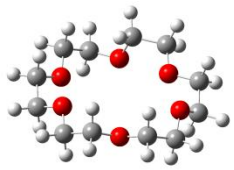
Table S5: Energies, enthalpies, and free energies (in Hartree) of the structures calculated with B3LYP/6-311+G(d,p)-CPCM(THF)//B3LYP/6-31G(d):

Structure	ZPE	ΔE	ΔH	ΔG	E	H	G	IF (cm^{-1})	Infrared
18-Crwon-6	0.371412	0.390058	0.391002	0.324791	-922.491764	-922.490820	-922.557031		
A	0.495501	0.524121	0.525065	0.436174	-1755.399699	-1755.398755	-1755.487646		
PhAcy	0.109992	0.116237	0.117181	0.079807	-308.225453	-308.224509	-308.261883		
^{t}BuOH	0.136139	0.142457	0.143401	0.107587	-233.493552	-233.492608	-233.528423		
KO^{t}Bu Cubic	0.495918	0.533467	0.534412	0.425598	-3331.599074	-3331.598130	-3331.706943		
KPh	0.098811	0.106332	0.107276	0.064198	-907.605305	-907.604361	-907.647439		
TS1	0.603454	0.639573	0.640517	0.534472	-2063.641559	-2063.640615	-2063.746660	-1150.36	9673.2742
B	0.471728	0.500406	0.501350	0.411235	-1830.134824	-1830.133880	-1830.223995		
TS2	0.581908	0.617955	0.618899	0.510923	-2138.338353	-2138.337409	-2138.445385	-369.32	1416.5191
C	0.584876	0.620509	0.621453	0.514045	-2138.394382	-2138.393438	-2138.500846		

E	0.584602	0.619340	0.620284	0.517455	-2138.399445	-2138.398501	-2138.501330		
TSf	0.583541	0.618729	0.619673	0.515313	-2138.379566	-2138.378622	-2138.482982	-43.85	32.0001
TS3z	0.692094	0.734409	0.735353	0.613597	-2446.622609	-2446.621665	-2446.743421	-908.77	13734.8322
D	0.698220	0.741931	0.742875	0.615383	-2446.654911	-2446.653967	-2446.781459		
TS3e	0.692138	0.735285	0.736229	0.612146	-2446.625828	-2446.624884	-2446.748966	-1201.55	11129.8971
F	0.697670	0.740708	0.741653	0.616635	-2446.657179	-2446.656235	-2446.781253		
TS2'	0.581489	0.617403	0.618347	0.511975	-2138.334482	-2138.333538	-2138.439911	-402.77	1517.3192
C'	0.584710	0.620178	0.621123	0.514650	-2138.390832	-2138.389887	-2138.496360		
Z-Pdt	0.226104	0.238814	0.239758	0.185679	-616.511749	-616.510805	-616.564884		
E-pdt	0.225800	0.238712	0.239657	0.185165	-616.513008	-616.512063	-616.566555		
A'	0.429150	0.452731	0.453675	0.376301	-1164.466692	-1164.465748	-1164.543122		
B'	0.405863	0.431175	0.432119	0.348346	-1239.212420	-1239.211476	-1239.295249		
TS2''	0.517995	0.549409	0.550353	0.453714	-1547.603312	-1547.602368	-1547.699007	-395.93	1359.4311
C''	0.518209	0.550489	0.551433	0.450992	-1547.600418	-1547.599473	-1547.699914		
D'	0.630538	0.670170	0.671114	0.551713	-1855.999275	-1855.998330	-1856.117732		
TSf	0.624534	0.664718	0.665662	0.545488	-1855.951102	-1855.950158	-1856.070332	-1322.55	17182.3000
TS3z	0.516568	0.548584	0.549528	0.450749	-1547.576559	-1547.575615	-1547.674394	-82.33	92.1114
E'	0.517995	0.549409	0.550353	0.453714	-1547.603312	-1547.602368	-1547.699007		
B'	0.493589	0.524507	0.525451	0.429483	-1869.963649	-1869.962705	-1870.058673		
TSa	0.540088	0.574884	0.575828	0.471125	-2002.693016	-2002.692071	-2002.796774	-301.73	628.0017
TSb	0.533718	0.568399	0.569344	0.464801	-2002.703376	-2002.702432	-2002.806975	-1190.0-12.3	12213.1932.338
7	0.449440	0.479279	0.480223	0.386002	-1787.790438	-1787.789494	-1787.883716		

Coordinates of the DFT optimized geometries:

18-Crown-6

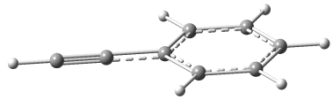


0 1

C	-3.73730900	-0.37089400	-0.37043600
H	-4.77301400	-0.73047400	-0.23595600
H	-3.56261000	-0.24416400	-1.45023500
C	-3.57240300	0.97642400	0.30788000
H	-4.45686400	1.60457800	0.09667600
H	-3.51608500	0.83157200	1.39890600
O	-2.81371200	-1.28189000	0.18758900
O	-2.39857400	1.58849100	-0.18439700
C	-2.09541800	2.81287000	0.44672100
H	-2.92094600	3.53557300	0.31231100
H	-1.94595800	2.67320900	1.52987200
C	-2.55769900	-2.40796500	-0.62404600

H	-3.46302000	-3.03064700	-0.74229800
H	-2.22926000	-2.09380700	-1.62733800
C	-0.83556500	3.39449300	-0.16632300
H	-0.92137500	3.36307000	-1.26459200
H	-0.74800100	4.45488300	0.13317900
C	-1.46713400	-3.24181200	0.02037400
H	-1.76342100	-3.51126200	1.04871700
H	-1.35173200	-4.17991300	-0.55159300
O	-0.27129500	-2.49652600	0.02347100
O	0.29051100	2.66387000	0.27285100
C	0.82363300	-3.18181800	0.58756200
H	1.11981900	-4.03924500	-0.04053300
H	0.56824500	-3.57051000	1.58963200
C	1.98755700	-2.21911500	0.72933400
H	1.64691800	-1.33793100	1.29068400
H	2.78812300	-2.71351500	1.30926300
O	2.45095600	-1.85820900	-0.55672900
C	1.49652200	3.12518700	-0.29888300
H	1.46985000	3.04259900	-1.39748900
H	1.66132400	4.18858800	-0.04630400
C	2.65914000	2.31290600	0.23840200
H	3.60090100	2.85063000	0.02692700
H	2.56238500	2.22720100	1.33321800
O	2.67449300	1.03707100	-0.36858900
C	3.66831400	0.19180800	0.16603400
H	3.50718900	0.04517100	1.24742800
H	4.67395800	0.63806100	0.05274400
C	3.66767700	-1.14298700	-0.57362900
H	4.48749500	-1.75490400	-0.15276100
H	3.88315800	-0.96580000	-1.63194800

PhAcy



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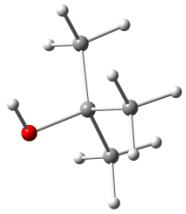
C	1.51254700	-1.20860500	0.00001300
C	0.11992700	-1.21313000	-0.00001100
C	-0.59417800	-0.00002100	-0.00003200
C	0.11990800	1.21312000	-0.00001300
C	1.51251400	1.20862600	0.00001500
C	2.21296400	0.00001200	0.00002400
H	2.05301100	-2.15130300	0.00002200
H	-0.42860100	-2.14998200	-0.00002200
H	-0.42866300	2.14994700	-0.00002400
H	2.05297500	2.15132600	0.00002500
H	3.29955900	0.00003500	0.00004400
C	-2.02414400	-0.00001300	-0.00007200
C	-3.23418700	0.00000400	-0.00001400
H	-4.30038500	0.00001800	0.00048200

tBuOH



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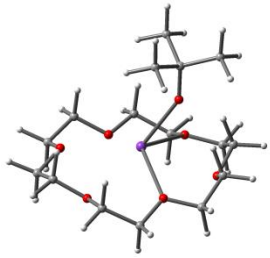
O	0.01325700	-0.00030100	1.45215800
H	0.94382300	0.00193000	1.72867300
C	-0.00533400	-0.00001600	0.01400800
C	0.69529500	-1.26277800	-0.51013500
H	0.66006200	-1.31840800	-1.60442800
H	1.75232700	-1.27372300	-0.21211500
H	0.21745200	-2.15886700	-0.10059900
C	-1.49012500	-0.00531200	-0.35745200
H	-1.98043900	-0.89360600	0.05421000
H	-1.98681500	0.87932300	0.05448300
H	-1.62211400	-0.00562200	-1.44478800
C	0.68598500	1.26812200	-0.50945600
H	0.65016000	1.32422200	-1.60370500
H	0.20160600	2.16038300	-0.09925200
H	1.74295100	1.28667700	-0.21154400

18-Crown-6-KOtBu (A)



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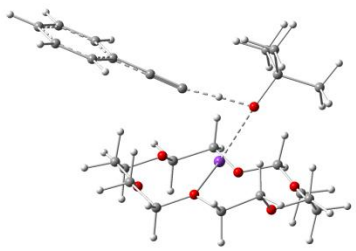
C	-3.84032500	1.17533600	0.72395900
H	-4.60186100	1.22252300	1.51989900
H	-4.36045100	1.18033500	-0.24689400
C	-2.94734500	2.39401100	0.82426900
H	-3.58484400	3.29329600	0.85306700
H	-2.36515600	2.36090900	1.75907700
O	-3.06163200	-0.00301900	0.85699700
O	-2.08417200	2.43116800	-0.29908100
C	-1.28913200	3.60862500	-0.34661000
H	-1.92976400	4.49702500	-0.47293000
H	-0.72011700	3.72139300	0.58877600
C	-3.83793200	-1.18293600	0.72377000
H	-4.59871900	-1.23227900	1.52029300
H	-4.35881700	-1.18838000	-0.24667000

