Electronic Supplementary Information

for

Divergent Reactivity of a New Dinuclear Xanthene-Bridged Bis(iminopyridine) Di-Nickel Complex with Alkynes

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1. ^{1}H and ^{13}C NMR Spectra

i. Spectra of Metal Complexes

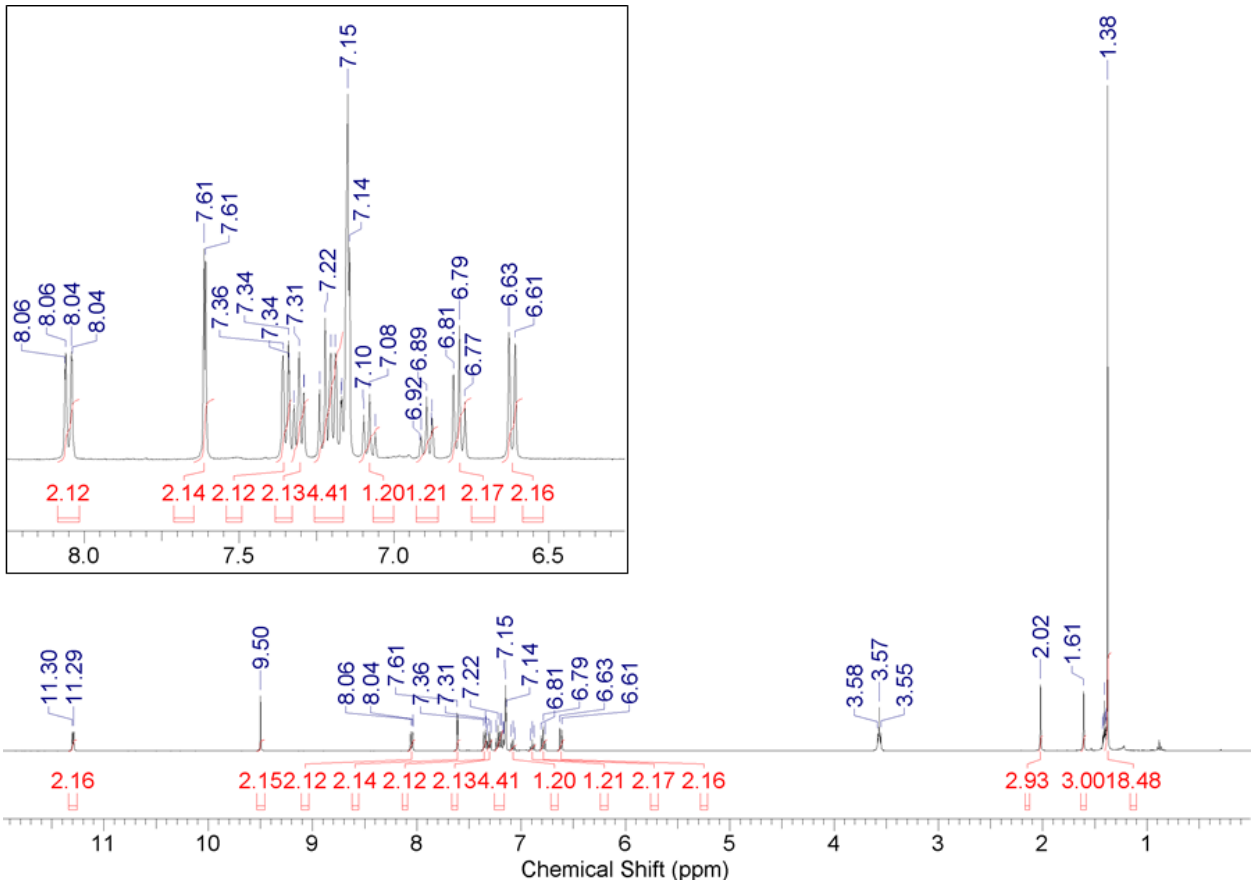

Figure S1. ^{1}H spectrum of *2*.

The peak at 3.57 ppm corresponds to THF.

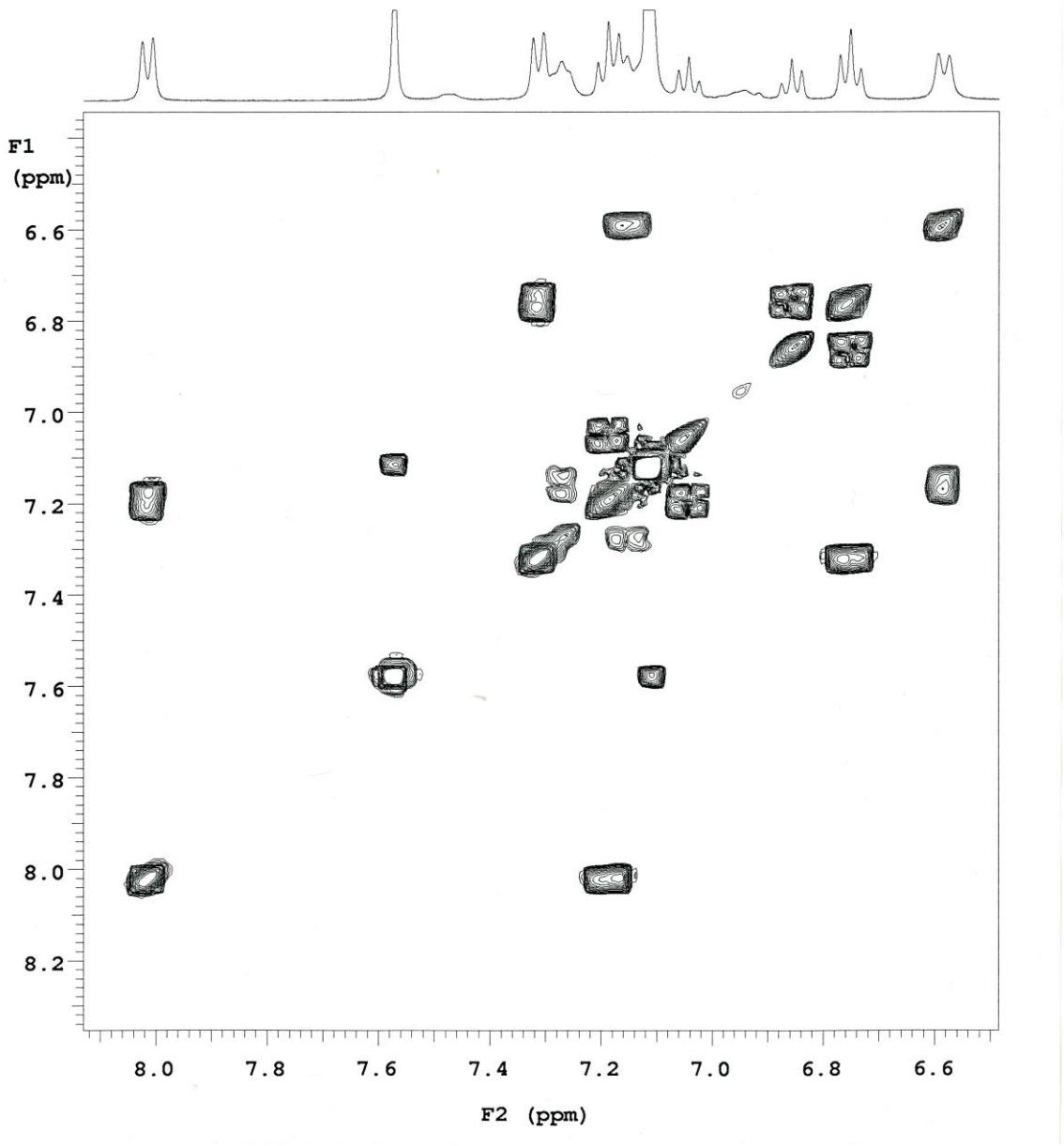

Figure S2. gCOSY NMR spectrum of *2*.

Only the aromatic region is shown. Evidence for a peak hidden by benzene (7.15 ppm) is shown through coupling between 7.15 ppm and 7.61 ppm (meta-coupling on the xanthene backbone). Evidence for two signals in the multiplet region (7.15 ppm to 7.25 ppm) is shown through multiple, different coupling patterns (7.08 ppm to the multiplet to 8.05 ppm and 6.63 ppm to the multiplet to 7.31 ppm).

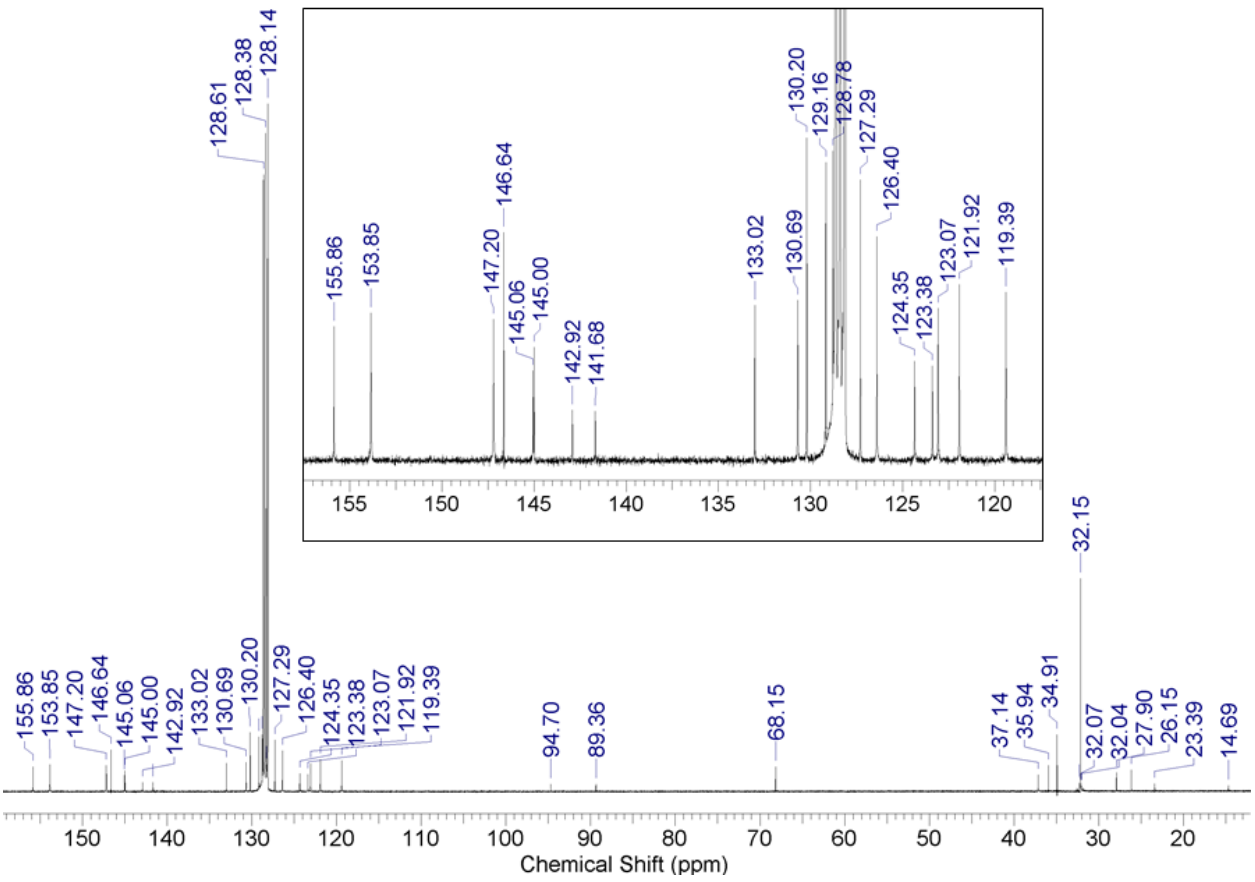

Figure S3. ^{13}C spectrum of *2*.

The peaks at 68.15 ppm and 26.15 ppm correspond to THF.

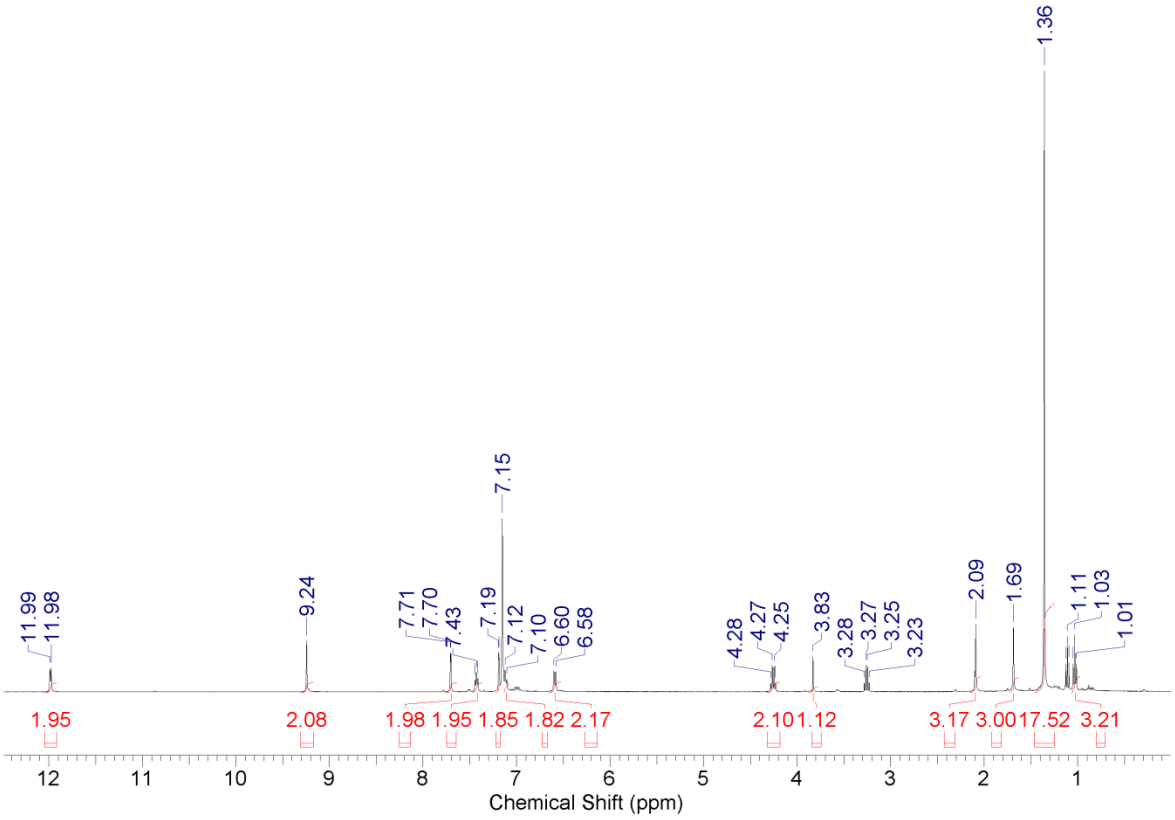

Figure S4. ^{1}H NMR spectrum of *3*.

The peaks at 3.26 ppm and 1.11 ppm correspond to ether.