C	-0.32064600	3.50907400	-1.50879500
H	-0.86853100	3.36809100	-2.45515300
H	0.23824500	4.45711400	-1.57776100
C	-2.94220900	-2.39973300	0.82242400
H	-2.35918900	-2.36599900	1.75669100
H	-3.57769900	-3.30044100	0.85121000
O	-2.08007700	-2.43413700	-0.30179900
O	0.54993200	2.42770900	-1.26247200
C	-1.28229500	-3.60964800	-0.35097400
H	-1.92090000	-4.49947300	-0.47756000
H	-0.71223900	-3.72187100	0.58384200
C	-0.31497900	-3.50672300	-1.51384100
H	0.24611800	-4.45335900	-1.58413400
H	-0.86394000	-3.36615200	-2.45963400
O	0.55324100	-2.42354100	-1.26714900
C	1.70797400	2.38720500	-2.08880000
H	1.41839100	2.32468100	-3.15020100
H	2.29985200	3.30572500	-1.94552200
C	2.54000100	1.18519300	-1.69413300
H	3.53319000	1.26926600	-2.16795500
H	2.64630800	1.13314400	-0.59824500
O	1.87876000	0.00385900	-2.15191300
C	2.54157300	-1.17760000	-1.69689300
C	1.71093100	-2.37985600	-2.09378300
H	2.30406200	-3.29788900	-1.95257100
H	1.42094400	-2.31554900	-3.15497000
K	-0.23731000	0.00066900	-0.10447000
H	3.53474300	-1.25945200	-2.17115000
H	2.64811300	-1.12780600	-0.60094500
O	1.87624400	0.00083500	1.16528000
C	2.49758000	-0.00107800	2.38807600
C	4.04361600	-0.00348500	2.22788500
H	4.58110600	-0.00496200	3.18753300
H	4.35479100	-0.89029500	1.66077400
H	4.35765100	0.88302000	1.66188600
C	2.10027300	1.25866200	3.20888700
H	2.36774000	2.15981200	2.64237500
H	1.01173600	1.26906700	3.36032300
H	2.58302500	1.31338600	4.19610700
C	2.09618600	-1.26076000	3.20701700
H	1.00762300	-1.26780800	3.35851000
H	2.36068800	-2.16190600	2.63909900
H	2.57879000	-1.31858500	4.19413300

TS1



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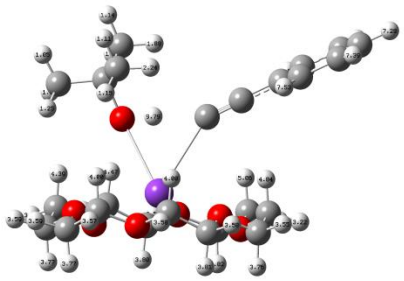
C	0.70530100	-0.33604600	3.59024000
H	1.21936500	-1.13411300	4.15036400
H	0.22363500	0.33722500	4.31814100
C	1.73349200	0.41150900	2.76768800

H	2.53761400	0.76748700	3.43317500
H	2.16431700	-0.26362000	2.01636400
O	-0.26001600	-0.88848600	2.71414800
O	1.10459200	1.51685200	2.12497400
C	2.00314000	2.22505100	1.28054900
H	2.85330200	2.61214100	1.86669400
H	2.39482200	1.56063300	0.49839700
C	-1.13577500	-1.82066700	3.32257600
H	-0.56745100	-2.68315100	3.70756000
H	-1.67013200	-1.35581900	4.16697700
C	1.27774000	3.39749700	0.65714300
H	0.80679800	4.01046400	1.44213300
H	2.00837600	4.02631000	0.12284500
C	-2.12872600	-2.29953200	2.28444400
H	-1.60498500	-2.65696500	1.38556800
H	-2.72069000	-3.12541700	2.71274600
O	-2.98242100	-1.20874800	1.94212300
O	0.28976700	2.92162700	-0.24723300
C	-4.01158800	-1.59409100	1.04287000
H	-4.72286300	-2.27185700	1.54510700
H	-3.58446100	-2.11156900	0.17507400
C	-4.75377100	-0.35831900	0.57944600
H	-5.65661400	-0.66620100	0.02732000
H	-5.06993600	0.24358100	1.44643900
O	-3.90022500	0.40013000	-0.26476900
C	-0.41699000	3.96688400	-0.88860400
H	-0.90262500	4.61702800	-0.14322600
H	0.27019800	4.58797900	-1.48687700
C	-1.46807100	3.37313600	-1.80284700
H	-1.93872500	4.18593400	-2.37989200
H	-1.00006200	2.67507900	-2.51478400
O	-2.43575100	2.70317200	-1.00995600
C	-3.53667700	2.21406700	-1.76074400
C	-4.51472200	1.54863800	-0.81454300
H	-5.42295000	1.27239600	-1.37555800
H	-4.80595300	2.25412400	-0.01956600
K	-1.02378700	0.36926400	0.32210000
H	-4.04286000	3.04236800	-2.28322600
H	-3.19765300	1.48670500	-2.51457700
O	-0.87997000	-1.85882900	-0.99738100
C	-1.07901300	-2.50903000	-2.22620100
C	-0.62289800	-1.59902500	-3.39290000
H	-0.75978000	-2.07518600	-4.37334300
H	-1.20229400	-0.66528600	-3.38477300
H	0.43550400	-1.34062500	-3.28007600
C	-0.27904200	-3.83152600	-2.26545300
H	0.79276600	-3.63021900	-2.16216300
H	-0.58311200	-4.47031900	-1.42745300
H	-0.43746500	-4.38711700	-3.19984500
C	-2.57910400	-2.82142900	-2.39498800
H	-2.91374900	-3.50604000	-1.60536700
H	-3.16456000	-1.89673800	-2.31746400
H	-2.79731200	-3.29049700	-3.36399100
H	0.36930700	-1.59157200	-0.81897200
C	1.61269600	-1.19117000	-0.64580800
C	2.82307800	-0.97402500	-0.64849900
C	4.22677600	-0.70219800	-0.65069800
C	4.77355500	0.28870300	-1.49415700

C	5.10820700	-1.41391100	0.19079300
C	6.14040500	0.55745000	-1.49015900
H	4.10766500	0.83548000	-2.15589500
C	6.47421500	-1.14149200	0.19009100
H	4.70255900	-2.18626400	0.83791800
C	6.99866700	-0.15425000	-0.64817800
H	6.53924200	1.32371200	-2.15082200
H	7.13441400	-1.70465200	0.84548500
H	8.06511800	0.05548600	-0.64794200

Int1A



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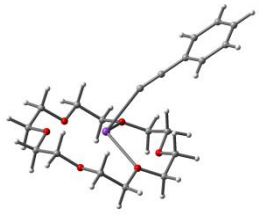
C	0.30871500	0.22409100	3.77058100
H	0.73304900	-0.51236900	4.47243900
H	-0.17309400	1.02150500	4.35969000
C	1.42781400	0.79314200	2.92465700
H	2.22084600	1.17176600	3.59123000
H	1.84601400	0.00981300	2.27759300
O	-0.63739300	-0.39914700	2.91825900
O	0.90967600	1.85542400	2.12813000
C	1.90610000	2.42515800	1.28596900
H	2.71610600	2.85941000	1.89574400
H	2.33154100	1.65469800	0.62888200
C	-1.66462000	-1.09122400	3.60085300
H	-1.23520100	-1.85408400	4.27124500
H	-2.26238200	-0.39576000	4.21260200
C	1.27941500	3.52800400	0.46120000
H	0.75405500	4.24137700	1.11639900
H	2.07474200	4.07276300	-0.07278100
C	-2.54756100	-1.77608400	2.57883600
H	-1.93833400	-2.40152500	1.91104700
H	-3.27422700	-2.41719500	3.10536600
O	-3.22957700	-0.78043000	1.82210400
O	0.36879800	2.95979900	-0.47110700
C	-4.11203600	-1.34548100	0.86389900
H	-4.90974200	-1.91585500	1.36952000
H	-3.56441900	-2.02309100	0.19641400
C	-4.74670400	-0.23240900	0.05792100
H	-5.55506200	-0.65346600	-0.56225100
H	-5.18866900	0.51747600	0.73326000
O	-3.76025600	0.36860900	-0.76765200
C	-0.24088400	3.91913200	-1.31088200
H	-0.83486600	4.63339600	-0.71765400
H	0.52150100	4.48965400	-1.86716000
C	-1.13796000	3.20658800	-2.30128300
H	-1.53602300	3.94098200	-3.02052800
H	-0.55661600	2.45738400	-2.86126800
O	-2.19839000	2.58456300	-1.59125900

C	-3.14945400	1.95877700	-2.43667900
C	-4.27107700	1.40672200	-1.58193000
H	-5.06970800	1.02553300	-2.24004100
H	-4.69575700	2.21233600	-0.96163800
K	-0.97285300	0.47290700	0.25250400
H	-3.56695200	2.68616900	-3.15220400
H	-2.68089800	1.14400300	-3.01127400
O	-0.93404000	-2.22386700	-0.58431600
C	-0.87812700	-3.12033000	-1.69974500
C	-0.43543900	-2.35332300	-2.95989500
H	-0.38337300	-3.01324300	-3.83519200
H	-1.14856000	-1.54833200	-3.17991700
H	0.54997800	-1.90445200	-2.79968200
C	0.11355500	-4.25577300	-1.39043900
H	1.11431900	-3.84481500	-1.22098500
H	-0.19536500	-4.78746500	-0.48303500
H	0.16847100	-4.97828600	-2.21453200
C	-2.29228600	-3.67987800	-1.88685800
H	-2.61709200	-4.20880800	-0.98309000
H	-3.00048600	-2.86658500	-2.08604500
H	-2.33127700	-4.38246900	-2.72770700
H	0.00691800	-1.85492400	-0.43580100
C	1.54983200	-0.96606800	-0.27944400
C	2.78212600	-0.85652800	-0.37131400
C	4.20041700	-0.71611000	-0.47855100
C	4.78026300	0.15807500	-1.42543300
C	5.07531600	-1.44292400	0.35974700
C	6.16246600	0.29919700	-1.52439700
H	4.12291100	0.71814500	-2.08502800
C	6.45677500	-1.29921900	0.25632400
H	4.64802900	-2.12460100	1.08979900
C	7.01097200	-0.42720300	-0.68473000
H	6.58143500	0.97814600	-2.26405400
H	7.10663900	-1.87282200	0.91361800
H	8.08949700	-0.31724500	-0.76428600