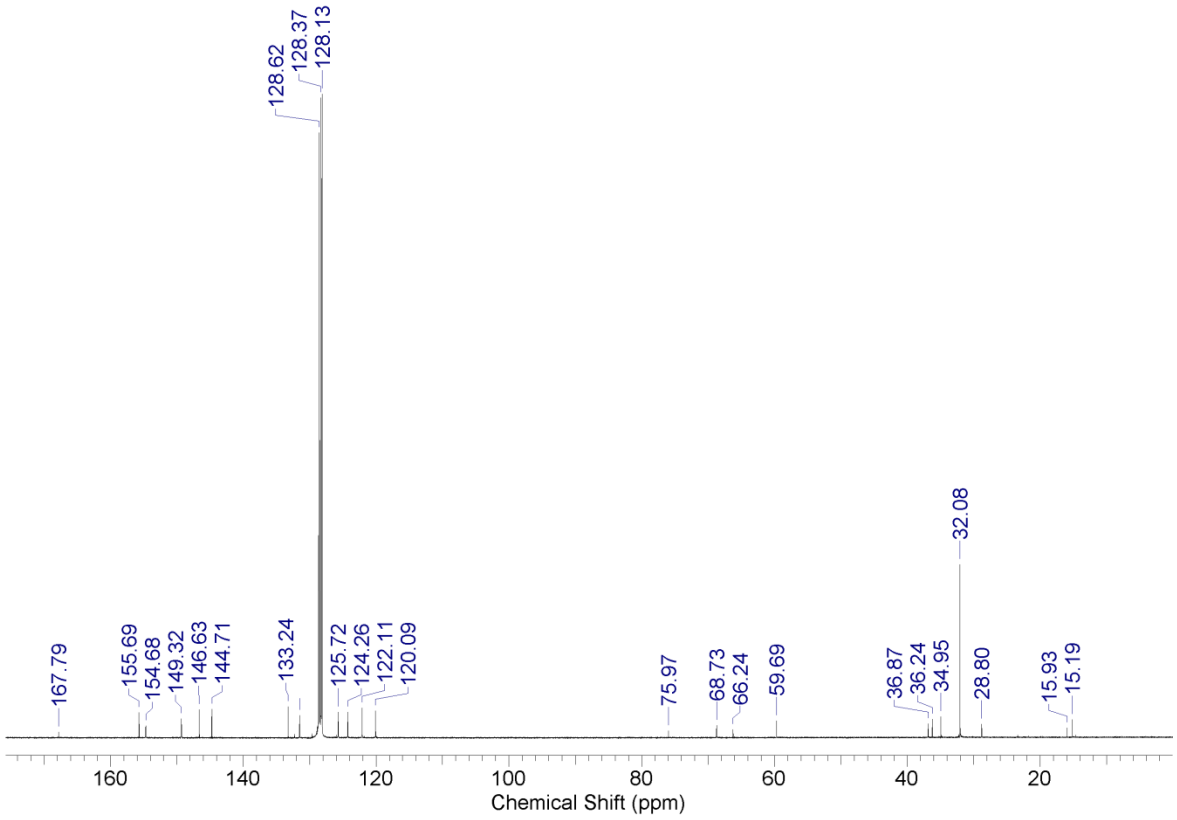

Figure S5. ^{13}C NMR spectrum of *3*.

The peaks at 66.24 ppm and 15.93 ppm correspond to ether.

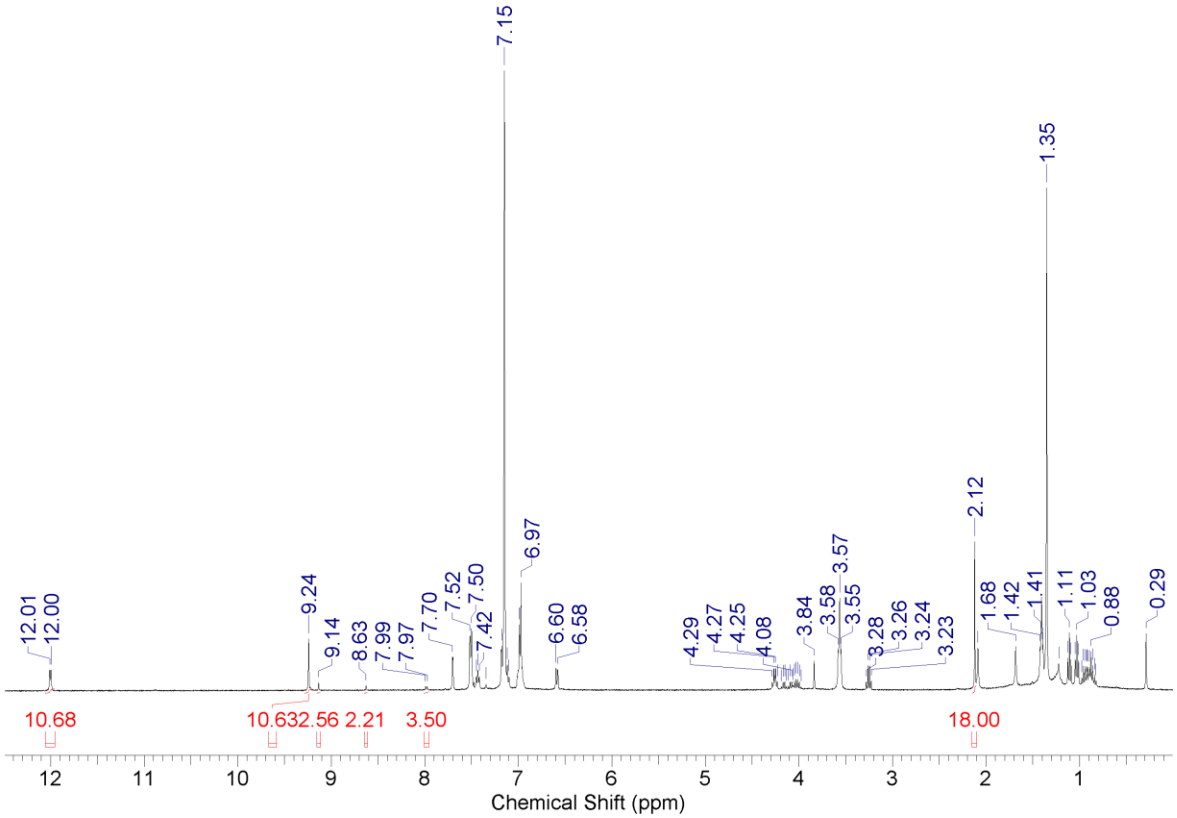

Figure S6. Reaction mixture of *2* with 2 equivalents of ethyl propiolate.

The peaks at 12.00 ppm, 9.24 ppm, 7.70 ppm, 7.42 ppm, 6.59 ppm, 4.26 ppm, 3.84 ppm, 2.09 ppm, 1.68 ppm, 1.35 ppm, and 1.03 ppm correspond to ***3***. The peak at 9.14 ppm corresponds to the 1,2,4-isomer. The peaks at 8.63 ppm and 7.99 correspond to the 1,3,5-isomer. The peaks at 7.51 ppm and 6.97 ppm correspond to diphenylacetylene. The peaks at 3.57 ppm and 1.41 ppm correspond to THF. The peaks at 3.26 ppm and 1.11 ppm correspond to ether. The peaks at 1.23 ppm and 0.88 ppm correspond to hexane.

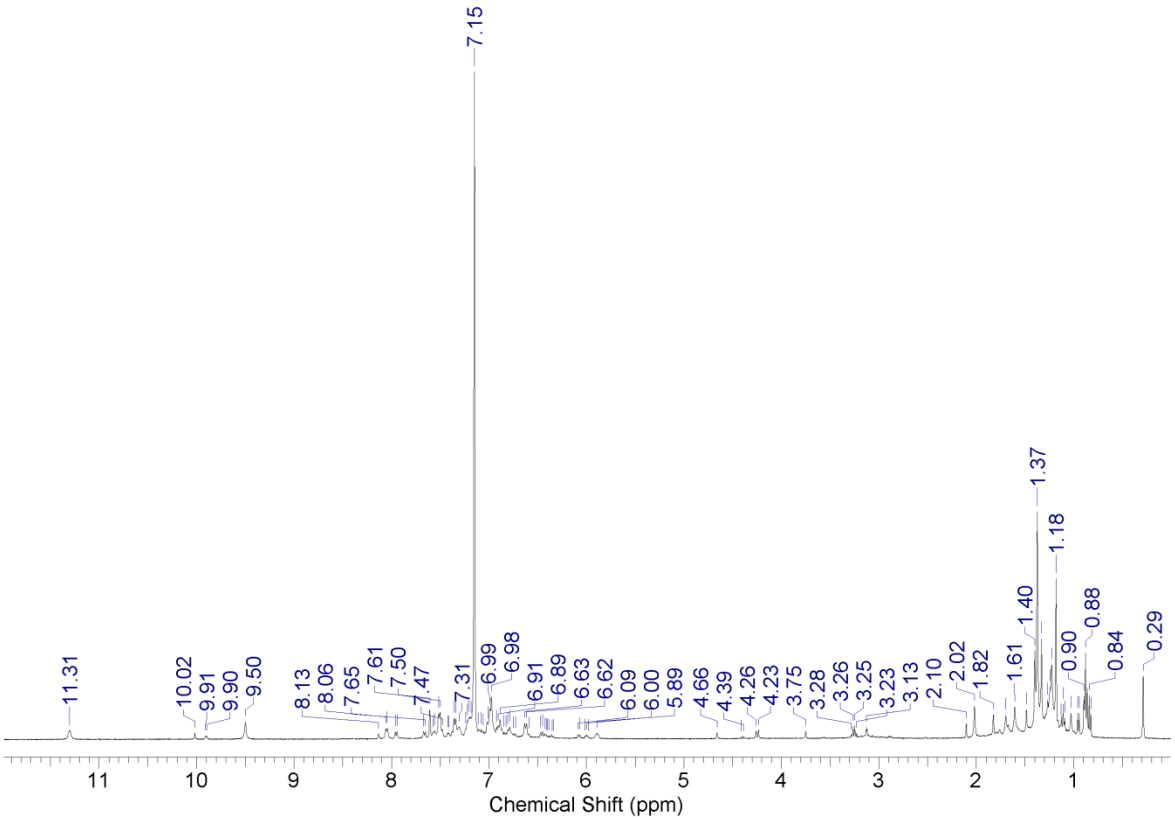

Figure S7. Reaction mixture of *2* with 1 equivalent of methyl propargyl ether (full spectra).

The peaks at 11.31 ppm and 9.50 ppm correspond to **2**.

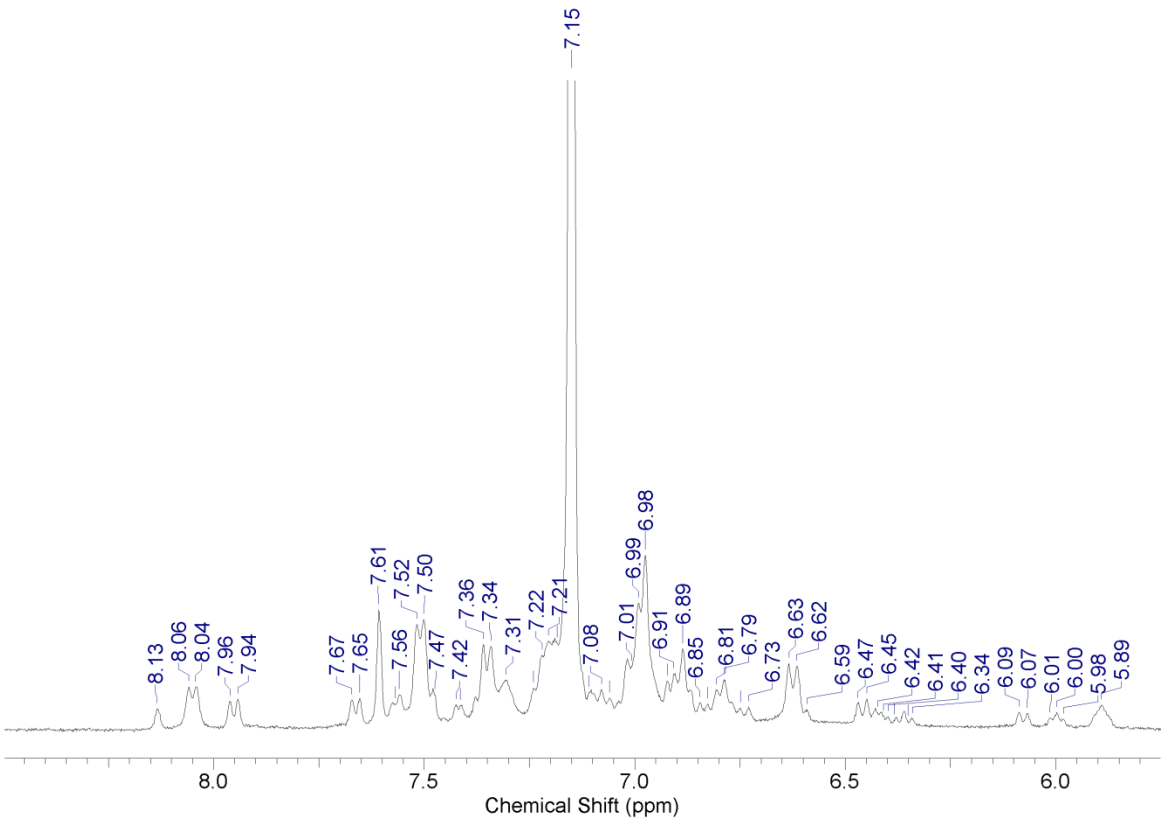

Figure S8. Reaction mixture of *2* with 1 equivalent of methyl propargyl ether (aromatic region).

The peaks at 8.05 ppm, 7.61 ppm, 7.35 ppm, 7.31 ppm, 7.21 ppm, 7.08 ppm, 6.89 ppm, 6.79 ppm, and 6.62 ppm correspond to ***2***. The peaks at 7.51 ppm and 6.98 ppm correspond to diphenylacetylene.

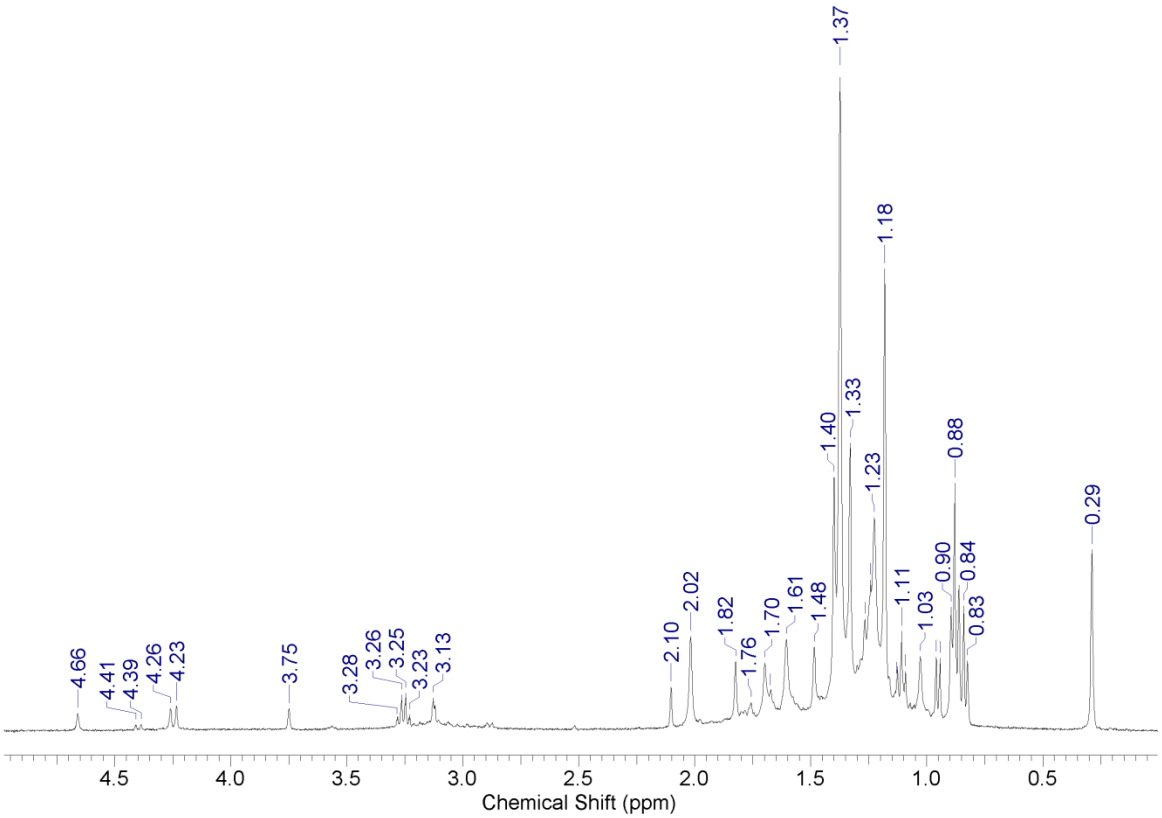

Figure S9. Reaction mixture of *2* with 1 equivalent of methyl propargyl ether (aliphatic region).

The peaks at 2.02 ppm, 1.61 ppm, and 1.37 ppm correspond to ***2***. The peaks at 4.41 ppm and 4.39 ppm correspond to the 1,2,4-isomer (2H and 2H respectively). The peak at 4.26 ppm corresponds to the 1,3,5-isomer (6H). The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peak at 2.10 ppm corresponds to toluene. The peaks at 1.23 ppm and 0.88 ppm correspond to hexane.

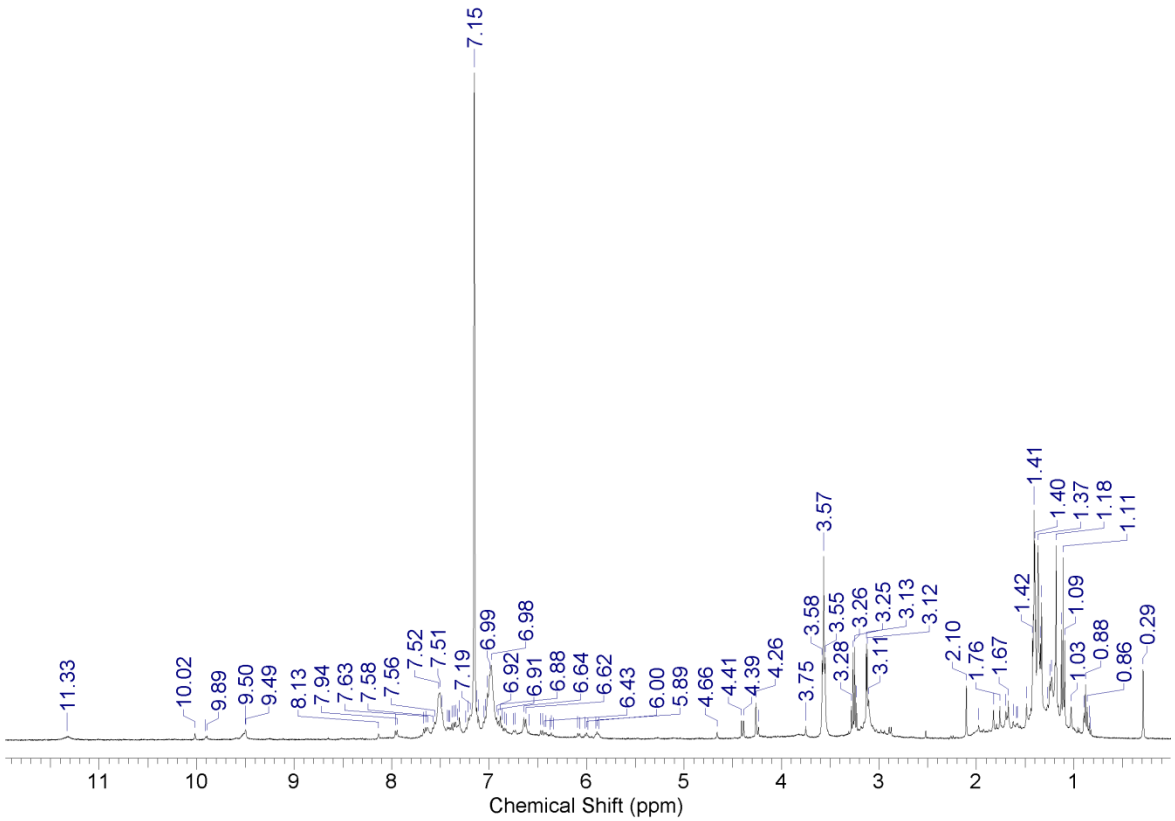

Figure S10. Reaction mixture of *2* with 2 equivalents of methyl propargyl ether (full spectrum).

The peaks at 11.33 ppm and 9.50 ppm correspond to ***2***.

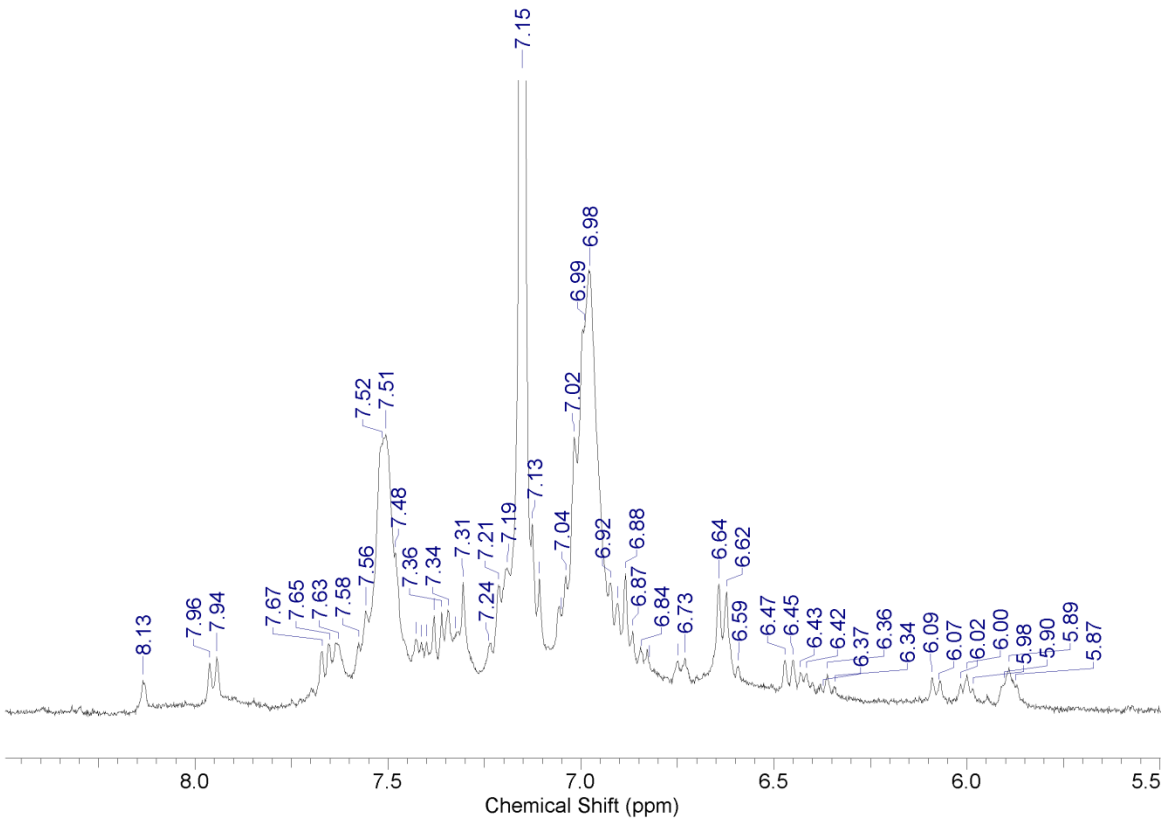

Figure S11. Reaction mixture of *2* with 2 equivalents of methyl propargyl ether (aromatic region).

The peaks at 7.61 ppm, 7.35 ppm, 7.31 ppm, 7.21 ppm, 6.88 ppm, 6.79 ppm, and 6.63 ppm correspond to **2**. The peaks at 7.51 ppm and 6.98 ppm correspond to diphenylacetylene.

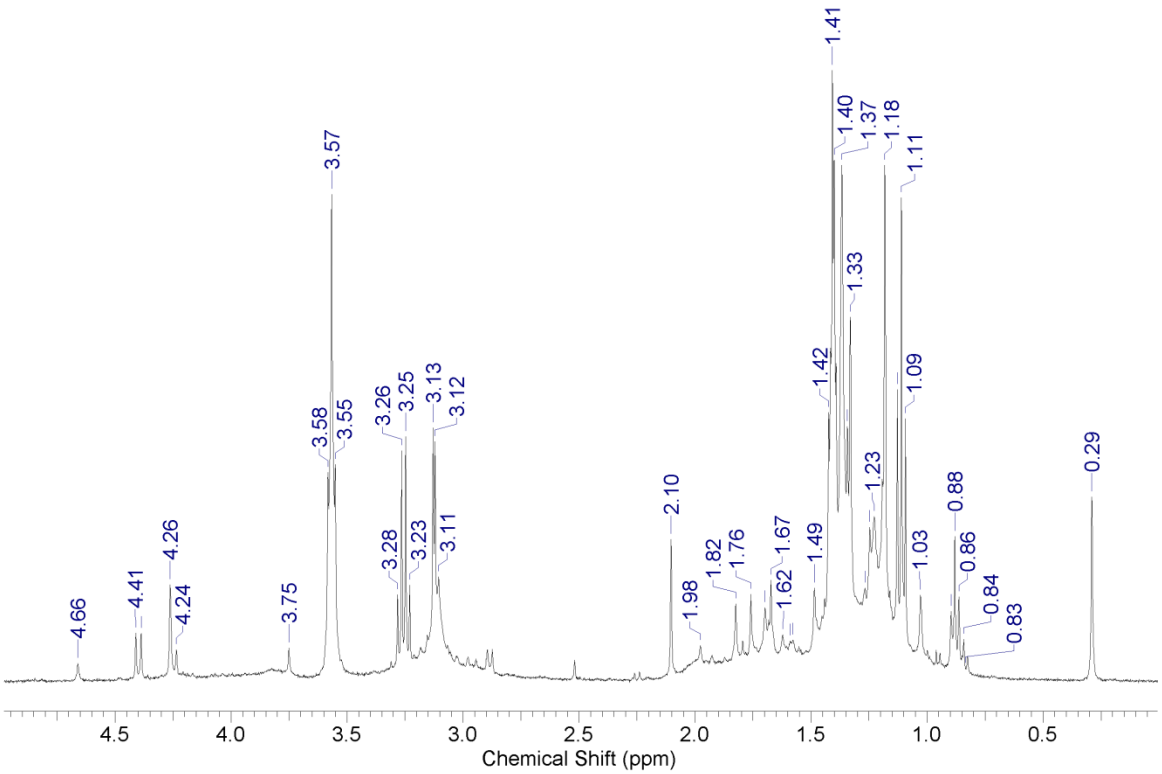

Figure S12. Reaction mixture of *2* with 2 equivalents of methyl propargyl ether (aliphatic region).

The peaks at 1.62 ppm and 1.37 ppm correspond to ***2***. The peaks at 4.41 ppm and 4.39 ppm correspond to the 1,2,4-isomer (2H and 2H respectively). The peak at 4.26 ppm corresponds to the 1,3,5-isomer (6H). The peaks at 3.57 ppm and 1.41 ppm correspond to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peak at 2.10 ppm corresponds to toluene. The peaks at 1.23 ppm and 0.88 ppm correspond to hexane.

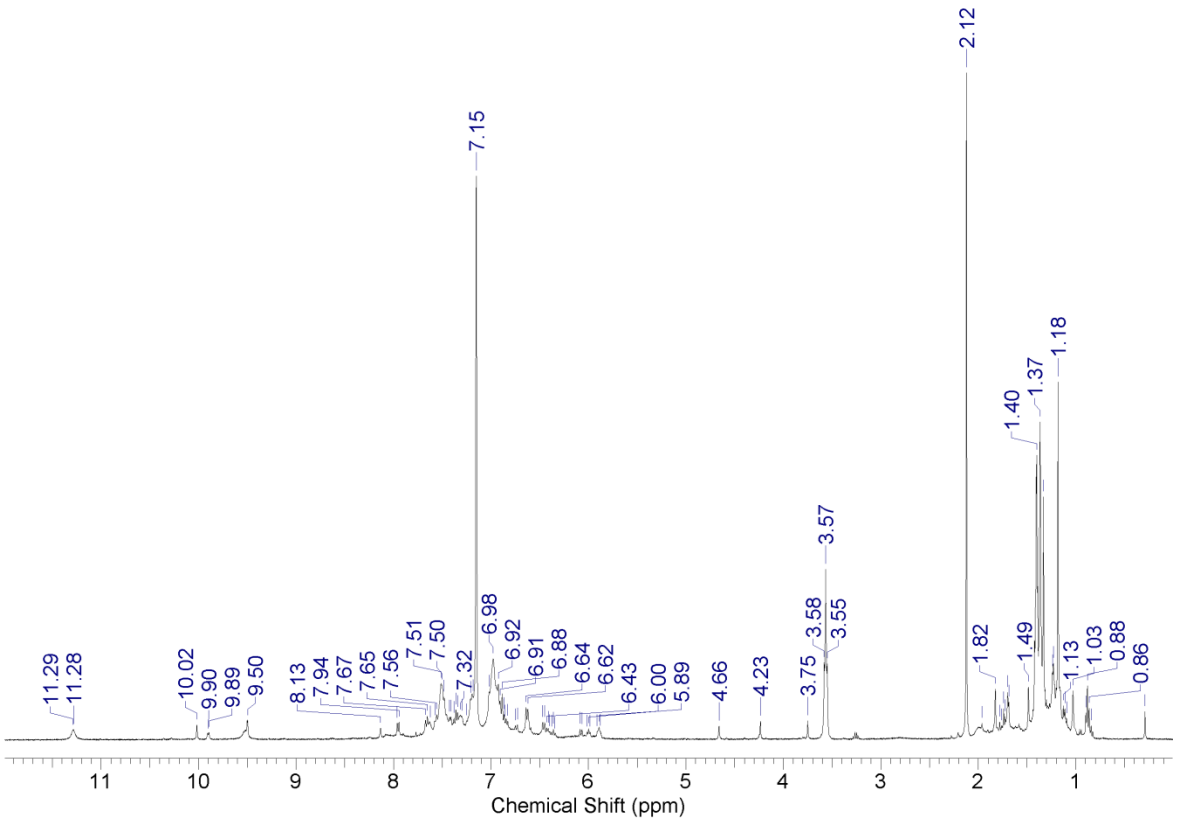

Figure S13. Reaction mixture of *2* with 1 equivalent of phenylacetylene (full spectrum).

The peaks at 11.29 ppm and 9.50 ppm correspond to **2**.