Crown-KPh (B)



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C	-4.28321200	-1.18297700	-1.75883700
H	-4.81741700	-1.22082000	-2.72232400
H	-5.03211300	-1.20650100	-0.95142600
C	-3.37858300	-2.39286900	-1.65025200
H	-3.97427400	-3.29807300	-1.85325800
H	-2.57959800	-2.33362500	-2.40600700
O	-3.50413400	-0.00049800	-1.67393800
O	-2.82612800	-2.44453900	-0.34476200
C	-2.02000700	-3.59666400	-0.13106100
H	-2.62821300	-4.51075600	-0.22929300
H	-1.20899100	-3.63732300	-0.87376300
C	-4.28353000	1.18174400	-1.75915800
H	-4.81777800	1.21916800	-2.72263800

H	-5.03241200	1.20530400	-0.95172900
C	-1.42223000	-3.53640200	1.26059400
H	-2.22025000	-3.45153800	2.01656800
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C	-3.37921400	2.39190400	-1.65095400
H	-2.58028400	2.33268800	-2.40677100
H	-3.97516300	3.29690200	-1.85412000
O	-2.82664500	2.44403000	-0.34553000
O	-0.54908900	-2.42858800	1.32258700
C	-2.02083500	3.59643600	-0.13216400
H	-2.62930100	4.51033200	-0.23060600
H	-1.20986300	3.63713000	-0.87491200
C	-1.42298100	3.53671300	1.25948300
H	-0.87697700	4.47629700	1.44527300
H	-2.22094600	3.45180500	2.01551100
O	-0.54950600	2.42917700	1.32173100
C	0.26977000	-2.38475100	2.48303300
H	-0.35324700	-2.31971500	3.38971900
H	0.87969500	-3.30008100	2.54850200
C	1.18655200	-1.18260500	2.38833200
H	1.92938700	-1.23783900	3.20169800
H	1.70962700	-1.17899000	1.42118500
O	0.40203400	0.00054000	2.52115100
C	1.18630200	1.18380600	2.38794200
C	0.26927400	2.38579500	2.48225200
H	0.87900300	3.30126800	2.54753600
H	-0.35380000	2.32085900	3.38890500
K	-1.12204300	0.00005300	0.01085900
H	1.92912500	1.23946700	3.20128900
H	1.70938500	1.17998500	1.42079900
C	1.44175100	-0.00001900	-1.03238500
C	2.68463400	0.00003600	-1.09019500
C	4.10986000	-0.00001400	-1.16747800
C	4.84684100	1.20692200	-1.20416700
C	4.84668800	-1.20701000	-1.20528600
C	6.23779900	1.20456400	-1.27277500
H	4.30096100	2.14629100	-1.18254800
C	6.23764500	-1.20476400	-1.27389100
H	4.30068700	-2.14632700	-1.18453000
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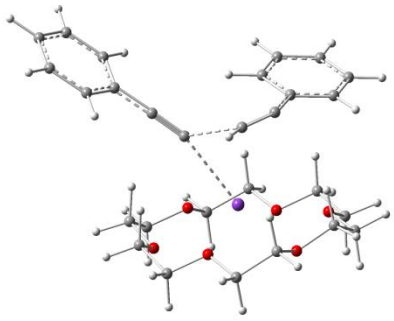

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H	2.75912300	0.76650600	-2.64611800
O	3.59265800	0.07451400	-0.26459900
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C	1.77852900	3.23398400	-2.31129100
H	2.39079100	3.83864900	-3.00092100
H	1.13057200	2.57680800	-2.90973900
C	4.39457200	-0.56226100	0.71537400
H	5.18022300	-1.16720800	0.23433300
H	4.88461500	0.18962700	1.35482200
C	0.92555500	4.15411600	-1.46253200
H	1.56649400	4.76804900	-0.80895900
H	0.36412800	4.83322400	-2.12546300
C	3.52891300	-1.47816300	1.55385900
H	3.01678500	-2.20322000	0.90689200
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O	2.58548200	-0.69707900	2.27678400
O	0.03852000	3.36464500	-0.69379700
C	1.73991500	-1.48902700	3.09830200
H	2.33971400	-2.06865800	3.81951000
H	1.16377900	-2.19745000	2.48370400
C	0.79955500	-0.57960800	3.86088100
H	0.21748000	-1.18698800	4.57367400
H	1.37790000	0.16092200	4.43691900
O	-0.06020300	0.06869000	2.94291200
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H	-2.64888000	3.74631300	1.23637500
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O	-1.08975200	2.49011600	1.79612500
C	-1.88940300	1.54888900	2.50531500
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H	-1.68314500	0.27790100	4.21968500
H	-0.54840800	1.65543300	4.18974700
K	0.83204000	0.76617800	0.30343900
H	-2.73210600	2.06199400	2.99811400
H	-2.28859200	0.79552400	1.81232100
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C	-2.90254200	-0.39694200	-0.76851000
C	-4.28961700	-0.72509000	-0.72125800
C	-4.74063700	-1.91701500	-0.10971100
C	-5.26370100	0.13305400	-1.28064100
C	-6.09616400	-2.23042200	-0.05983300
H	-4.00568600	-2.59105000	0.32119500
C	-6.61788700	-0.18614500	-1.22870500
H	-4.93523100	1.05098000	-1.76019100
C	-7.04452800	-1.36855100	-0.61784500
H	-6.41596100	-3.15516400	0.41522000
H	-7.34629700	0.49085900	-1.66941400
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C	-0.36374700	-0.25972600	-2.38318700
C	0.52622100	-1.14999800	-2.46671700
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C	2.83230900	-3.91971000	-1.36807400
H	2.99675100	-2.22131500	-2.68682300
C	2.00074800	-4.64855700	-0.51149500
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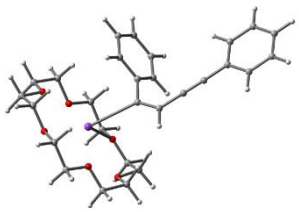
Crown-Kcis1 (C)



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H	-2.95035200	-4.33092200	0.12991500
H	-1.73491800	-3.26698200	-0.62979600
O	-3.42811200	-1.55523700	-1.65940800
O	-2.75845200	-2.44431300	0.98279300
C	-1.82160700	-2.84255800	1.98048100
H	-2.06527800	-3.85405200	2.34526600
H	-0.80288500	-2.85378100	1.56920900
C	-4.36875700	-1.05041800	-2.59087000
H	-4.47435200	-1.74050500	-3.44400100
H	-5.35754100	-0.93924200	-2.11772400
C	-1.89082800	-1.86973500	3.13968300
H	-2.91761600	-1.81273400	3.53647400
H	-1.23223900	-2.23540300	3.94388000
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H	-2.87677800	0.19782300	-3.51696900
H	-4.56300500	0.62204200	-3.91522500
O	-3.91027700	1.23016300	-2.03755200
O	-1.46131500	-0.59805400	2.68768000
C	-3.53430500	2.53897900	-2.44349200
H	-4.22642900	2.91361800	-3.21515300
H	-2.51747600	2.53267300	-2.86500800
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H	-0.53298600	-0.02032900	4.45081200
C	-0.72695500	1.63088700	3.09815000
H	-0.43378800	2.32481500	3.90297600
H	0.15476300	1.40571600	2.48072700
O	-1.74697200	2.21614700	2.29310900
C	-1.32290700	3.42231200	1.67324100
C	-2.43625700	3.93699300	0.78445300

H	-2.17709400	4.94805800	0.43108400
H	-3.37543300	4.00304300	1.35664800
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H	-1.09471000	4.18452200	2.43680400
H	-0.41763500	3.24739200	1.07446100
C	0.79727300	0.46801200	-0.32407900
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H	1.46479600	2.48904400	-0.29244400
C	1.15739300	-0.94602200	-0.32978800
C	1.76299900	-1.58355200	0.78473400
C	0.80231700	-1.79045500	-1.41393600
C	1.99653500	-2.95776200	0.80886400
H	2.06220600	-0.97041100	1.63120200
C	1.05771100	-3.16090300	-1.39605100
H	0.33792600	-1.34000500	-2.29002000
C	1.64768900	-3.76515000	-0.27986200
H	2.47652500	-3.40208800	1.67981700
H	0.79751700	-3.76440000	-2.26469900
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C	5.77299500	0.79839300	-0.53524300
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C	6.71087000	1.85236300	-0.58956700
C	7.62669200	-0.78262800	-0.60776400
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C	8.07647200	1.58809100	-0.65159300
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C	8.54370200	0.27110400	-0.66125600
H	7.98002300	-1.81114200	-0.61495400
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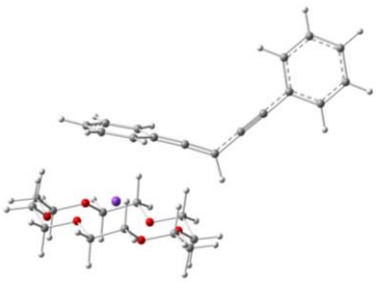

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H	6.07879600	-1.20825800	-1.90639700
H	4.33858700	-1.21161100	-2.32102300
O	3.50315000	-2.44683800	-0.19542400
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C	5.05830900	1.18184400	-1.48991700
H	6.07879900	1.20817400	-1.90644800
H	4.33859200	1.21151800	-2.32107000
C	3.19267100	-3.58567000	0.59018200
H	3.41443000	-4.50905200	0.03054600
H	3.79345000	-3.59089900	1.51352300