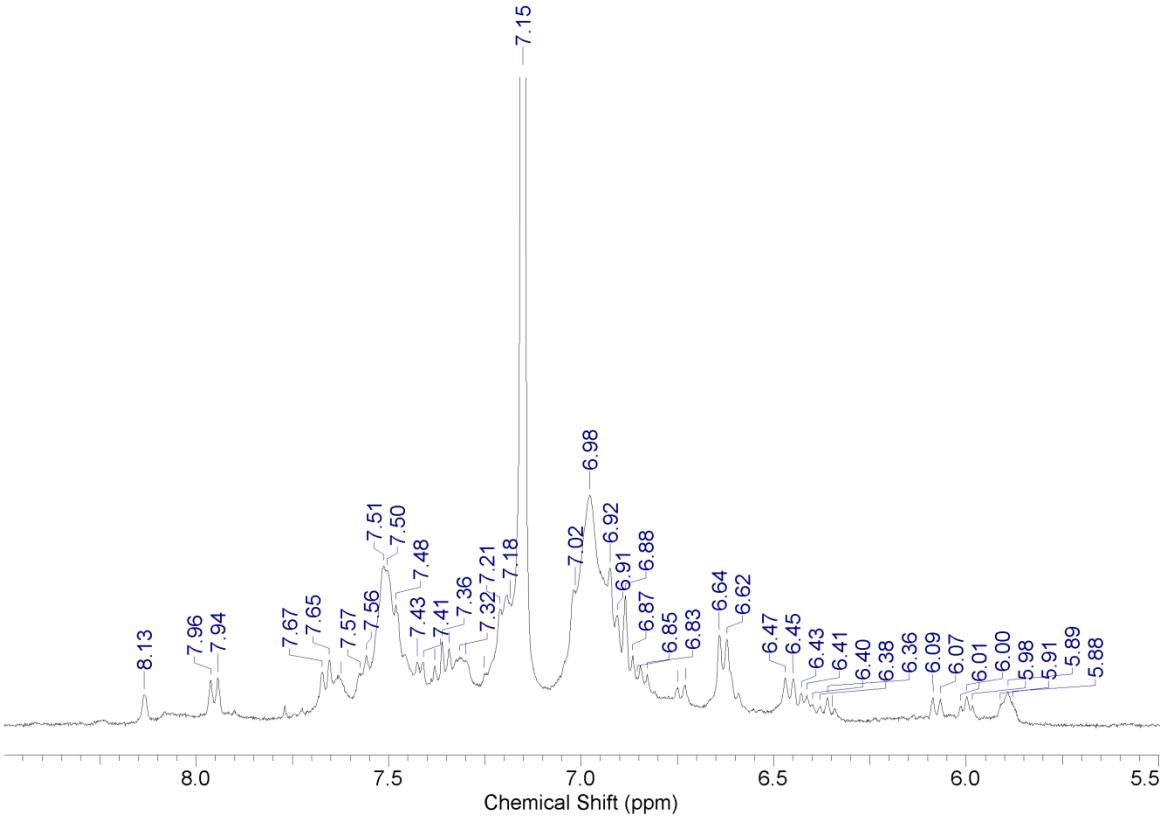

Figure S14. Reaction mixture of *2* with 1 equivalent of phenylacetylene (aromatic region).

The peaks at 7.61 ppm, 7.35 ppm, 7.31 ppm, 7.21 ppm, 6.88 ppm, 6.79 ppm, and 6.63 ppm correspond to **2**. The peaks at 7.51 ppm and 6.98 ppm correspond to diphenylacetylene.

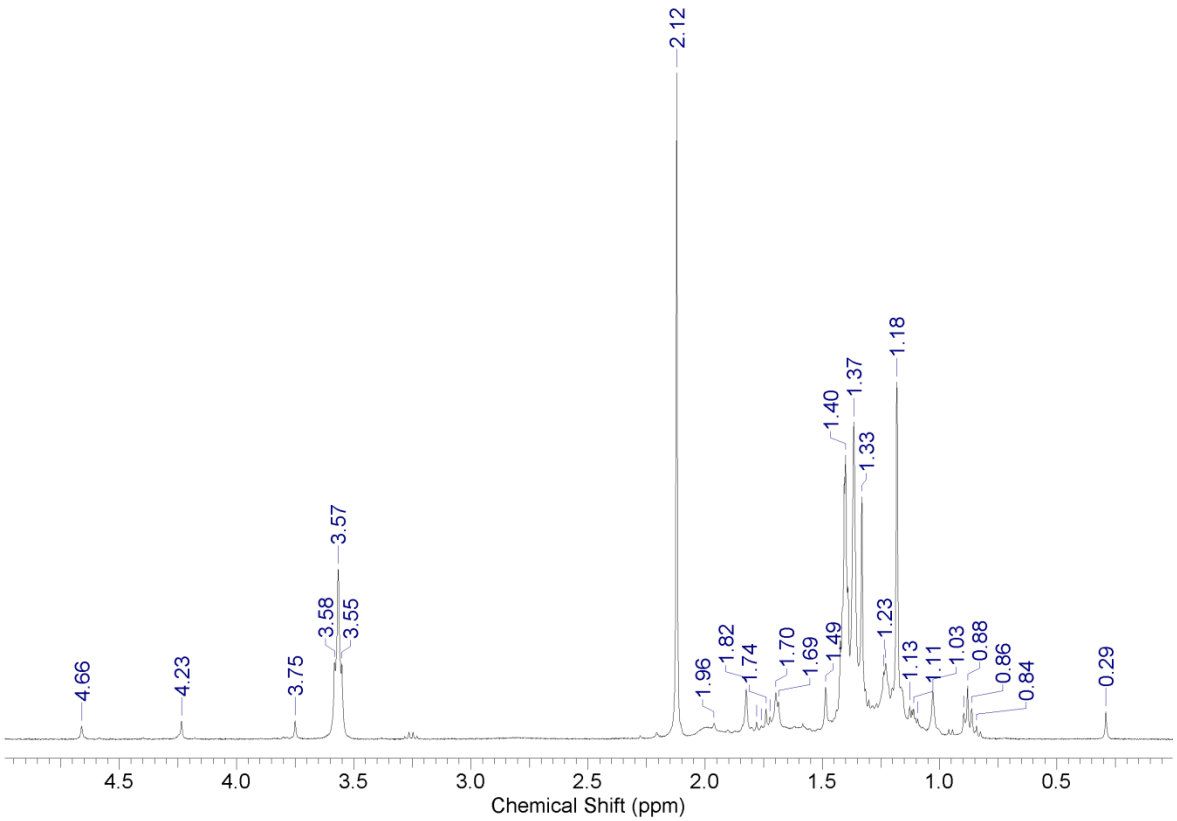

Figure S15. Reaction mixture of 2 with 1 equivalent of phenylacetylene (aliphatic region).

The peak at 1.37 ppm corresponds to **2**. The peaks at 3.57 ppm and 1.41 ppm correspond to THF. The peak at 2.12 ppm corresponds to hexamethylbenzene. The peaks at 1.23 ppm and 0.88 ppm correspond to hexane. The peak at 1.11 ppm corresponds to ether.

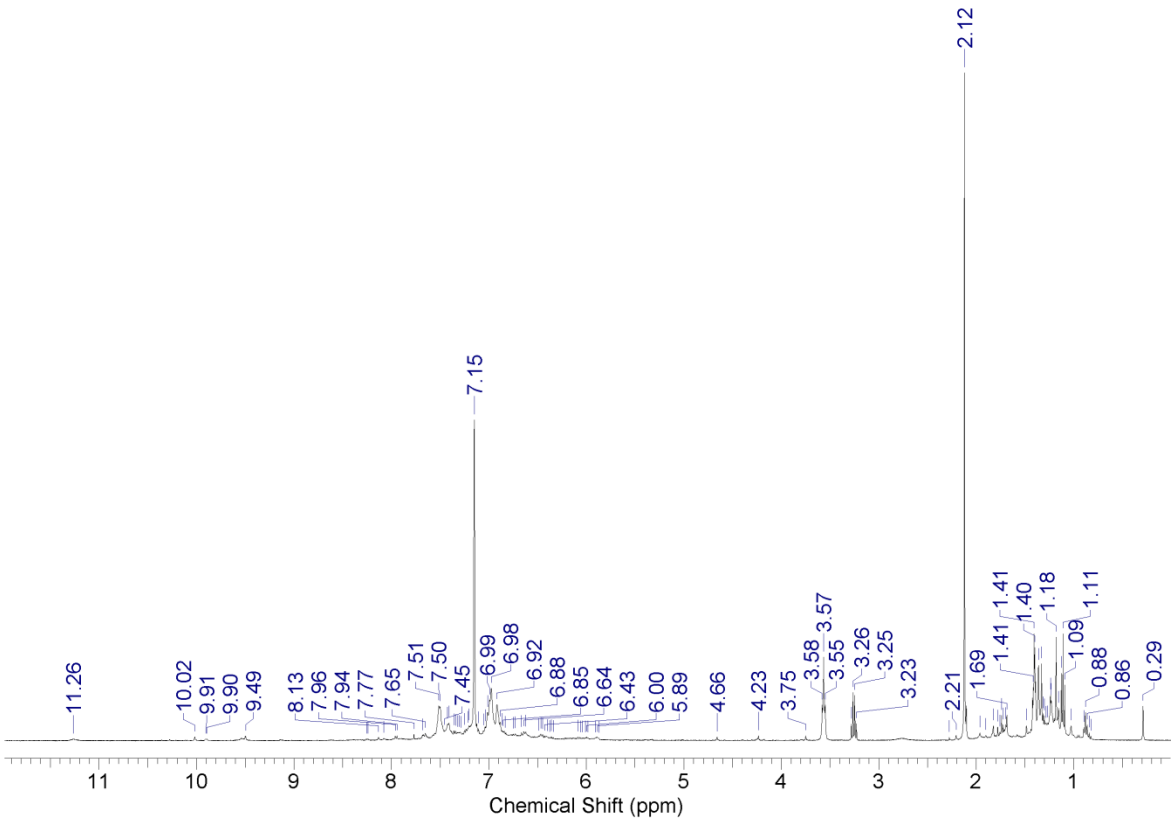

Figure S16. Reaction mixture of *2* with 2 equivalents of phenylacetylene (full spectrum).

The peaks at 11.26 ppm and 9.49 ppm correspond to **2**.

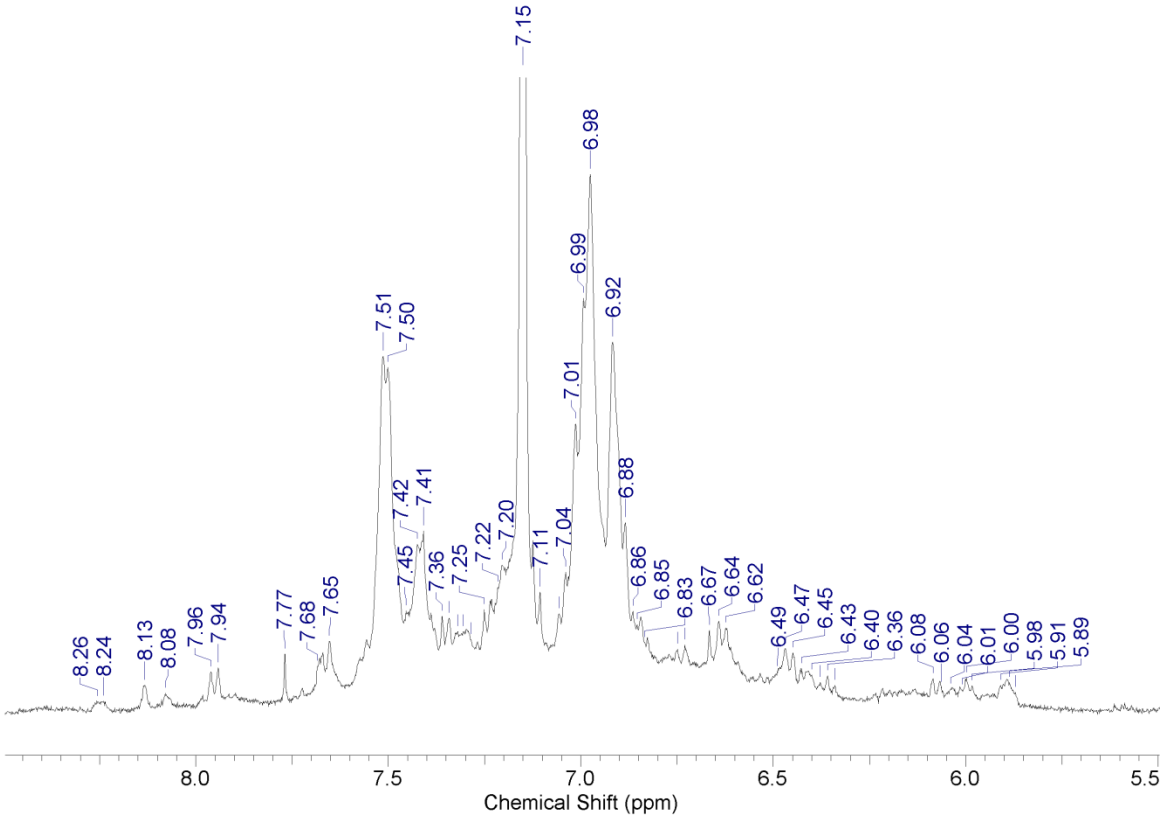

Figure S17. Reaction mixture of *2* with 2 equivalents of phenylacetylene (aromatic region).

The peaks at 7.61 ppm, 7.35 ppm, 7.31 ppm, 7.21 ppm, 6.88 ppm, 6.79 ppm, and 6.63 ppm correspond to ***2***. The peaks at 7.51 ppm and 6.98 ppm correspond to diphenylacetylene.

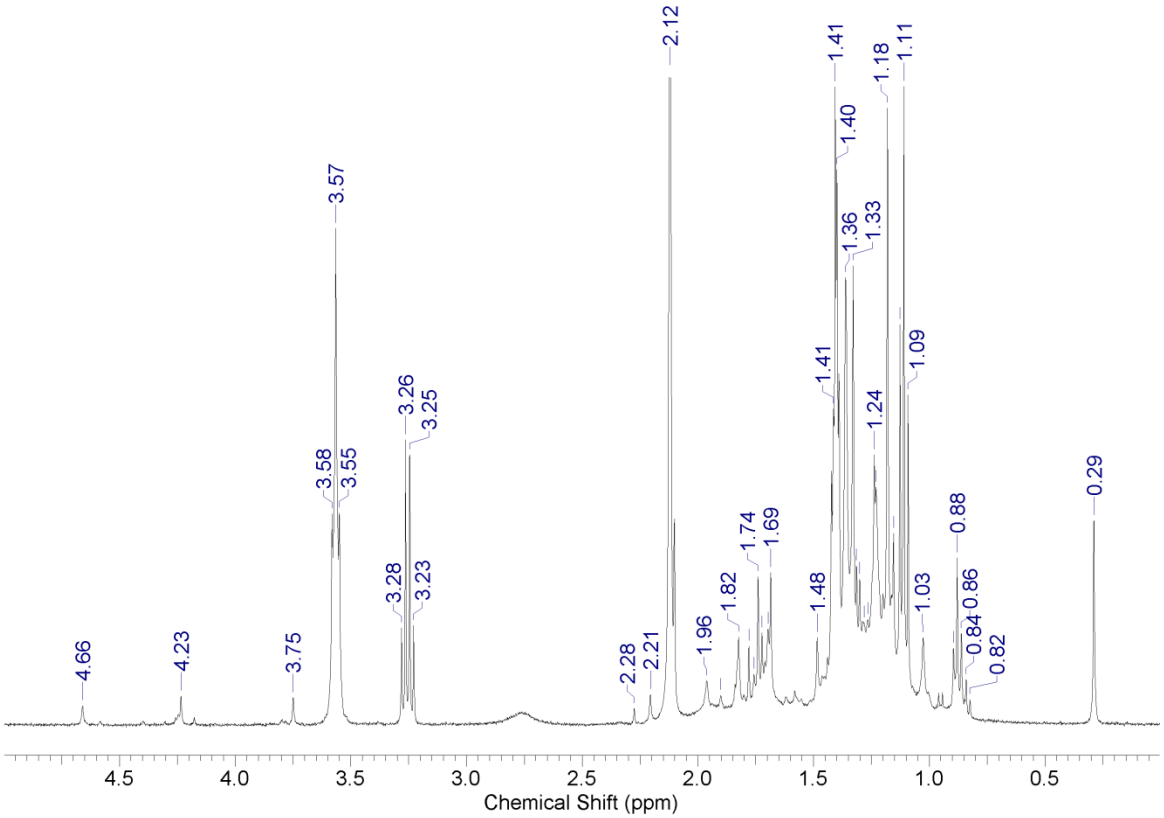

Figure S18. Reaction mixture of *2* with 1 equivalent of phenylacetylene (aliphatic region).

The peak at 1.36 ppm corresponds to ***2***. The peaks at 3.57 ppm and 1.41 ppm correspond to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peak at 2.12 ppm corresponds to hexamethylbenzene. The peaks at 1.23 ppm and 0.88 ppm correspond to hexane.

ii. Example Calculation for Determining Yields of Catalysis

Using the Results from Ethyl propiolate Cyclotrimerization. The peak at 9.09 ppm corresponds to the 3 aromatic protons on the 1,3,5-isomer. The integration value associated with these protons is 1.17, thus the value of one proton is equal to 1/3 of 1.17, so 0.39. The peak at 2.11 ppm corresponds to the 18 benzyl protons on the internal integration standard, hexamethylbenzene. The integration value associated with these protons was calibrated to 18.00, thus the value of one proton is equal to 1.00. Since 0.10 mmol of hexamethylbenzene was added to the reaction mixture, an integration value of 1.00 is equal to 0.10 mmol. Therefore, the value of 0.39 for one proton on the 1,3,5-isomer is equal to 0.039 mmol. If 1.00 mmol of ethyl propiolate was used for the reaction, and 3 mol of alkyne are needed for 1 mol of benzene isomer, the expected yield of the reaction is 0.33 mmol. Thus, percent yield of the 1,3,5-isomer is 0.039 / 0.33 X 100 = 12%. The peaks at 8.60 ppm, 7.98 ppm, and 7.47 ppm correspond to the 3 aromatic protons on the 1,2,4-isomer. Each peak corresponds to a single proton, thus the value of one proton is equal to the integration value (1.80, 1.90, 2.03 respectively). During catalysis, diphenylacetylene is released from the complex, producing signals at 7.50 ppm and 6.99 ppm. Due to proximity, the peak at 7.47 ppm for the 1,2,4-isomer was omitted from calculations. An average of the remaining values was used to determine the value of one proton on the 1,2,4-isomer. Percent yield for the 1,2,4-isomer was calculated as described for the 1,3,5-isomer.

iii. Spectra of Catalytic Reaction Mixtures

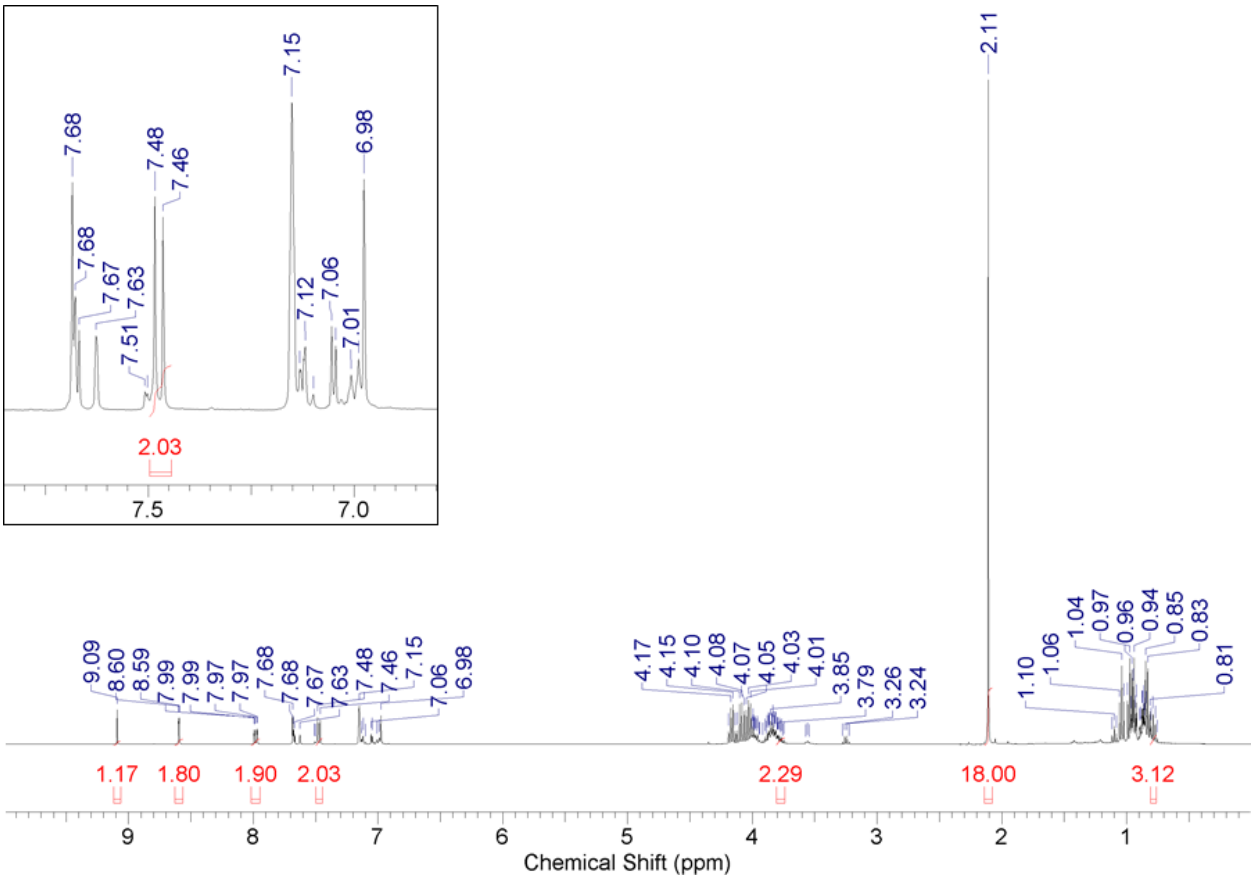

Figure S19. Reaction mixture of ethyl propiolate with 1 mol% catalyst at room temperature for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.79 ppm and 0.81 ppm correspond to the starting material (2H and 3H respectively). The peak at 9.09 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.60 ppm, 7.98 ppm, and 7.47 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.11 corresponds to the internal integration standard hexamethylbenzene (18H, 0.10 mmol). Except for the small peaks at 7.50 ppm and 6.99 ppm (diphenylacetylene), all other peaks in the aromatic region correspond to cyclooctatetraene products.

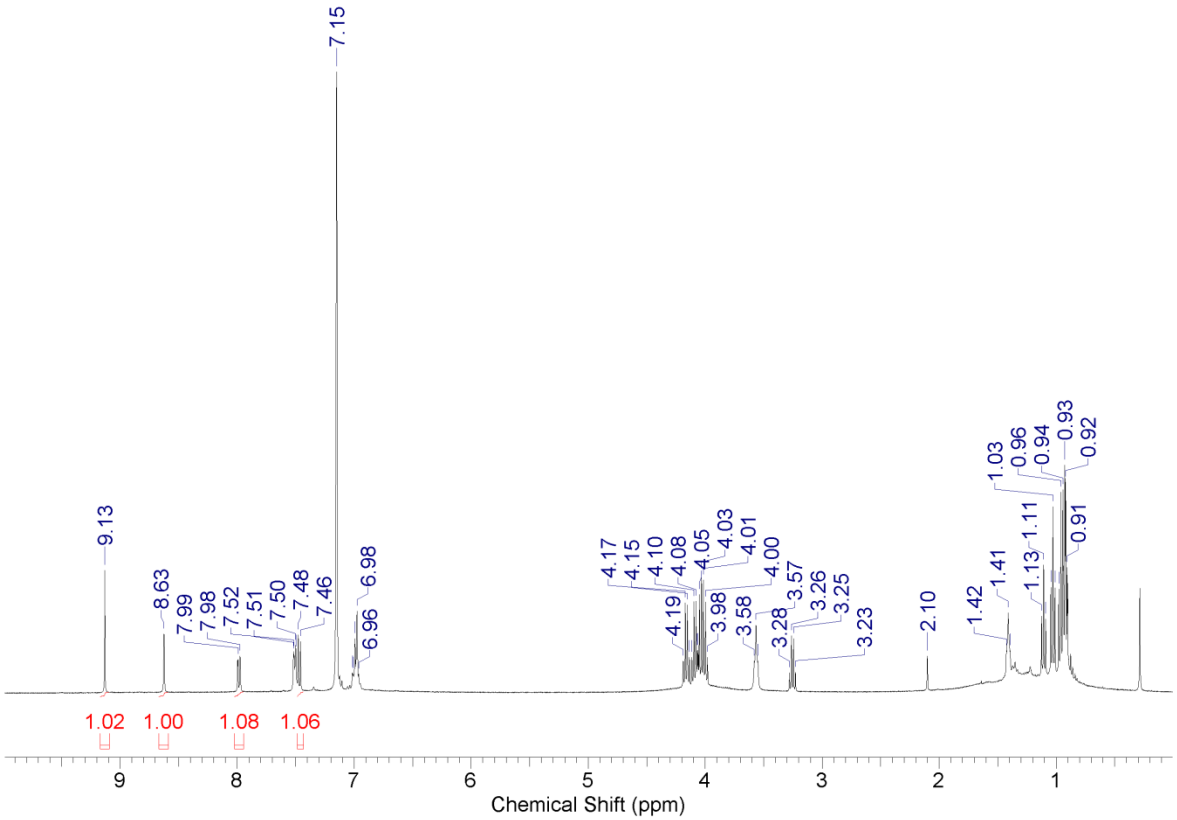

Figure S20. Reaction mixture of ethyl propiolate with 5 mol% catalyst at room temperature for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The lack of peaks at 3.79 ppm and 0.81 ppm, indicates the consumption of all starting material. The peak at 9.13 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.63 ppm, 7.98 ppm, and 7.47 ppm correspond to the 1,2,4-isomer (1H each). The peaks at 3.57 and 1.41 correspond to THF. The peaks at 3.25 and 1.11 correspond to ether. The peaks at 7.50 and 6.98 correspond to diphenylacetylene. The lack of other peaks in the aromatic region indicates the absence of cyclooctatetraene products.

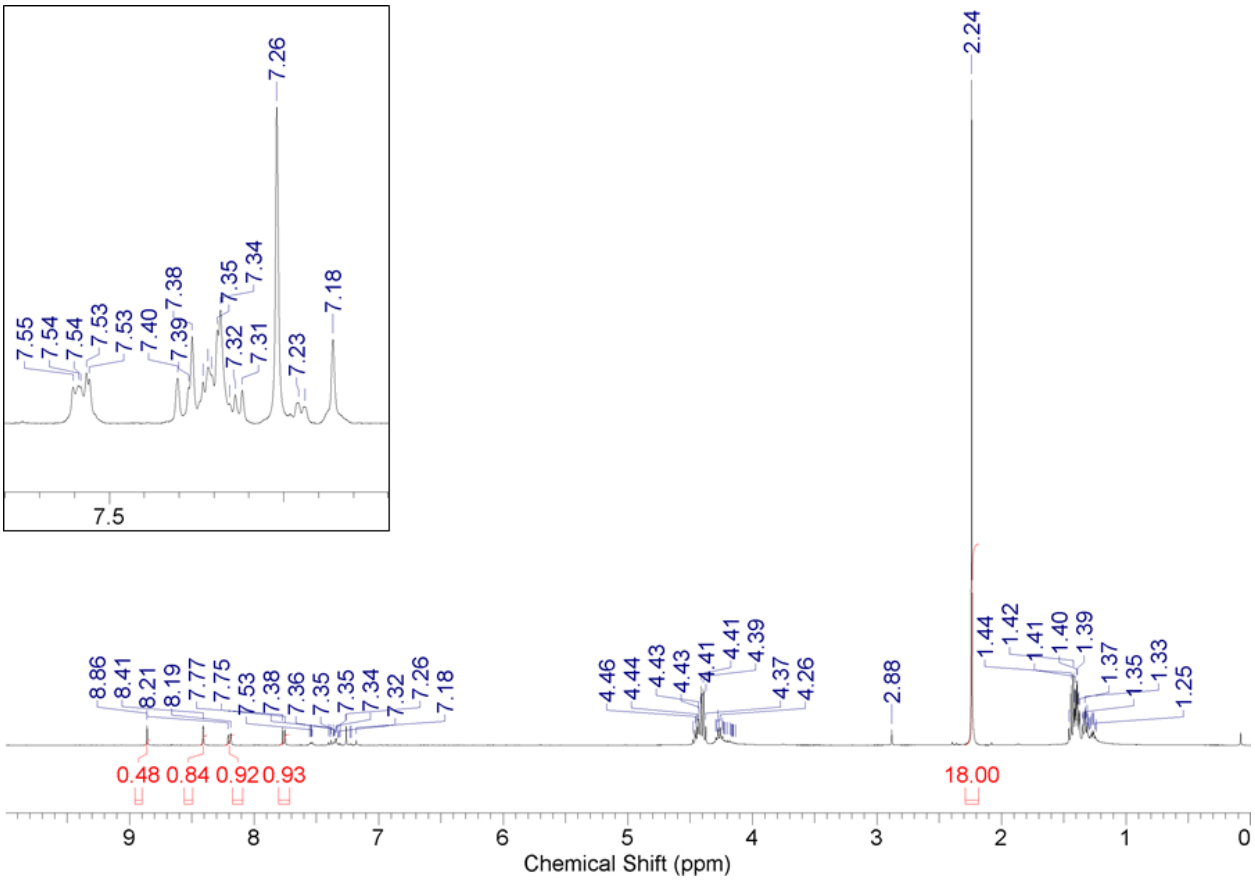

Figure S21. Reaction mixture of ethyl propiolate with 1 mol% catalyst at room temperature for 24 hours (reaction in THF, NMR in $CDCl_3$).

Solvent was removed in vacuo and the resulting product redissolved in $CDCl_3$. Due to the volatility of the starting material, only trace amounts remained and were ignored in calculations. The peak at 8.86 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.41 ppm, 8.20 ppm, and 7.76 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.24 corresponds to the internal integration standard hexamethylbenzene (18H, 0.10 mmol). Except for the peaks at 7.54 ppm and 7.36 ppm (diphenylacetylene), all other peaks in the aromatic region correspond to cyclooctatetraene products.

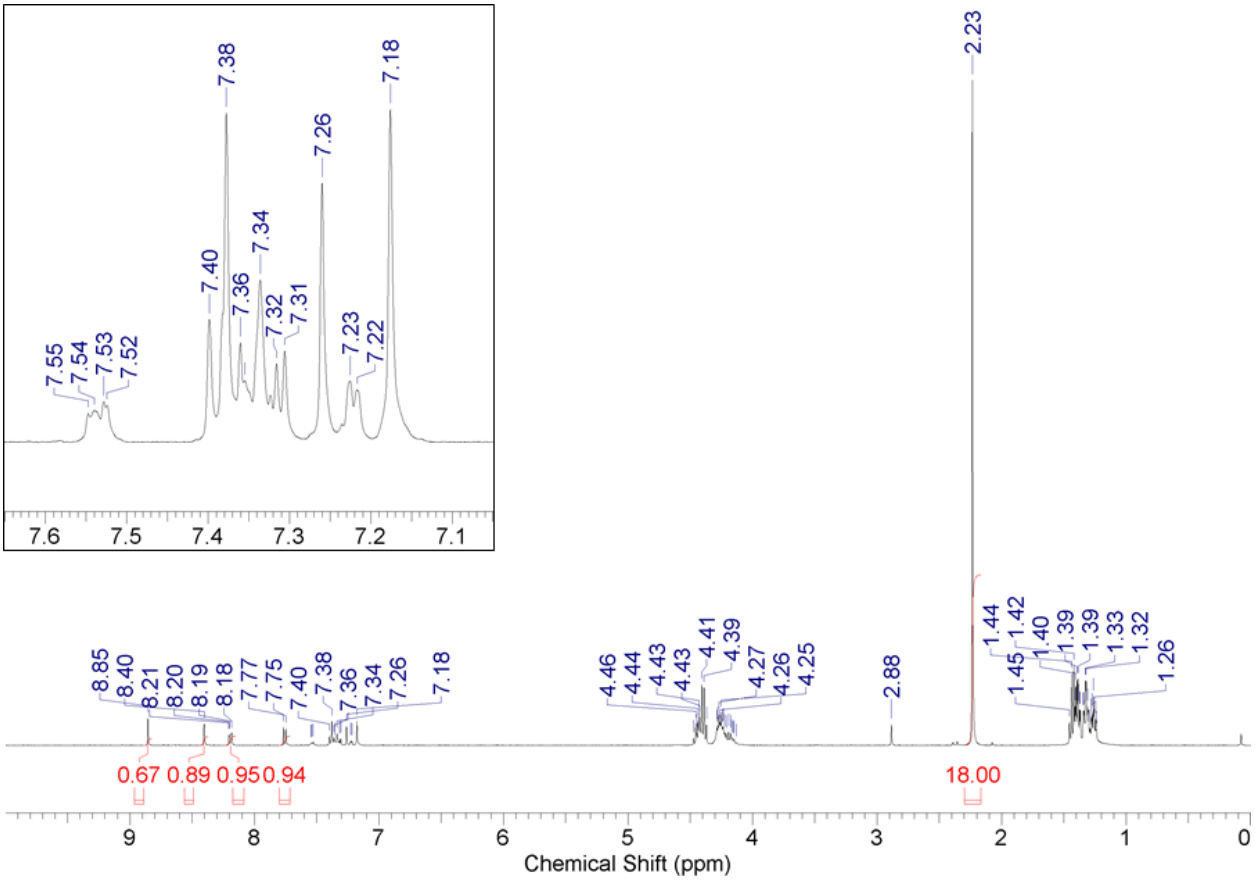

Figure S22. Reaction mixture of ethyl propiolate with 1 mol% catalyst at room temperature for 24 hours (reaction in ether, NMR in $CDCl_3$).