C	4.86107200	2.38784200	-0.59597100
H	5.51973700	2.31708000	0.28440000
H	5.13587200	3.29615400	-1.15697200
C	1.71837500	-3.55661300	0.93564300
H	1.12053000	-3.47213600	0.01587900
H	1.45031400	-4.49927800	1.44050900
O	1.47403500	-2.44962900	1.78945600
O	3.50316400	2.44683100	-0.19551400
C	0.12078000	-2.36710500	2.22367600
H	-0.16529300	-3.28891500	2.75574900
H	-0.55436900	-2.23155800	1.36650700
C	-0.01450100	-1.18856400	3.16431800
H	-1.03609700	-1.17896400	3.57567000
H	0.69643400	-1.28427600	4.00082300
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H	3.79347000	3.59094500	1.51339700
H	3.41445900	4.50905300	0.03039000
C	1.71839500	3.55665500	0.93551400
H	1.45034100	4.49933900	1.44035000
H	1.12055000	3.47215500	0.01575200
O	1.47404300	2.44970100	1.78936200
C	0.12078700	2.36720100	2.22358100
C	-0.01450400	1.18869800	3.16426800
H	-1.03610300	1.17911700	3.57561300
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H	-0.16528200	3.28903400	2.75561800
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C	-1.71756800	-0.00002100	-0.51778000
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C	-0.08849800	1.22898300	-1.90915300
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C	0.99915700	1.20287700	-2.76306500
H	-0.54404000	2.17797900	-1.63641400
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H	-0.54403500	-2.17806700	-1.63633300
C	1.60507000	-0.00007200	-3.18724400
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C	-6.66735600	-0.00000300	-0.29565800
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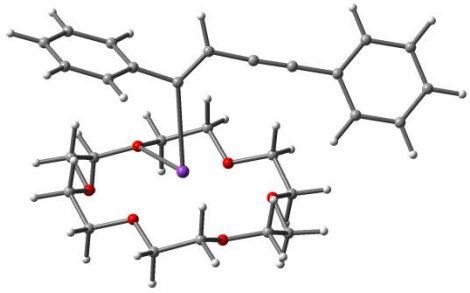

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O	-2.53540000	2.53230400	-1.06882700
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C	-3.94508500	-0.37887000	1.56986700
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H	-2.66929900	4.07838900	-2.44908900
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C	-3.13469000	-0.62547300	2.82503800
H	-3.27822300	0.19795700	3.54360500
H	-3.48964800	-1.55671300	3.29549200
C	-0.62447800	3.65278600	-1.96799500
H	-0.50003200	2.82603800	-2.68451800
H	-0.31048100	4.58639300	-2.46257300
O	0.15563800	3.42345700	-0.80360500
O	-1.76684800	-0.74030300	2.47266900
C	1.55204700	3.39777400	-1.06439200
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C	2.29144400	3.15073000	0.23462400
H	3.37323100	3.26027800	0.05494300
H	1.99205000	3.89909900	0.98587800
O	1.99349800	1.84253600	0.68802500
C	-0.92610700	-1.12745200	3.54471200
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C	0.49542200	-1.24021800	3.03332700
H	1.12990100	-1.66305000	3.82941500
H	0.52954300	-1.91428000	2.16459200
O	0.95518300	0.05638300	2.67291700
C	2.31500500	0.05954300	2.24928900
C	2.70335500	1.47103800	1.86400500
H	3.78723500	1.50344500	1.67687600
H	2.46756200	2.16657100	2.68499000
K	-0.68701100	0.80226100	0.33883800
H	2.96905700	-0.27642300	3.07054900
H	2.45473300	-0.61598300	1.39397400
C	-0.62015000	-1.62802200	-1.19745600
C	0.44440100	-2.46617900	-1.34253200
C	-1.95009800	-2.20056200	-1.39261700
C	-2.44189000	-3.26625100	-0.59702300

C	-2.85057200	-1.65941600	-2.34509600
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H	-1.77899900	-3.70535100	0.14503700
C	-4.13827100	-2.16588900	-2.50852500
H	-2.50578200	-0.83795300	-2.97063400
C	-4.60378400	-3.21005500	-1.70020900
H	-4.08036100	-4.57346200	-0.11243000
H	-4.78883700	-1.74090500	-3.27133800
H	-5.61329700	-3.59510300	-1.81946300
C	1.79695000	-2.07084400	-1.15245900
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H	3.96961800	0.68931400	-0.82704700
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H	7.46463100	-2.83092100	-0.74278000
H	8.12268400	-0.43610100	-0.57049100
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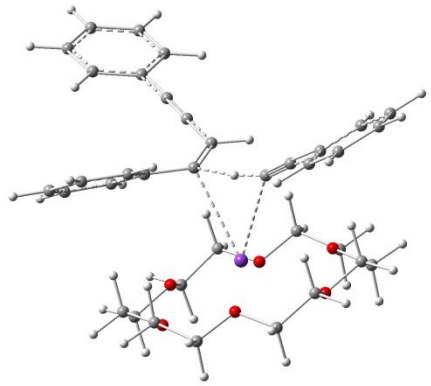
TS3z



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H	-1.42685300	-4.50872300	-2.56461800
H	-1.30713900	-2.73055200	-2.51607400
O	-3.14118900	-2.37060000	-0.66671900
O	-0.65236800	-3.71517400	-0.80587600
C	0.70700100	-3.88169800	-1.19614000
H	0.81972800	-4.80276400	-1.79148100

H	1.04342100	-3.03178800	-1.80364000
C	-4.44128700	-2.25509500	-0.10850800
H	-5.20357400	-2.30822200	-0.90279600
H	-4.62547400	-3.08024100	0.59819000
C	1.56201400	-3.99890200	0.04714700
H	1.20456300	-4.82955600	0.67726000
H	2.59751900	-4.21994200	-0.25753700
C	-4.56601400	-0.92384700	0.59973600
H	-4.30383300	-0.10636400	-0.08459300
H	-5.61158900	-0.79195800	0.92352600
O	-3.69900900	-0.91631800	1.72899800
O	1.51008100	-2.77880100	0.76753800
C	-3.76998700	0.30562100	2.45652700
H	-4.80285100	0.48449500	2.79800300
H	-3.46030000	1.14436600	1.81835500
C	-2.86928000	0.20894400	3.66873500
H	-3.02372600	1.09890200	4.30036300
H	-3.12968900	-0.68184200	4.26273900
O	-1.51673100	0.13663800	3.24478700
C	2.35925400	-2.76477900	1.90271500
H	2.05698700	-3.54840300	2.61630500
H	3.40222300	-2.95750300	1.60360500
C	2.28329300	-1.40602200	2.56550700
H	3.01377600	-1.37275500	3.39034000
H	2.53512400	-0.61467000	1.84586700
O	0.96496500	-1.21967600	3.06944600
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C	-0.59846400	0.07189300	4.32301000
H	-0.69304600	0.96501200	4.96205500
H	-0.79973100	-0.81605400	4.94357000
K	-0.91444200	-1.15958600	0.73132700
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H	0.98918400	2.00155300	0.83812500
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C	2.64098700	-0.71973200	-1.88983400
C	0.70156600	-0.08299900	-3.17128300
C	3.11655600	-1.44928900	-2.97975600
H	3.21554200	-0.69549900	-0.96997900
C	1.18791200	-0.79413000	-4.26719500
H	-0.24559900	0.44647600	-3.24331400
C	2.39867500	-1.48820000	-4.17905300
H	4.06187100	-1.98320700	-2.89718300
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C	2.93888400	1.75745800	0.04414800
C	4.13694600	1.99394100	0.08032800
C	5.53794500	2.23876600	0.06392000
C	6.33715200	1.75566700	-0.99551500
C	6.16605000	2.96320100	1.09956100
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H	5.86021100	1.20277600	-1.79930000
C	7.53921200	3.19155500	1.07487000
H	5.56029200	3.34322700	1.91702900
C	8.31861300	2.70627100	0.02142000
H	8.30745200	1.61092900	-1.83741100

H	8.00430500	3.75329400	1.88131400
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C	-2.93814700	2.18841100	-0.83331700
C	-4.12945200	2.95071500	-1.04232900
C	-4.41658200	4.07859700	-0.24544200
C	-5.04960500	2.59418600	-2.05024200
C	-5.58117200	4.81514500	-0.44780700
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C	-6.21264800	3.33490500	-2.24728300
H	-4.83197000	1.73481900	-2.67800000
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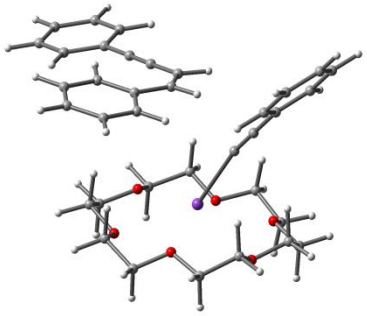

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H	0.78693100	-0.62395600	3.70501600
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H	-1.92496800	-1.76395600	3.80517000
H	-1.42058600	-0.51062000	2.64162200
C	3.94494900	-2.36360000	2.17290800
H	4.59127100	-1.94221600	2.95996900
H	4.00987800	-3.46238200	2.22653400
C	-2.36981800	-2.23862000	1.76933800
H	-2.38671800	-3.33071300	1.91560200
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C	4.42594300	-1.88073200	0.82082400
H	4.23711500	-0.80361600	0.70838400
H	5.51050700	-2.06682100	0.74449600
O	3.73310200	-2.60397400	-0.19298200
O	-1.88699200	-1.92618000	0.47332900
C	4.11415700	-2.19218900	-1.50314100
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H	3.93300800	-1.11494900	-1.62480700
C	3.30493000	-2.97870200	-2.51270500
H	3.70597100	-2.79146100	-3.52198400
H	3.38446300	-4.05821000	-2.30558700
O	1.94798000	-2.56318900	-2.44398600

C	-2.69452400	-2.47351400	-0.55630800
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H	-2.79467500	-2.46427500	-2.69187900
H	-2.01012600	-1.02333900	-1.99210300
O	-0.83933400	-2.74300900	-2.03921700
C	-0.26200300	-2.55412000	-3.32231900
C	1.09673900	-3.22382800	-3.35769600
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H	1.00029600	-4.29147500	-3.10059000
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H	-0.14684600	-1.48061200	-3.53819800
C	-0.79518500	1.99632500	-0.28460800
C	-1.73023100	1.80395700	-1.25253800
H	-1.35502700	1.72239400	-2.27311400
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C	-2.17190700	2.36480400	1.82549200
C	0.24179400	2.17702600	1.93160700
C	-2.21215000	2.54714800	3.20638200
H	-3.09160400	2.39087600	1.25254300
C	0.19321900	2.35819300	3.31320800
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C	-1.03271600	2.54355600	3.95767600
H	-3.16851200	2.70660400	3.69878600
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C	-3.13341300	1.67089300	-1.12880800
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C	2.48738200	0.81199700	-0.50277500
C	3.31508600	1.71082400	-0.73934000
C	4.26619800	2.74038600	-1.01716200
C	4.49010500	3.19821400	-2.33566200
C	5.02361800	3.33950000	0.01507900
C	5.42047500	4.19913900	-2.60432900
H	3.91616900	2.75238000	-3.14337700
C	5.95301300	4.34009700	-0.25799900
H	4.86464600	3.00359500	1.03623500
C	6.15952400	4.77797600	-1.56898100
H	5.56995400	4.53164900	-3.62947500
H	6.52020100	4.78314500	0.55800900
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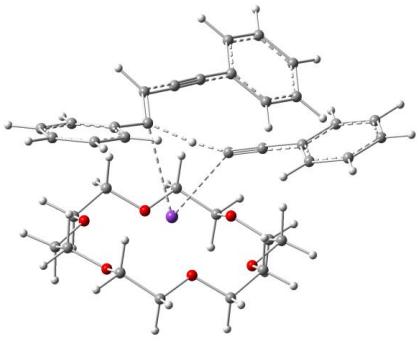
TS3e



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C	4.29397200	1.53477200	-0.97977000
H	5.38042600	1.71561600	-1.03206300
H	3.95847000	1.76322700	0.04296000
O	2.19957100	2.30449900	-1.83568200
O	4.00160300	0.18475400	-1.30906700
C	4.69556400	-0.74492600	-0.48510800
H	5.78398200	-0.59240200	-0.57402000
H	4.41267900	-0.61794100	0.56802400
C	1.47139700	3.11231600	-2.74773200
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H	1.71607900	2.82949500	-3.78429900
C	4.36228500	-2.14693500	-0.94635800
H	4.60992400	-2.26346100	-2.01392600
H	4.97275900	-2.86325500	-0.37279800
C	-0.01058000	2.93926900	-2.49782800
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O	-0.38252900	1.60876300	-2.83970500
O	2.98254900	-2.39309700	-0.73369300
C	-1.77375000	1.37011600	-2.65646000
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C	-2.09124700	-0.03715700	-3.11387800
H	-3.18406000	-0.18036500	-3.10714600
H	-1.73348700	-0.18506100	-4.14545700
O	-1.46869900	-0.96633300	-2.24058900
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H	2.81307300	-3.91423300	-2.13625600
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H	0.87770100	-3.60932300	0.22420300
O	0.39477400	-3.05071900	-1.71925200
C	-1.01479600	-3.23213100	-1.62095500
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H	-1.31090200	-2.50132600	-3.62790000
K	1.01984900	-0.22934700	-0.95363600
H	-1.28036600	-4.27500900	-1.86041600
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C	0.81059900	-0.66627000	2.08366700
C	0.09281700	-1.70813000	2.58970100
C	2.15304300	-0.40860800	2.61780400

C	3.08019600	-1.43341600	2.92107000
C	2.59099200	0.92569000	2.79602900
C	4.35902500	-1.14290900	3.39593800
H	2.78334900	-2.46791000	2.76764500
C	3.86543100	1.21449700	3.28267400
H	1.89915700	1.73265100	2.56731800
C	4.76085200	0.18305600	3.58411200
H	5.04568600	-1.95546700	3.62649200
H	4.16203300	2.25082600	3.43145800
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C	-2.33288500	-2.35000500	1.76083600
C	-3.63995400	-2.65324700	1.28973200
C	-4.21299900	-1.90276100	0.23793400
C	-4.39582200	-3.70624700	1.84837300
C	-5.48961600	-2.20009100	-0.23195600
H	-3.63522000	-1.09119100	-0.19461100
C	-5.67142100	-3.99575700	1.37115100
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C	-4.25494000	4.82317700	1.20933500
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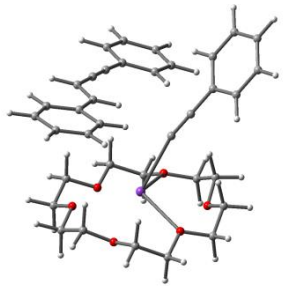

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H	6.02758000	0.06275900	-1.09117900
H	4.65380000	0.85101700	-0.26539600
O	3.22154600	1.29990000	-2.38113800

O	4.24193600	-1.00087100	-1.11314100
C	4.45946400	-1.74407900	0.07782900
H	5.53788100	-1.90985900	0.23595500
H	4.06411000	-1.20265100	0.95090500
C	2.80338700	2.18499400	-3.41003000
H	3.38258700	3.12130000	-3.36110000
H	2.96890000	1.72926000	-4.39973600
C	3.77801200	-3.08960100	-0.05610200
H	4.13342500	-3.59411900	-0.96878200
H	4.04723200	-3.71639600	0.80954100
C	1.33475600	2.50070300	-3.21591100
H	1.15283500	2.82892600	-2.18276800
H	1.05043900	3.31005300	-3.90930200
O	0.57321100	1.32869500	-3.49426500
O	2.37310700	-2.90496200	-0.11270400
C	-0.82092800	1.52916600	-3.27539100
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C	-1.54942400	0.23417900	-3.56909700
H	-2.63534900	0.42217000	-3.57594800
H	-1.26074700	-0.14379400	-4.56330800
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H	-2.91982500	-1.88065900	-2.87723100
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H	-1.93083400	-2.34481900	-0.64324400
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C	-1.19892900	-1.60066300	2.94288000
C	1.10624600	-0.67906800	3.38790400
C	1.51583900	-1.60953400	4.36404300
C	1.99911100	0.35269600	3.03055200
C	2.76934900	-1.51224500	4.96016200
H	0.84927900	-2.41457700	4.66173400
C	3.25409700	0.44676500	3.63250600
H	1.68713500	1.07221000	2.27472200
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H	4.62180100	-0.40677700	5.07067800
C	-2.41574700	-1.57622900	2.22284000
C	-3.46066100	-1.56566700	1.59433100
C	-4.64868700	-1.50254600	0.81347400
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H	-6.01503100	0.28341200	-1.75693400
H	-7.68005600	-3.02642100	0.43115900
H	-7.88027000	-1.31456100	-1.36163600
H	-1.10428100	-2.37145300	3.70763200
C	0.32774100	1.74177200	0.16615100
C	-0.16997800	2.82399200	0.52569300
C	-0.75137000	4.05976200	0.94592900
C	-0.06908800	5.28724600	0.78531600
C	-2.03483300	4.10288400	1.53696300
C	-0.64094100	6.49046300	1.19168200
H	0.92134900	5.27546600	0.33814900
C	-2.60243300	5.30819100	1.94259400
H	-2.57402100	3.16963600	1.67365800
C	-1.91163000	6.51128900	1.77289200
H	-0.09076100	7.41935800	1.05587100
H	-3.59139200	5.30933900	2.39611400
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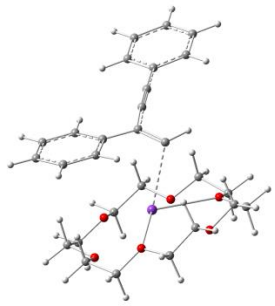
Crw-KPh-Gem (C')



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H	-1.18459100	3.19949000	-1.97711300
O	-0.23379500	3.13762100	0.40981700
O	-2.84038900	2.95748600	-0.75397500
C	-3.63376300	2.39018900	-1.78894300
H	-4.11336700	3.18630700	-2.38269700
H	-3.00290500	1.78383800	-2.45569500
C	0.76449200	3.45576900	1.36144800
H	1.43440000	4.23870500	0.97044600
H	0.30985000	3.82778500	2.29405200
C	-4.71345500	1.53209800	-1.16245600
H	-5.24920900	2.10981500	-0.39263800
H	-5.43918400	1.23547100	-1.93699000
C	1.58031400	2.20823900	1.63332800
H	1.99190100	1.81699000	0.69217300
H	2.41853800	2.46252500	2.30268100
O	0.73901000	1.23717700	2.24571200
O	-4.11482000	0.37934700	-0.58834300
C	1.41534200	0.01597300	2.51560400
H	2.27921200	0.19474700	3.17687300
H	1.78603700	-0.43379200	1.58302000
C	0.45584100	-0.92240000	3.21629700

H	1.00300400	-1.82264200	3.53976700
H	0.04269600	-0.43141600	4.11200600
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C	-4.31226300	-1.73196300	0.50491600
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H	-3.86022400	-2.20797300	-0.37702900
O	-3.30782000	-1.41415600	1.45909500
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H	-2.05436400	-1.64674400	3.75062300
K	-1.43917900	0.57448700	0.29750100
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C	0.13464400	0.71085800	-2.09052700
C	0.82735200	-0.43611600	-1.76465900
C	0.14614600	-1.76869200	-1.68711800
C	0.73985100	-2.88721500	-1.07298200
C	-1.13303800	-1.94367000	-2.25335900
C	0.08453600	-4.11893500	-1.01534500
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H	0.57621200	-4.96605800	-0.54102600
H	-2.76323300	-3.28277800	-2.66869400
H	-1.68792900	-5.23748900	-1.54929600
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C	5.49113300	-1.25532200	-0.17533200
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C	7.50353500	0.08930800	-0.08317600
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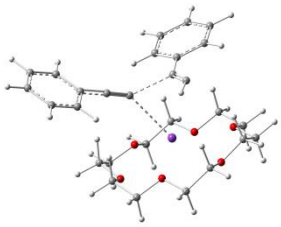
TS2’