Solvent was removed in vacuo and the resulting product redissolved in $CDCl_3$. Due to the volatility of the starting material, only trace amounts remained and were ignored in calculations. The peak at 8.85 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.40 ppm, 8.20 ppm, and 7.76 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.23 corresponds to the internal integration standard hexamethylbenzene (18H, 0.10 mmol). Except for the peaks at 7.54 ppm and 7.36 ppm (diphenylacetylene), all other peaks in the aromatic region correspond to cyclooctatetraene products.

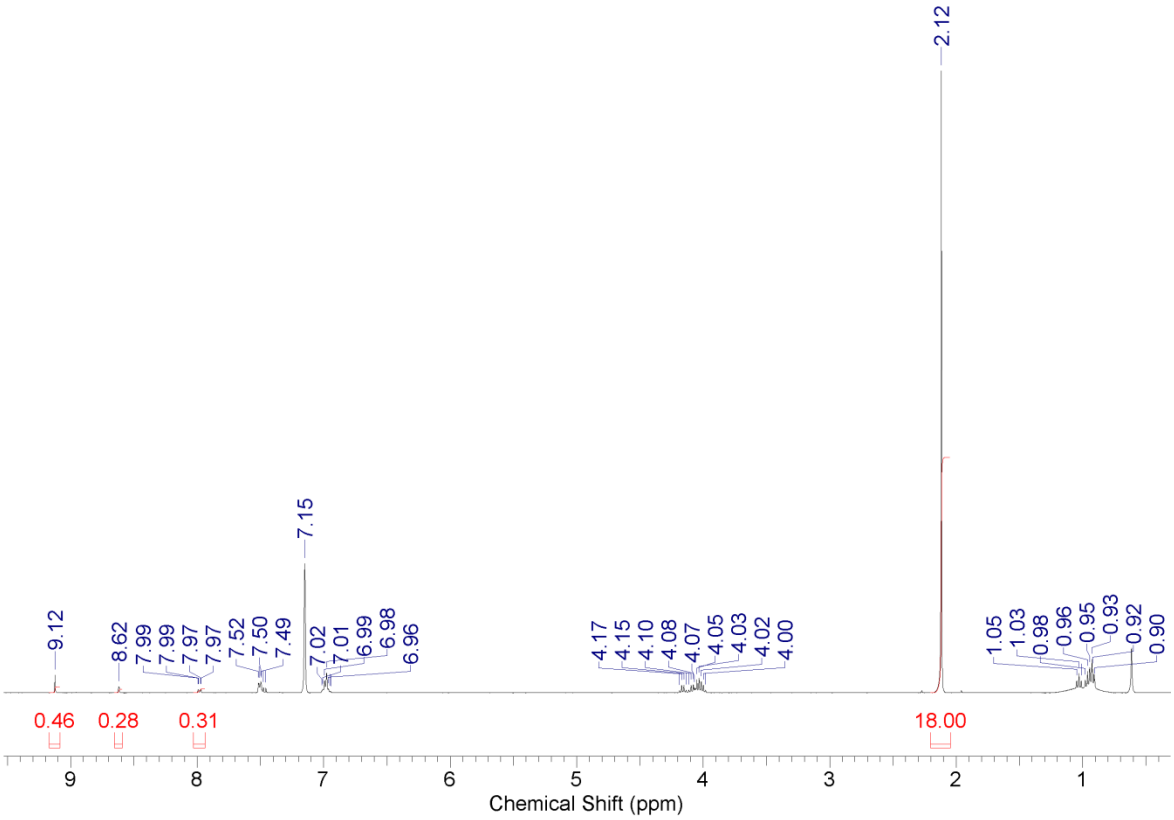

Figure S23. Reaction mixture of ethyl propiolate with 5 mol% catalyst at room temperature for 24 hours (reaction in acetonitrile, NMR in C_6D_6).

Solvent was removed in vacuo and the resulting product redissolved in C_6D_6. Due to the volatility of the starting material, only trace amounts remained and were ignored in calculations. The peak at 9.12 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.62 ppm, 7.98 ppm, and 7.48 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.12 corresponds to the internal integration standard hexamethylbenzene (18H, 0.10 mmol). The peaks at 7.50 and 6.98 correspond to diphenylacetylene. The lack of other peaks in the aromatic region indicates the absence of cyclooctatetraene products.

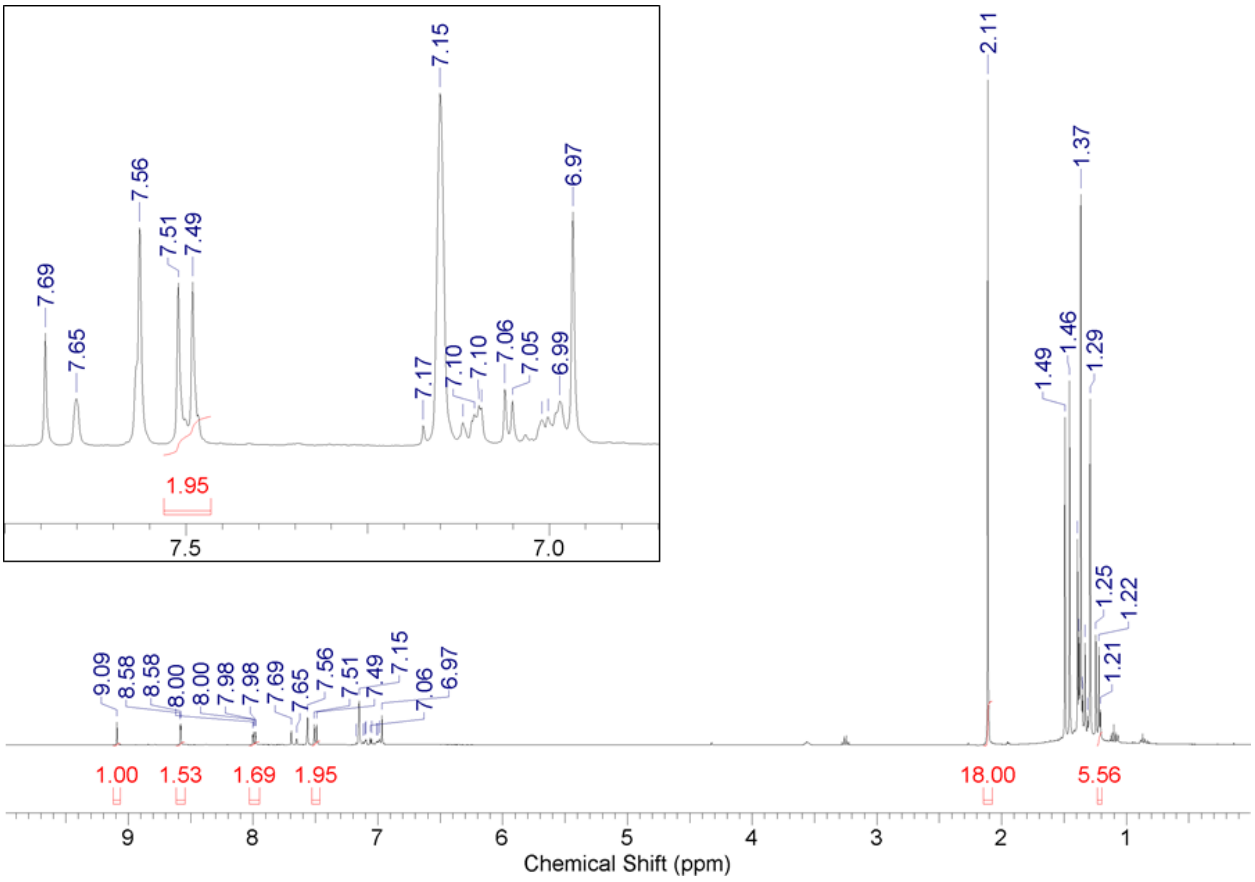

Figure S24. Reaction mixture of *tert*-butyl propiolate with 1 mol% catalyst at room temperature for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The peak at 1.22 ppm corresponds to the starting material (9H). The peak at 9.09 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.58 ppm, 7.99 ppm, and 7.50 ppm correspond to the 1,2,4-isomer (1H each). Due to the proximity of the peak at 7.50 ppm to diphenylacetylene, it was ignored in calculations. The peak at 2.11 corresponds to the internal integration standard hexamethylbenzene (18H, 0.10 mmol). Except for the other small peak 6.99 ppm (diphenylacetylene), all other peaks in the aromatic region correspond to cyclooctatetraene products.

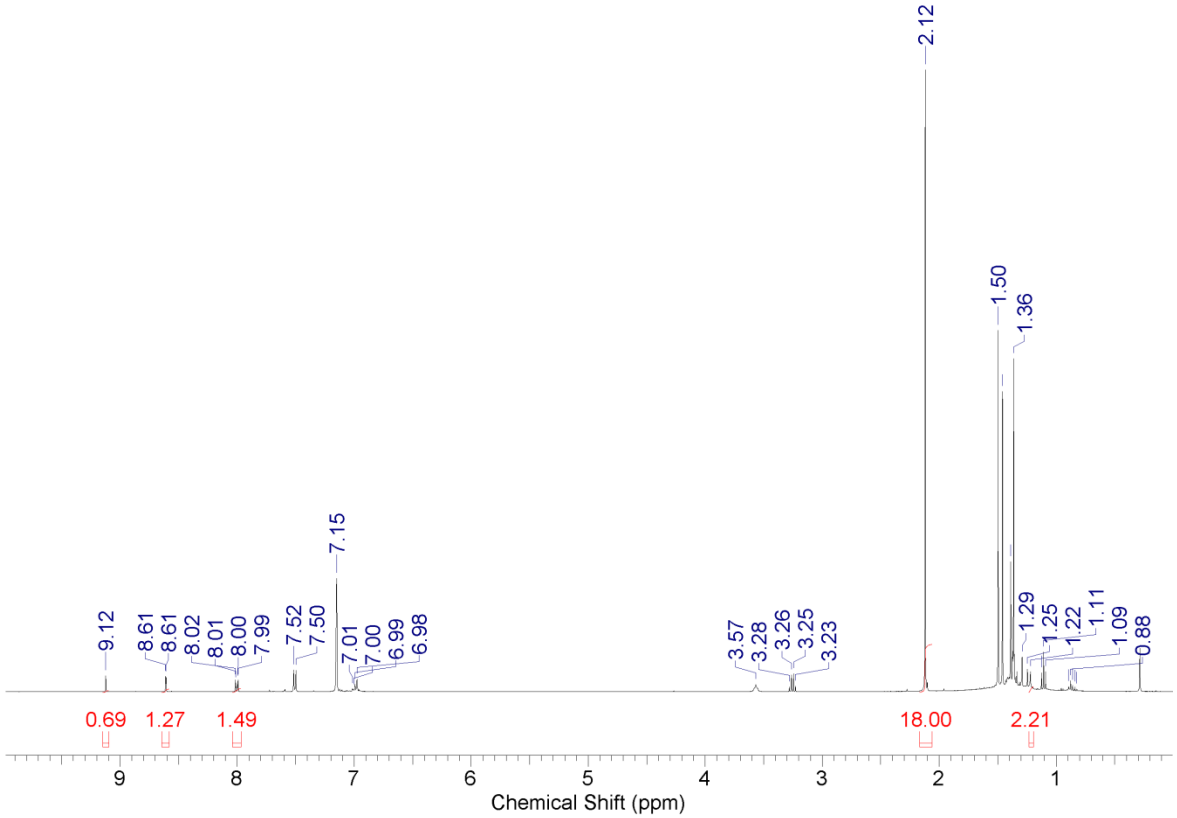

Figure S25. Reaction mixture of *tert*-butyl propiolate with 5 mol% loading catalyst at room temperature for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The peak at 1.22 ppm corresponds to the starting material (9H). The peak at 9.12 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.61 ppm, 8.00 ppm, and 7.51 ppm correspond to the 1,2,4-isomer (1H each). Due to the proximity of the peak at 7.51 ppm to diphenylacetylene, it was ignored in calculations. The peak at 2.11 corresponds to the internal integration standard hexamethylbenzene (18H, 0.04 mmol). The peak 6.99 ppm also corresponds to diphenylacetylene. The peak at 3.57 corresponds to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peaks at 1.29 ppm and 0.88 ppm correspond to hexane. The lack of other peaks in the aromatic region indicates the absence of cyclooctatetraene products.

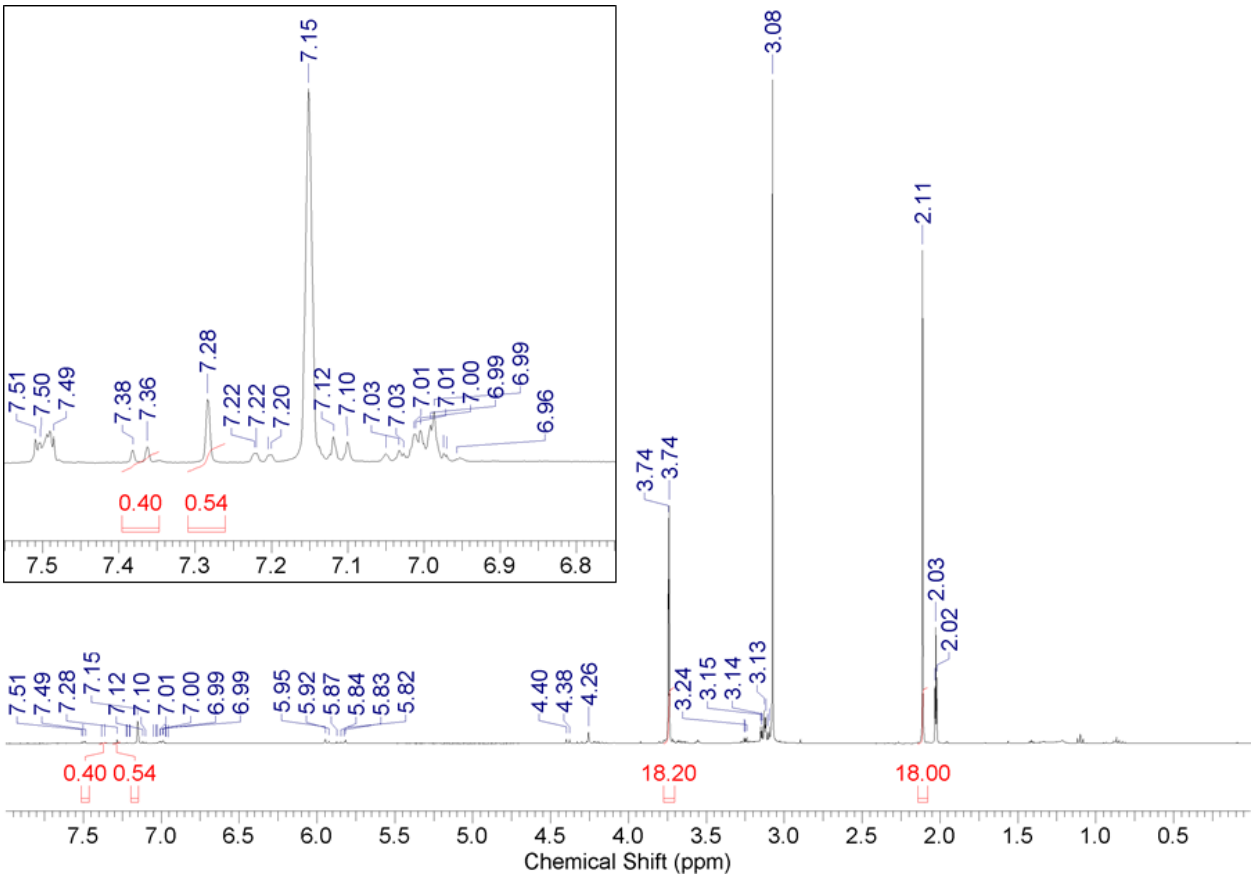

Figure S26. Reaction mixture of methyl propargyl ether with 1 mol% catalyst at room temperature for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.74 ppm, 3.08 ppm, and 2.03 ppm correspond to the starting material (2H, 3H, and 1H respectively). The peak at 7.28 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 7.37 and 7.21 correspond to the 1,2,4-isomer (1H each). The peak at 2.11 corresponds to the internal integration standard hexamethylbenzene (18H, 0.08 mmol). The peaks at 7.50 and 6.98 correspond to diphenylacetylene. The peaks from 5.95 ppm to 5.82 ppm correspond to cyclooctatetraene products.