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O	-0.79409500	3.11431700	-0.13139300
O	-1.25876500	1.66332000	2.29409000
C	-1.66588700	0.45378600	2.92790200
H	-2.53711400	0.64040000	3.57732300
H	-1.93932500	-0.29490300	2.17101400
C	-0.24693300	4.20686600	-0.84607400
H	-1.04795000	4.80385800	-1.31228400
H	0.32150300	4.86645500	-0.17043100
C	-0.52262000	-0.05148000	3.78194200
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H	-0.87519700	-0.89566600	4.39664600
C	0.66002200	3.66993000	-1.93417900
H	0.10103100	2.96273300	-2.56410800
H	0.99799300	4.50539800	-2.56959100
O	1.77220600	3.02664400	-1.33141300
O	0.53858900	-0.47180400	2.93755800
C	2.64734300	2.42537800	-2.28107300
H	2.97037400	3.17042200	-3.02660300
H	2.13712800	1.60067100	-2.80192200
C	3.86868500	1.90939600	-1.55079300
H	4.60854300	1.55969500	-2.28929400
H	4.32626900	2.72376800	-0.96627600
O	3.48731900	0.84452400	-0.69539800
C	1.67675500	-0.93000900	3.64299000
H	2.12973600	-0.10754000	4.22019400
H	1.39811100	-1.72923700	4.34959100
C	2.67842500	-1.48530700	2.65224900
H	3.52123700	-1.93070800	3.20678100
H	2.20876500	-2.27366800	2.04597700
O	3.13983700	-0.43141800	1.81837400
C	4.08816700	-0.87295400	0.85511800
C	4.56856900	0.31830300	0.05429000
H	5.37787200	-0.01088700	-0.61786200
H	4.97639800	1.08831200	0.72901700
K	0.77148700	0.75617200	0.35147100
H	4.95505300	-1.33392600	1.35720800
H	3.64004600	-1.61995400	0.18481100
C	0.06800100	-0.16840900	-2.97398500
C	0.12671700	-1.03531100	-2.05844200
C	0.93545800	-2.17630400	-1.63815200
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C	0.60465200	-3.03282100	-0.57486600
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H	-0.60723400	0.62620600	-3.24266100
C	-1.43969100	-0.88699500	-0.55070600
C	-2.67777000	-0.96362100	-0.61613300
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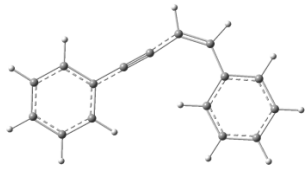
Z-pdt



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H	-3.86991800	-2.86191400	-0.14401000
H	-1.68942500	-1.68478100	-0.14951100
H	-3.72835900	2.09446900	0.12709100
H	-5.91046200	0.91633800	0.13096500
H	-5.98749700	-1.56576600	-0.00414000
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C	-0.23450000	1.54710100	-0.01329200
C	0.94497600	2.32504500	-0.02103700
H	0.77351900	3.40131200	-0.03435500
C	2.24152700	1.92135800	-0.01854400
H	2.97253100	2.72818500	-0.03567600
C	2.83702600	0.58655600	0.00116300
C	2.09935600	-0.61310800	0.06705800
C	4.24318700	0.49388700	-0.04490600
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H	1.01770400	-0.57266400	0.10865900
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H	4.83037000	1.40821000	-0.09411100
C	4.14237200	-1.91688100	0.03383000
H	2.15955400	-2.75772400	0.13547900
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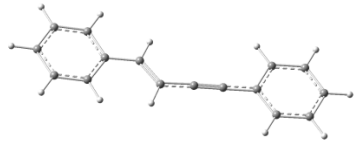
E-pdt



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C	5.49587600	-1.00381500	-0.00017400
C	6.02100500	0.29113400	0.00020200
H	5.56037600	2.39884100	0.00071400
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H	3.70759200	-2.20870700	-0.00061900
H	6.16307000	-1.86162400	-0.00035600
H	7.09684100	0.44332000	0.00031600
C	1.82826500	-0.30197100	-0.00022900
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H	-1.09133700	-1.72543700	-0.00062100
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H	-1.33594200	1.33395300	0.00018300
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C	-3.95059600	1.31888100	-0.00032400
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H	-3.46454800	2.29179900	-0.00064200
C	-5.19699500	-1.16766600	0.00048700
H	-3.22737300	-2.00757800	0.00092200
C	-5.97229000	-0.00342600	0.00006200
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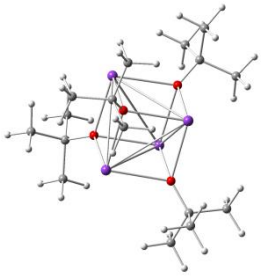
KtBuCubic



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O	0.89903500	-0.96155000	1.87619700
O	1.64725800	0.28818500	-1.57775200
O	-1.64698000	-1.36654500	-0.85005400
O	-0.90896700	2.04201200	0.53852200
C	-2.64312900	-2.19085400	-1.35320500

C	-4.00868200	-1.45412800	-1.37958800
H	-4.82571000	-2.07429100	-1.77205200
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H	-3.58059700	-4.14442800	-0.84643000
H	-1.85433300	-4.02275000	-0.45016600
H	-3.05324100	-3.18752400	0.55284700
C	-2.30988900	-2.63873300	-2.80125500
H	-2.20573800	-1.76159900	-3.45471700
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H	-0.89977900	4.22684300	-1.03176400
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H	-3.14930900	3.09861700	-0.52320700
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C	2.65745300	0.45558700	-2.51372600
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H	3.11555200	-0.21827000	-4.58473800
H	2.22963000	-1.39810900	-3.59741300
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H	3.61795000	2.12863200	-3.62330000
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C	4.01312500	-0.06025100	-1.96151000
H	4.28193100	0.48386200	-1.04548700
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H	4.84067000	0.05353200	-2.67454900
C	1.44781900	-1.54144600	3.01070300
C	0.77113400	-2.90414000	3.31686200
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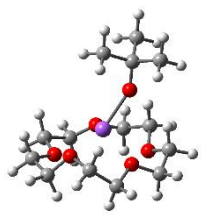
Na-Crown-OtBu (A')



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C	-1.23354400	1.72081600	1.91442000
H	-1.81514900	2.05649300	2.78882900
H	-1.90347900	1.37321100	1.11175800
C	-0.35987700	2.86090900	1.43070100
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C	1.47511400	3.14373000	-0.08880000
H	1.27149800	4.18232400	-0.39716400
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C	2.15330500	2.40525600	-1.22804600
H	3.09258800	2.91591800	-1.49233100
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C	1.60946300	-2.69165800	1.14036500
H	1.45846300	-3.67392000	1.61797100
H	2.49195600	-2.22494700	1.60925100
C	1.80818000	-2.89903000	-0.35796600
H	2.68450400	-3.53775700	-0.54231700
H	0.92275000	-3.39242600	-0.76793700
C	3.12420100	0.27462700	-1.71522000
H	2.59663600	0.23563100	-2.68083600
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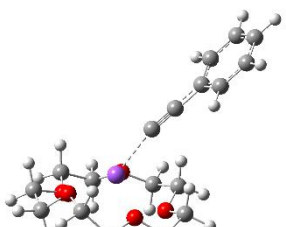
O	1.92177100	-1.66703300	-1.06841500
Na	0.13809400	0.01377200	-0.16947800
O	-1.94734600	-0.12599500	-0.44856500
C	-3.00075200	-0.39246400	-1.29060700
C	-2.49387500	-0.81880800	-2.69492500
H	-1.88008600	-0.01412100	-3.12226500
H	-1.86238600	-1.71254200	-2.60204200
H	-3.30462700	-1.04368200	-3.40328800
C	-3.87380200	-1.54220200	-0.71926700
H	-3.25833600	-2.44263700	-0.59620100
H	-4.25431400	-1.25801900	0.27020200
H	-4.73297600	-1.79510600	-1.35738200
C	-3.89484400	0.86558400	-1.45948700
H	-4.74993400	0.70461000	-2.13198600
H	-4.28378800	1.17647600	-0.48129500
H	-3.29228800	1.69149000	-1.85881400

<u>Na-Crown-Ph (B')</u>



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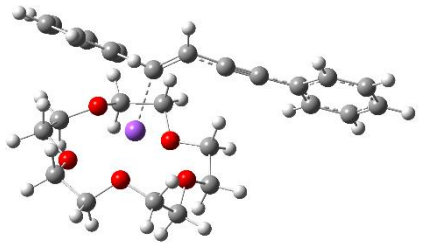
O	1.33459700	-2.03449300	0.97337800
C	1.03454400	-1.94409000	2.36035300
H	1.95323600	-1.75241300	2.93661600
H	0.58750900	-2.88448300	2.71728000
C	0.05644600	-0.79815200	2.54652200
H	-0.28509100	-0.77172200	3.59388700
H	-0.80943500	-0.92765100	1.88197200
O	0.74973500	0.40106000	2.21353500
C	-0.08075000	1.55979400	2.13182600
H	-0.50204200	1.80575100	3.11988200
H	-0.89653200	1.38325300	1.41652500
C	0.80328600	2.70216300	1.66798300
H	0.23027000	3.64134500	1.65669300
H	1.65127600	2.81864000	2.35995900
O	1.28736500	2.39608000	0.36396200
C	2.46273100	3.07902000	-0.02023300
H	2.26401500	4.14426000	-0.22078100
H	3.22032600	3.01492200	0.77664700
C	2.99440500	2.42023200	-1.27997700
H	3.91686000	2.92915700	-1.60004200
H	2.25577700	2.49299300	-2.09264700
O	3.25365000	1.05385000	-0.97578000
C	2.40342500	-2.88924500	0.62355100
H	2.23572200	-3.91332300	0.99560600
H	3.34746600	-2.52461100	1.06201200
C	2.46411500	-2.92133400	-0.90034200
H	3.27911100	-3.57951200	-1.23510600
H	1.51771700	-3.31026900	-1.28579800
C	3.85005200	0.31389400	-2.03089500
H	3.24449100	0.39033600	-2.94690400
H	4.86085700	0.69345200	-2.24833800
C	3.92879800	-1.13439700	-1.58780700
H	4.48650100	-1.72158800	-2.33389900
H	4.46521700	-1.19303200	-0.62923700
O	2.59959100	-1.61936300	-1.46764800
Na	1.03641700	0.00911800	-0.29709200
C	-1.28088100	-0.04845700	-0.69994800
C	-2.52171600	-0.06624000	-0.67915700
C	-3.94932300	-0.08315000	-0.66375100
C	-4.66807600	-1.27235800	-0.40428100
C	-4.70038700	1.09043300	-0.90241100
C	-6.06057400	-1.28449400	-0.38296100
H	-4.10909900	-2.18629100	-0.22326600
C	-6.09277000	1.07354000	-0.88021300
H	-4.16639400	2.01387800	-1.10845900
C	-6.78443100	-0.11271400	-0.61993000
H	-6.58615100	-2.21571800	-0.18150600
H	-6.64362900	1.99273400	-1.06889700

H	-7.87142800	-0.12415300	-0.60373200

Na-Crw-PhP (E')



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O	0.71832700	-1.86560900	1.21549800
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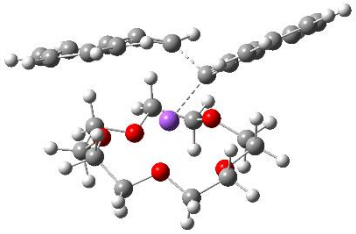
H	1.19145500	-3.69012800	0.34353800
H	2.59015300	-2.68333600	0.82233300
C	1.60008000	-2.03364200	-0.97864400
H	2.31878100	-2.57380300	-1.61542200
H	1.90591000	-0.98060500	-0.90556200
O	0.28350800	-2.13460500	-1.51333400
C	0.08107900	-1.43412400	-2.73740400
H	0.73944800	-1.82834600	-3.52746000
H	0.28815600	-0.36309500	-2.59916800
C	-1.36887500	-1.64834500	-3.13202000
H	-1.56862000	-1.17847000	-4.10689800
H	-1.56954000	-2.72676500	-3.21711900
O	-2.18926200	-1.07982700	-2.12008600
C	-3.50891000	-1.59058200	-2.04428700
H	-4.12257300	-1.23748500	-2.88805300
H	-3.48978200	-2.69109400	-2.06754300
C	-4.12223400	-1.11514600	-0.74025200
H	-5.15202000	-1.49772900	-0.66247000
H	-4.14760800	-0.01682100	-0.70508900
O	-3.31936400	-1.62061000	0.32446500
C	0.37804000	-2.42026800	2.47248900
H	1.27918800	-2.63747300	3.06808500
H	-0.17154200	-3.36626200	2.33476100
C	-0.46568900	-1.38224000	3.20410500
H	-0.75896200	-1.76094400	4.19389800
H	0.12515400	-0.47187200	3.33803600
C	-3.80744700	-1.30781400	1.62280500
H	-3.95861600	-0.22333100	1.72562600
H	-4.76721400	-1.81571300	1.80743300
C	-2.77609400	-1.78055800	2.62923200
H	-3.16992200	-1.65762600	3.64991600
H	-2.56533300	-2.84781400	2.46455300
O	-1.60972600	-0.98956100	2.45017100
Na	-1.01283300	-0.62659100	0.04005600
C	-0.41083200	1.72453700	-0.25197000
C	0.75098100	2.43115800	-0.18574500
H	0.75791700	3.53183700	-0.12826500
C	2.05793200	1.86712900	-0.18313500
C	3.21582000	1.47223800	-0.17939800
C	4.58127900	1.07443500	-0.12130400
C	5.53158300	1.88227100	0.54368400
C	5.03740400	-0.12052400	-0.71968600
C	6.86967100	1.50565500	0.60924500

H	5.19744900	2.80583500	1.00670200
C	6.37751400	-0.49272300	-0.64736500
H	4.32836500	-0.74479500	-1.25544000
C	7.30254700	0.31548800	0.01761400
H	7.58075900	2.14508200	1.12676600
H	6.70358900	-1.41709600	-1.11864900
H	8.34809700	0.02407600	0.07090100
C	-1.65495400	2.50144700	-0.16222700
C	-2.66913400	2.37736800	-1.14330300
C	-1.93819100	3.34870600	0.93640800
C	-3.87243900	3.07488300	-1.04557500
H	-2.48551900	1.72574300	-1.99489700
C	-3.15425900	4.02294600	1.04706400
H	-1.18362000	3.46104900	1.71116800
C	-4.13173500	3.89699800	0.05629300
H	-4.61653300	2.97640600	-1.83460800
H	-3.33588200	4.66286200	1.90885100
H	-5.07596800	4.42935000	0.13916900

TS2''



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O	-0.80098400	-0.32123200	2.42949500
C	-0.23368700	-1.35033000	3.22804600
H	-1.02610600	-2.01145500	3.61240300
H	0.30743100	-0.92085300	4.08514100
C	0.2110700	-2.14558700	2.35796300
H	1.24558400	-2.89273500	2.97499500
H	1.45941000	-1.47749200	1.89396000
O	-0.5880000	-2.78443800	1.35207100
C	0.0698800	-3.46459500	0.36037100
H	1.28339500	-4.28805800	0.81197200
H	1.39614100	-2.76016700	-0.12478300
C	-0.27265900	-4.03618400	-0.64644500
H	0.26878000	-4.62655400	-1.40160000
H	-0.98497300	-4.69949200	-0.13268900
O	-0.97383300	-2.95907700	-1.25597200
C	-2.19038200	-3.31834200	-1.88756400
H	-2.00620300	-3.81866600	-2.85153600
H	-2.76017500	-4.00693100	-1.24505200
C	-2.99924700	-2.05506300	-2.11441500
H	-3.94713000	-2.31467600	-2.61151700
H	-2.44847200	-1.34887400	-2.75279300
O	-3.24130200	-1.46995300	-0.83925400
C	-1.92333900	0.33433200	2.99430300
H	-1.65405600	0.84483500	3.93317900
H	-2.71331000	-0.40008700	3.22337700
C	-2.40074800	1.36085500	1.97478200
H	-3.27950000	1.89820600	2.35762600
H	-1.60735000	2.08702800	1.77753300

C	-4.06611900	-0.31209200	-0.87216900
H	-3.69080300	0.40241300	-1.61818500
H	-5.10285800	-0.58226100	-1.12814600
C	-4.01952800	0.32410300	0.50396300
H	-4.70676200	1.18325300	0.53644200
H	-4.33784900	-0.40599500	1.26391900
O	-2.68430400	0.74898500	0.71974700
Na	-0.91656400	-0.77529800	-0.00503800
C	1.38353000	-0.18495500	-0.64519600
C	2.61097300	-0.02823300	-0.53212100
C	4.01830100	0.13478600	-0.37961700
C	4.55096500	1.12324800	0.47898700
C	4.92888400	-0.69009600	-1.07827900
C	5.92639500	1.27503000	0.63026900
H	3.86460700	1.76739800	1.02116000
C	6.30324700	-0.53176900	-0.92384900
H	4.53615900	-1.45172800	-1.74595800
C	6.81190700	0.44988100	-0.06878600
H	6.31143600	2.04405000	1.29597300
H	6.98325000	-1.17716100	-1.47513100
H	7.88538800	0.57177800	0.04974300
C	0.21061100	0.41897500	-2.16458000
C	-0.46907100	1.48818600	-2.14841900
C	-0.74244900	2.65282400	-1.35296200
C	0.27069500	3.23365200	-0.55339000
C	-2.00740200	3.27983500	-1.36534100
C	0.01919000	4.37986400	0.19882300
H	1.24740500	2.76092400	-0.53569200
C	-2.25785700	4.41590500	-0.59937100
H	-2.78636100	2.86755200	-2.00167600
C	-1.24577500	4.97630700	0.18652300
H	0.81652500	4.81124700	0.80050200
H	-3.24145400	4.88005800	-0.62972200
H	-1.43653600	5.87361000	0.76999300
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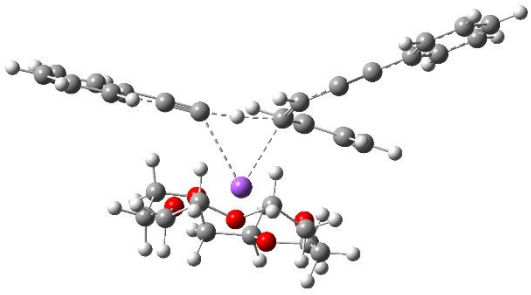
TS3z'



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O	-3.30175900	-0.76689500	1.05013100
C	-3.66953400	-0.23806000	2.31158000
H	-4.00193000	-1.04331800	2.98556000
H	-4.48540400	0.49236300	2.20449400
C	-2.43829900	0.45154100	2.87594100
H	-2.65999700	0.86306400	3.87314500
H	-2.13751900	1.26844500	2.20491700
O	-1.41653500	-0.53569600	2.94885800
C	-0.12780300	-0.07588200	3.33640200
H	-0.15587300	0.39027800	4.33383700