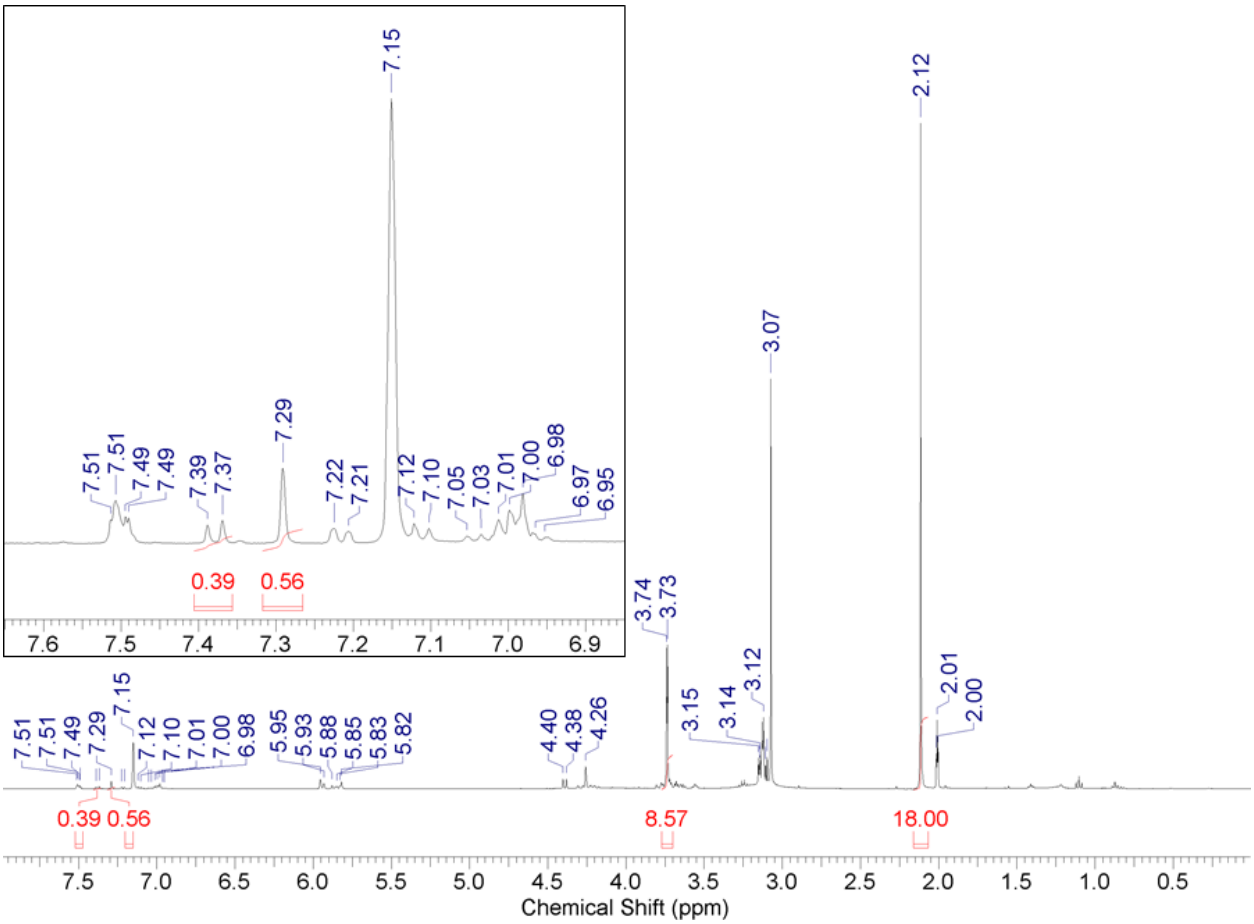

Figure S27. Reaction mixture of methyl propargyl ether with 1 mol% catalyst at 50 °C for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.74 ppm, 3.08 ppm, and 2.03 ppm correspond to the starting material (2H, 3H, and 1H respectively). The peak at 7.28 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 7.37 and 7.21 correspond to the 1,2,4-isomer (1H each). The peak at 2.11 corresponds to the internal integration standard hexamethylbenzene (18H, 0.12 mmol). The peaks at 7.50 and 6.98 correspond to diphenylacetylene. The peaks from 5.95 ppm to 5.82 ppm correspond to cyclooctatetraene products.

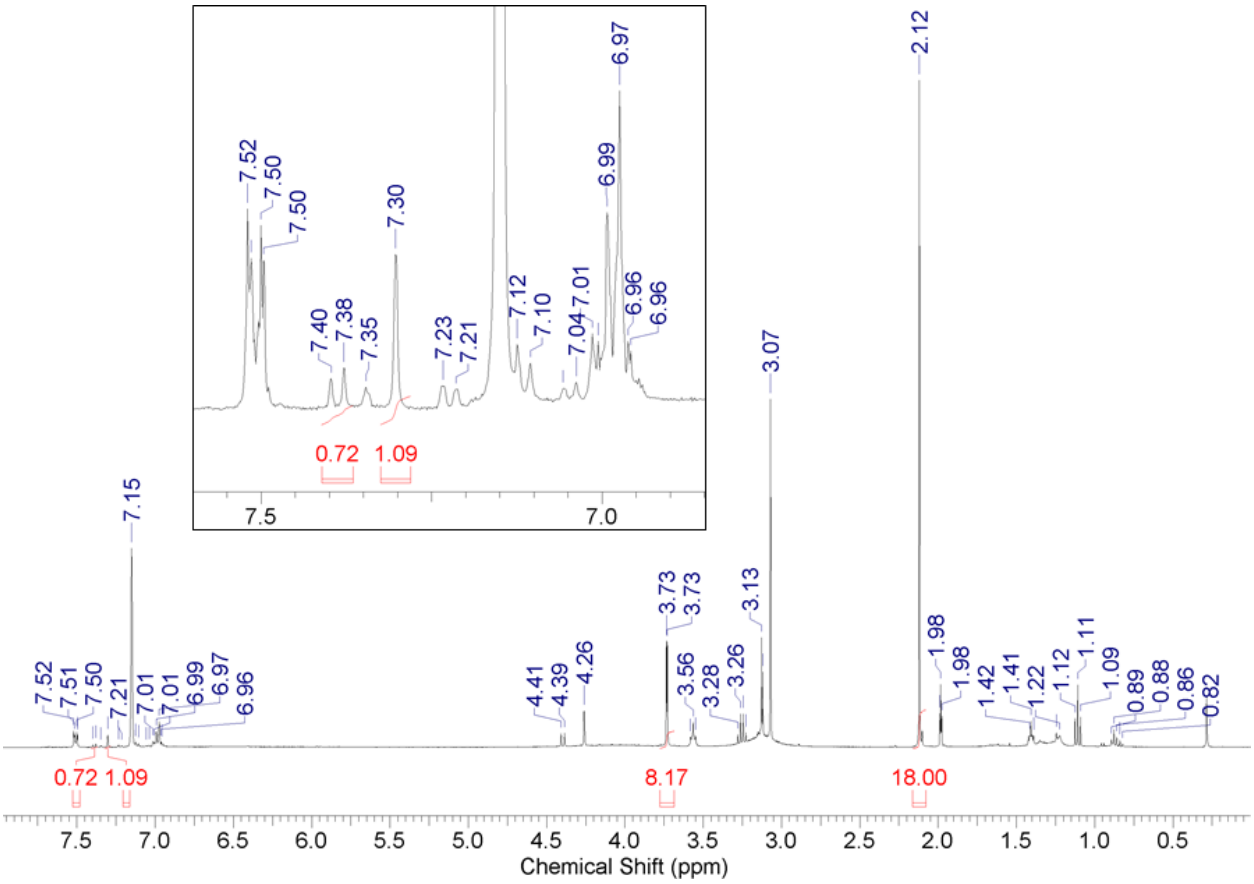

Figure S28. Reaction mixture of methyl propargyl ether with 5% loading catalyst at room temperature for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.73 ppm, 3.07 ppm, and 1.98 ppm correspond to the starting material (2H, 3H, and 1H respectively). The peak at 7.30 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 7.39 and 7.22 correspond to the 1,2,4-isomer (1H each). The peak at 2.12 corresponds to the internal integration standard hexamethylbenzene (18H, 0.03 mmol). The peaks at 7.51 and 6.98 correspond to diphenylacetylene. The peaks at 3.56 ppm and 1.41 ppm correspond to THF. The peaks at 3.26 ppm and 1.11 ppm correspond to ether. The peak at 0.88 ppm corresponds to hexane. The lack of peaks in the vinylic region indicates the absence of cyclooctatetraene products.

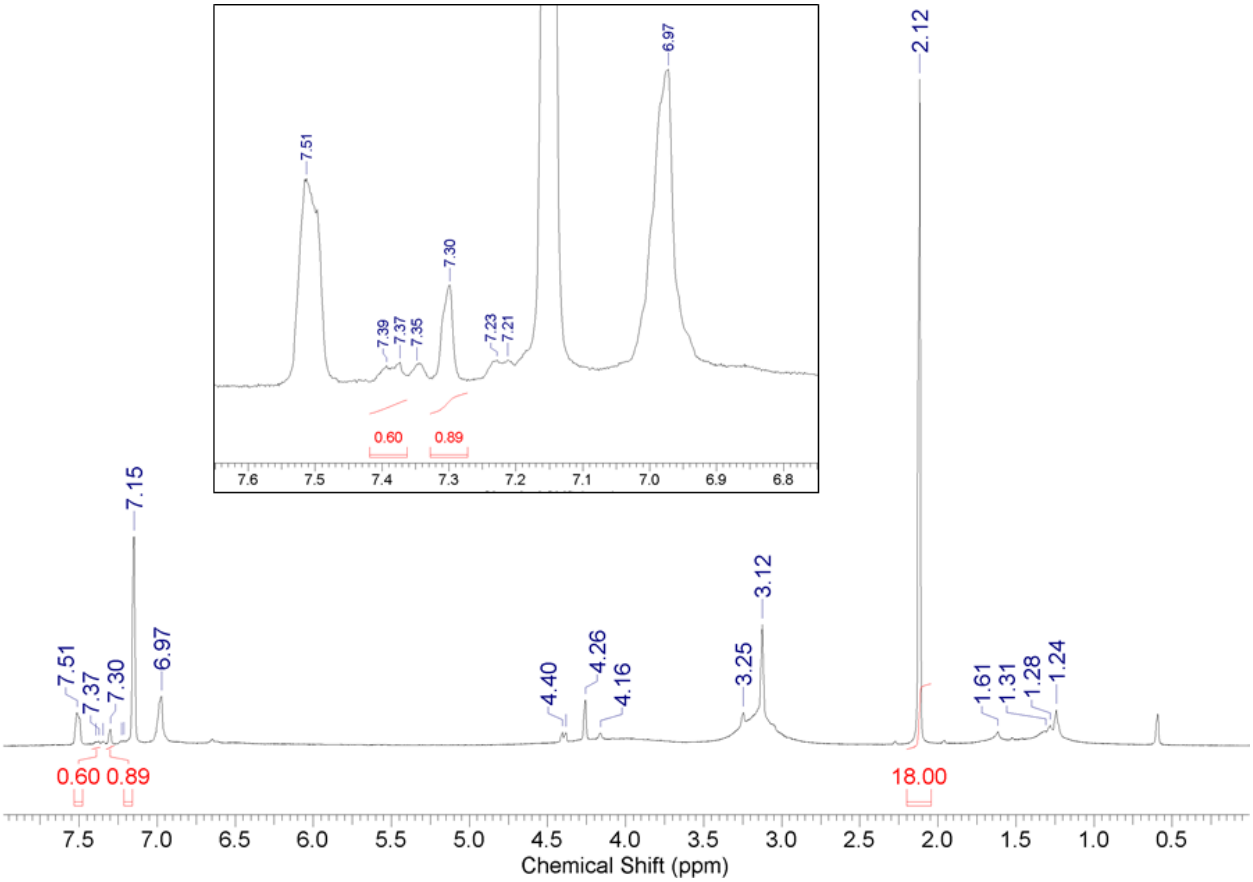

Figure S29. Reaction mixture of methyl propargyl ether with 5 mol% catalyst at room temperature for 24 hours (reaction in acetonitrile, NMR in C_6D_6).

Solvent was removed in vacuo and the resulting product redissolved in C_6D_6. Due to the volatility of the starting material, only trace amounts remained and were ignored in calculations. The peak at 7.28 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 7.37 and 7.21 correspond to the 1,2,4-isomer (1H each). The peak at 2.11 corresponds to the internal integration standard hexamethylbenzene (18H, 0.01 mmol). The peaks at 7.51 and 6.97 correspond to diphenylacetylene. The lack of peaks in the vinylic region indicates the absence of cyclooctatetraene products.