H	0.25537600	0.66013900	2.61465300
C	0.76800200	-1.30210000	3.37411900
H	1.78637500	-1.01952500	3.67803200
H	0.36825400	-2.01599100	4.10905800
O	0.77261900	-1.89388400	2.08055400
C	1.02859700	-3.28962700	2.06463700
H	2.07741700	-3.50385500	2.32273100
H	0.38132400	-3.79594700	2.79720100
C	0.73907700	-3.81731300	0.67262800
H	0.92180700	-4.90338700	0.65582800
H	1.39371300	-3.33774200	-0.06661900
O	-0.62766500	-3.53837100	0.37577200
C	-4.32223700	-1.39754000	0.30088600
H	-5.23283300	-0.77934900	0.27345500
H	-4.58540100	-2.36725100	0.75410000
C	-3.79219300	-1.54651400	-1.12358600
H	-4.51349100	-2.09825800	-1.74420500
H	-3.63755500	-0.55008700	-1.54345400
C	-1.06092800	-4.02795300	-0.88903800
H	-0.42952900	-3.62233300	-1.69251000
H	-1.00518700	-5.12764400	-0.91546700
C	-2.49892300	-3.58620900	-1.07978000
H	-2.90585000	-4.02804600	-2.00238900
H	-3.10356200	-3.93649500	-0.23085900
O	-2.50756600	-2.16738200	-1.16604400
Na	-0.98613500	-1.07667300	0.47087600
C	0.89709800	0.41844800	-0.66642000
C	1.58014000	1.38317100	0.01177500
C	1.55672900	-0.60002800	-1.49641500
C	2.75467700	-1.26461000	-1.14101600
C	0.93434300	-1.00614900	-2.70001400
C	3.30003900	-2.26304200	-1.94915200
H	3.25596800	-0.98357900	-0.22049100
C	1.49102000	-1.98927500	-3.51777100
H	0.00810100	-0.51746600	-2.99263900
C	2.67680400	-2.62998200	-3.14570100
H	4.22478000	-2.75176500	-1.64788500
H	0.99728600	-2.25711800	-4.44963900
H	3.10977300	-3.40022900	-3.77903600
C	2.97738000	1.64149000	0.03365400
C	4.17199800	1.89005700	0.07330300
C	5.57262700	2.13776900	0.08465300
C	6.12962500	3.13617800	0.91179200
C	6.44065600	1.38388500	-0.73480900
C	7.50243400	3.36748300	0.91811800
H	5.46981300	3.72350200	1.54344200
C	7.81193600	1.62242200	-0.72234600
H	6.01825100	0.61756600	-1.37782500
C	8.35073500	2.61331800	0.10302900
H	7.91321300	4.14176500	1.56137700
H	8.46473600	1.03332800	-1.36177500
H	9.42173500	2.79774100	0.10916300
H	0.98290800	2.10770100	0.58038900
C	-1.70429100	1.52755700	-0.65112900
C	-2.75140300	2.16146900	-0.75293700
C	-3.98571000	2.87634700	-0.84557700
C	-4.40821000	3.73491200	0.19161300
C	-4.82223700	2.73807400	-1.97355100

C	-5.61900600	4.41804800	0.10520800
H	-3.76661200	3.86336100	1.05869900
C	-6.03189200	3.42402100	-2.05435300
H	-4.50211900	2.09305100	-2.78688300
C	-6.43858600	4.26566800	-1.01600700
H	-5.92293800	5.07684200	0.91510100
H	-6.65892500	3.30476300	-2.93461900
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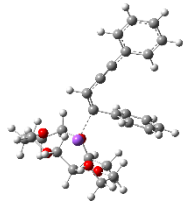
Na-Crw-PhPcis (C'')



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O	3.22994100	-2.11136000	-1.25312800
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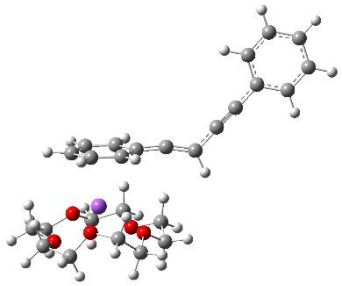
H	4.60950000	-3.04721300	-0.01295000
H	3.64188400	-4.14003000	-1.04314800
C	2.59017200	-3.34917200	0.67066600
H	2.79283200	-4.26165800	1.25358800
H	1.57743200	-3.41953200	0.24712300
O	2.71027400	-2.19161500	1.48441700
C	1.70617900	-2.04870100	2.48851800
H	1.74253100	-2.89021600	3.19765800
H	0.71156400	-2.00569900	2.02125700
C	1.99800700	-0.75001300	3.21864500
H	1.28633600	-0.61799800	4.04786200
H	3.01687700	-0.78006400	3.63487000
O	1.88516800	0.30647700	2.27956700
C	2.49672600	1.52932600	2.64819900
H	1.94114900	2.02439800	3.45963800
H	3.52722900	1.34771800	2.99231100
C	2.50887500	2.42695600	1.42478100
H	2.98836500	3.38470300	1.68011000
H	1.48478600	2.62241400	1.08035200
O	3.25163200	1.75410200	0.40596400
C	4.21974300	-1.64565200	-2.15491400
H	4.53442900	-2.44488900	-2.84520400
H	5.11009000	-1.30866200	-1.59921300
C	3.59915000	-0.50718900	-2.95655200
H	4.32440500	-0.12183000	-3.68730500
H	2.72678900	-0.88520400	-3.49773300
C	3.38798800	2.49402400	-0.80094700
H	2.40214700	2.82306400	-1.15858700
H	4.02225900	3.38057700	-0.64186900
C	4.03503500	1.58417700	-1.82782100
H	4.26270400	2.15599000	-2.74031000
H	4.97693000	1.18322900	-1.42447600
O	3.11466900	0.53831400	-2.11900100
Na	1.97537800	-0.34155600	-0.09188200
C	-0.44343900	-0.52097500	-0.30258500
C	-1.40705000	-1.48320700	-0.31545700

C	-0.80226000	0.89762300	-0.21666900
C	-1.38210000	1.46479000	0.94553600
C	-0.45432100	1.80265500	-1.25109700
C	-1.59141300	2.83815500	1.06528000
H	-1.67273400	0.80121900	1.75575600
C	-0.68808100	3.17325300	-1.13922700
H	-0.00359100	1.40378200	-2.15828400
C	-1.24779200	3.70918500	0.02561000
H	-2.04370400	3.23222000	1.97398800
H	-0.43277200	3.82967900	-1.96985400
H	-1.42181200	4.77833500	0.11679100
C	-2.81840200	-1.27248600	-0.32184000
C	-4.02670000	-1.09734800	-0.32183500
C	-5.42525100	-0.84208200	-0.31298400
C	-5.91303500	0.48134000	-0.23682600
C	-6.36259600	-1.89574600	-0.37654100
C	-7.28179900	0.73409200	-0.22530200
H	-5.19874000	1.29763700	-0.18646600
C	-7.72993500	-1.63352200	-0.36438300
H	-5.99947800	-2.91763100	-0.43591200
C	-8.19858700	-0.31918500	-0.28888700
H	-7.63658300	1.76039800	-0.16657500
H	-8.43501000	-2.45999100	-0.41461500
H	-9.26667900	-0.11781200	-0.28017200
H	-1.11437200	-2.53852800	-0.34116700

TS**f'**



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H	-1.81091000	1.18460700	3.42520900
H	-0.12513400	1.63834600	3.03802600
C	-0.65757200	-0.37837200	2.49041700
H	-0.29331000	-0.79715700	3.44123500
H	0.12368700	-0.48863900	1.72530000
O	-1.85690200	-1.03222600	2.07956800
C	-1.73245800	-2.42977900	1.84886600
H	-1.39334600	-2.94934200	2.75892800
H	-1.01191800	-2.61865200	1.04164700
C	-3.11038300	-2.93532900	1.46494700
H	-3.07898800	-4.02217000	1.29326100
H	-3.81549300	-2.73332500	2.28511500
O	-3.52704900	-2.24721900	0.29252900
C	-4.92395100	-2.26434300	0.05597500
H	-5.24703900	-3.23360500	-0.35567500
H	-5.46804500	-2.09079200	0.99677200
C	-5.25600500	-1.15677000	-0.92587700
H	-6.34001700	-1.15688900	-1.11881800

H	-4.72652400	-1.30817300	-1.87803000
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H	-2.94091100	2.84432700	2.11460800
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H	-2.85580300	4.26574000	0.03244300
H	-1.46204300	3.31103900	-0.54260300
C	-5.26111300	1.23276200	-1.04829500
H	-4.94801700	1.16899600	-2.10080100
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C	-0.00918200	0.82065400	-1.83682800
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C	-1.69987200	-0.64869500	-2.83801400
H	-1.50392100	-2.73757500	-2.30242200
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H	-2.50265300	-0.80046300	-3.55314000
C	4.04403700	0.07702600	0.38601600
C	5.25466900	0.05312900	0.24574800
C	6.66321900	0.01587800	0.04397400
C	7.20261900	-0.27320400	-1.22790900
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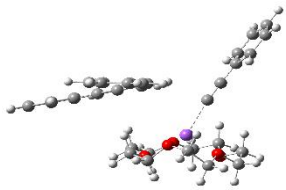
H	7.15250700	0.49038500	2.09014900
C	9.45368300	-0.05850700	-0.36131400
H	8.97604500	-0.53358700	-2.41093200
H	9.60458300	0.42532700	1.73572800
H	10.52886500	-0.08719300	-0.51759500
H	2.34367800	0.34874700	1.63451700

Na-Crw-PhPcisP (D')



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O	3.98262400	-2.40219300	-0.51650500
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H	5.68555400	-2.24923600	-1.69946900
C	4.04029600	-1.10449300	-2.50415900

H	4.57530700	-0.95382700	-3.45566200
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C	0.47324400	-0.63958100	-3.30681000
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H	3.66799000	-4.33912000	2.16651000
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H	-0.07814800	1.82323500	0.40826400

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