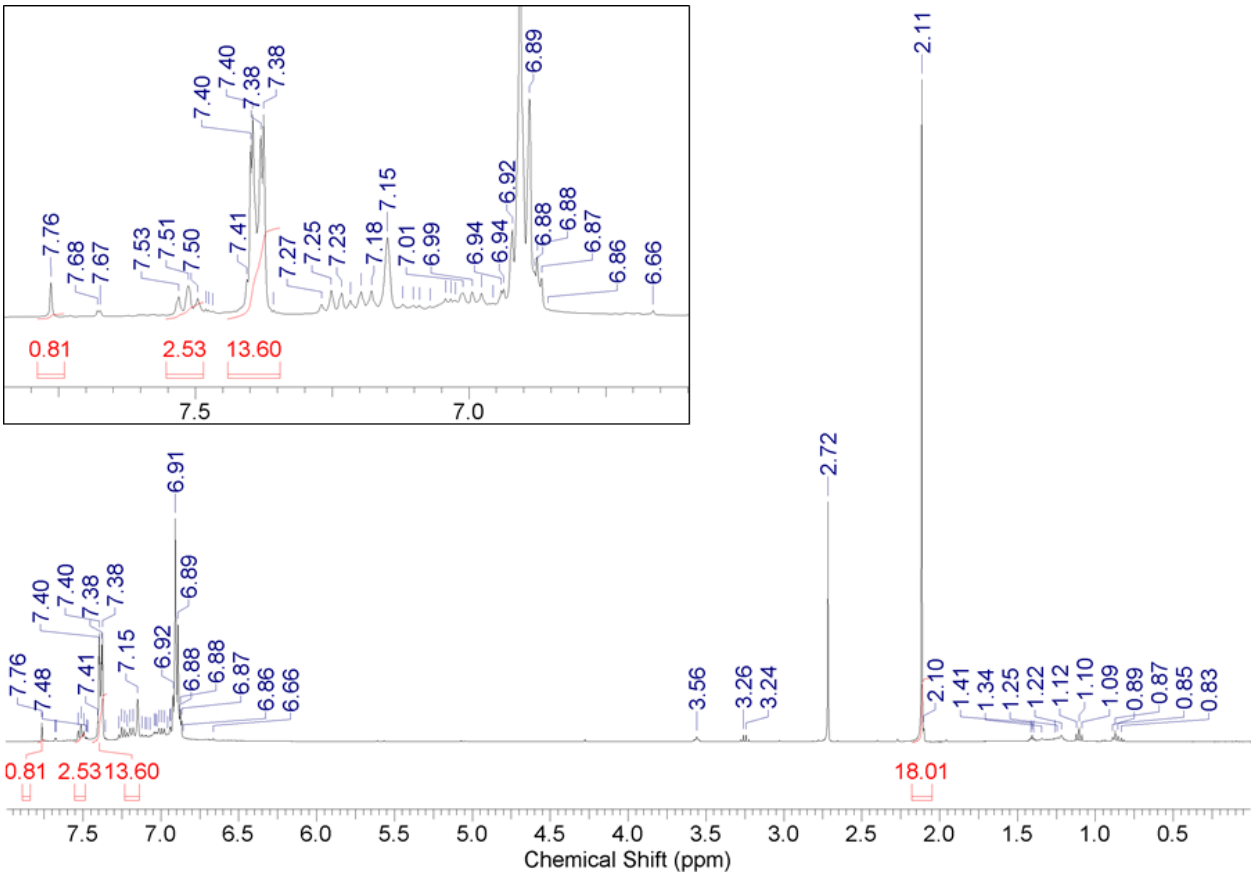

Figure S30. Reaction mixture of phenylacetylene with 1 mol% catalyst at room temperature for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 7.39 ppm, 6.91 ppm, and 2.72 ppm correspond to the starting material (2H, 3H, and 1H respectively). The peak at 7.76 ppm corresponds to the 1,3,5-isomer (3H). The peak at 7.51 corresponds to the 1,2,4-isomer (1H). The peak at 2.11 corresponds to the internal integration standard hexamethylbenzene (18H, 0.10 mmol). The peaks for diphenylacetylene (7.50 ppm and 6.99 ppm) are masked by the starting material and benzene products of the reaction. The peaks at 3.56 ppm and 1.41 ppm correspond to THF. The peaks at 3.26 ppm and 1.11 ppm correspond to ether. The peaks at 1.25 ppm and 0.88 ppm correspond to hexane. The lack of peaks in the vinylic region indicates the absence of cyclooctatetraene products.

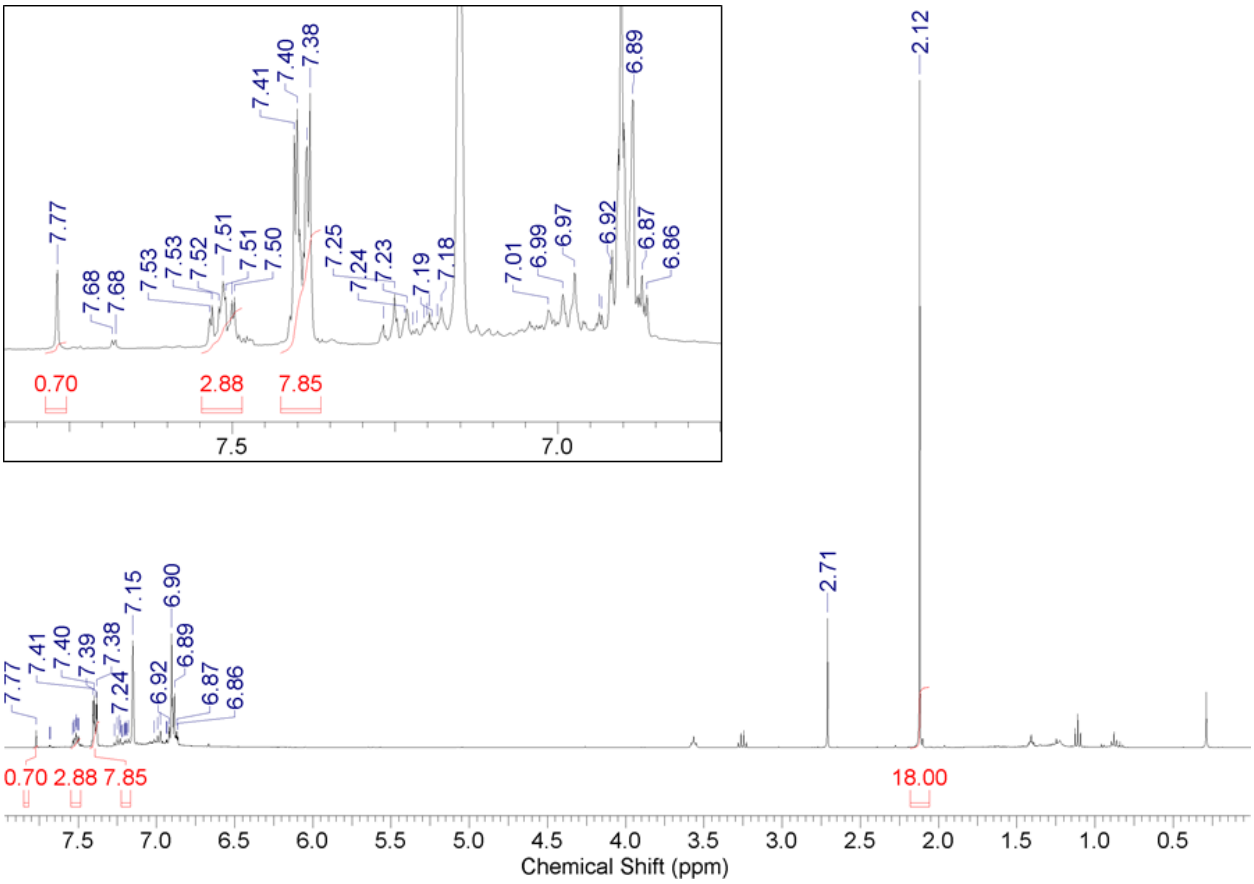

Figure S31. Reaction mixture of phenylacetylene with 5 mol% catalyst at room temperature for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 7.39 ppm, 6.90 ppm, and 2.71 ppm correspond to the starting material (2H, 3H, and 1H respectively). The peak at 7.77 ppm corresponds to the 1,3,5-isomer (3H). The peak at 7.51 corresponds to the 1,2,4-isomer (1H). The peak at 2.12 corresponds to the internal integration standard hexamethylbenzene (18H, 0.03 mmol). The peaks for diphenylacetylene (7.50 ppm and 6.99 ppm) are masked by the starting material and benzene products of the reaction. The lack of peaks in the vinylic region indicates the absence of cyclooctatetraene products.

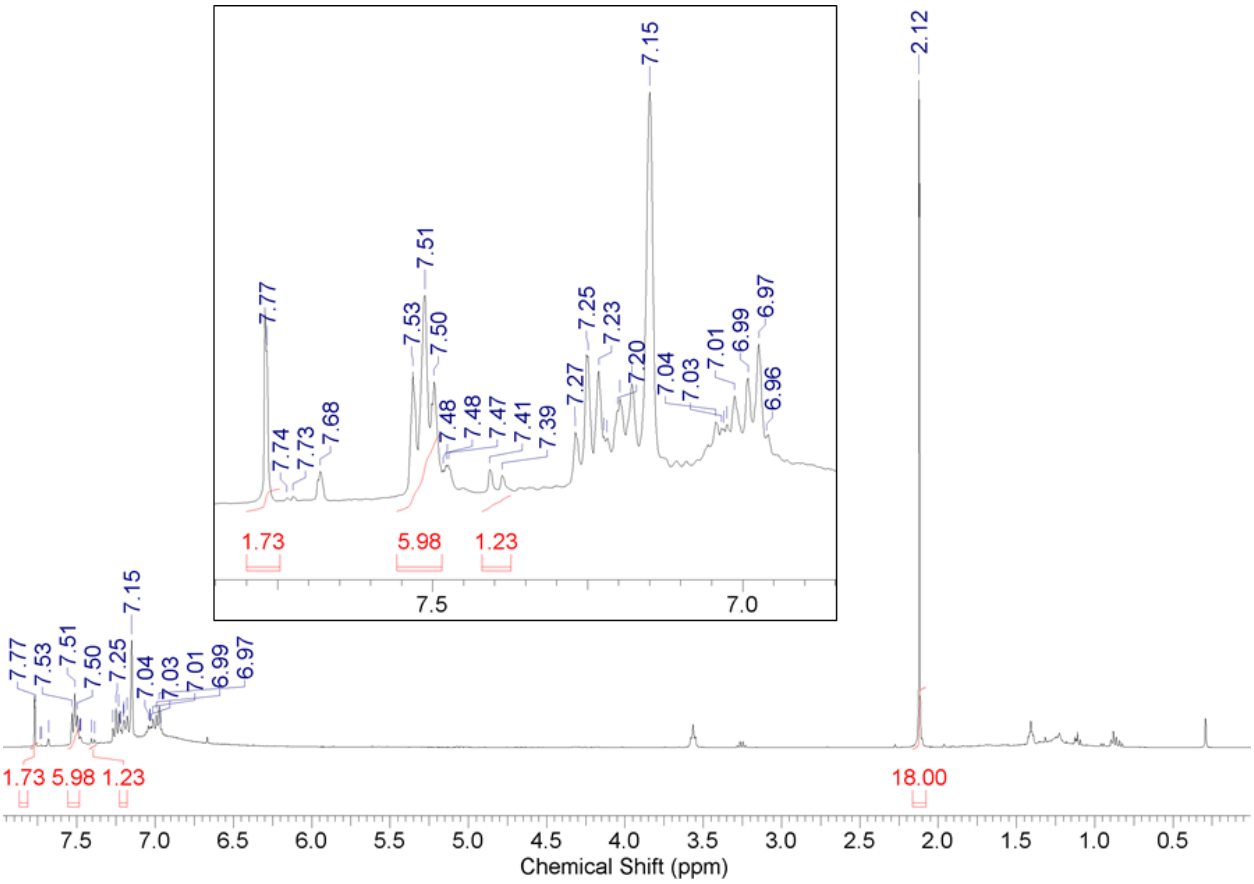

Figure S32. Reaction mixture of phenylacetylene with 5 mol% catalyst at 50 °C for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The peak at 7.39 ppm corresponds to the starting material (2H). The peak at 7.77 ppm corresponds to the 1,3,5-isomer (3H). The peak at 7.51 corresponds to the 1,2,4-isomer (1H). The peak at 2.12 corresponds to the internal integration standard hexamethylbenzene (18H, 0.03 mmol). The peaks for diphenylacetylene (7.50 ppm and 6.99 ppm) are masked by the starting material and benzene products of the reaction. The lack of peaks in the vinylic region indicates the absence of cyclooctatetraene products.

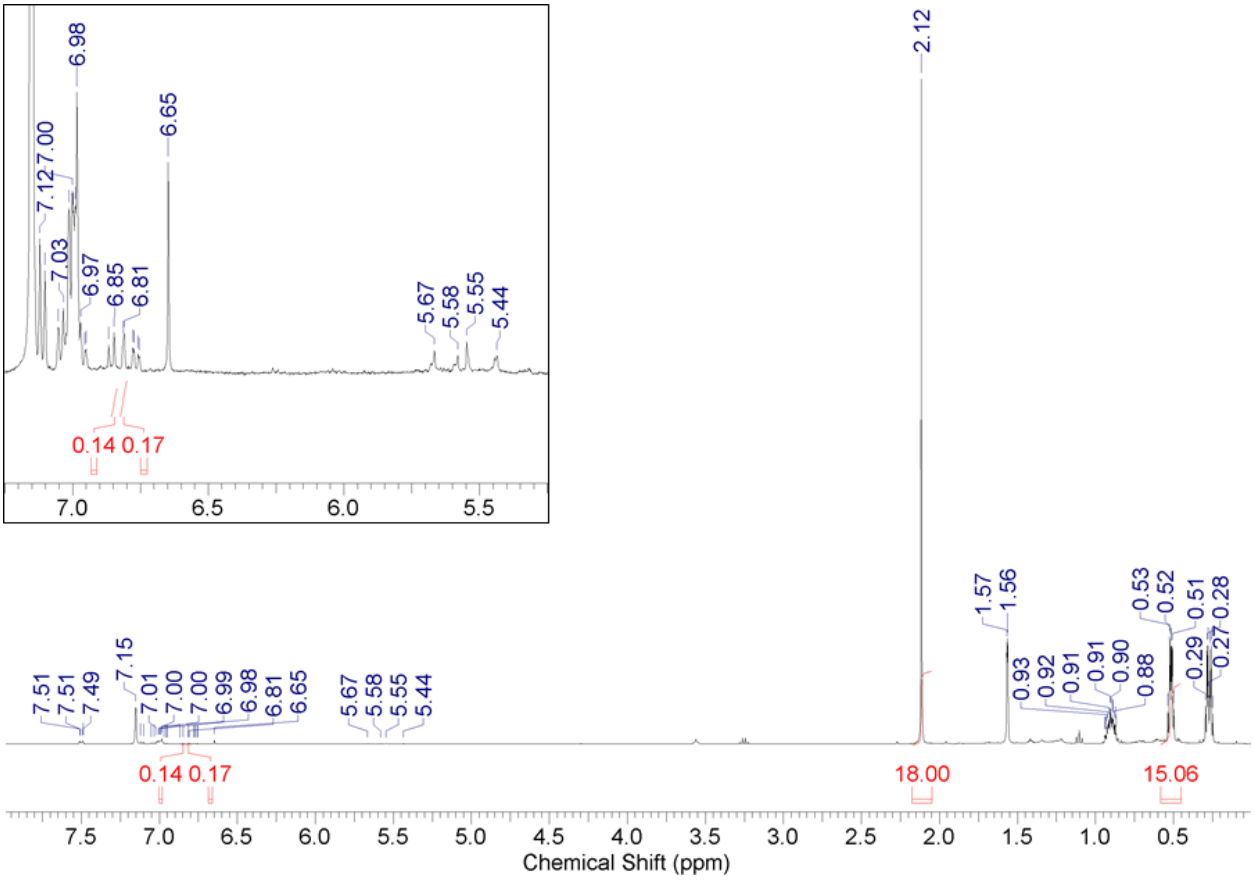

Figure S33. Reaction mixture of cyclopropylacetylene with 1 mol% catalyst at room temperature for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 1.57 ppm, 0.91 ppm, 0.52 ppm, and 0.28 ppm correspond to the starting material (1H, 1H, 2H, and 2H respectively). The peak at 6.85 ppm corresponds to the 1,3,5-isomer (3H). The peak at 6.81 corresponds to the 1,2,4-isomer (1H). The peak at 2.12 corresponds to the internal integration standard hexamethylbenzene (18H, 0.10 mmol). The peaks at 7.50 and 6.98 correspond to diphenylacetylene. The peaks from 5.67 ppm to 5.44 ppm correspond to cyclooctatetraene products.

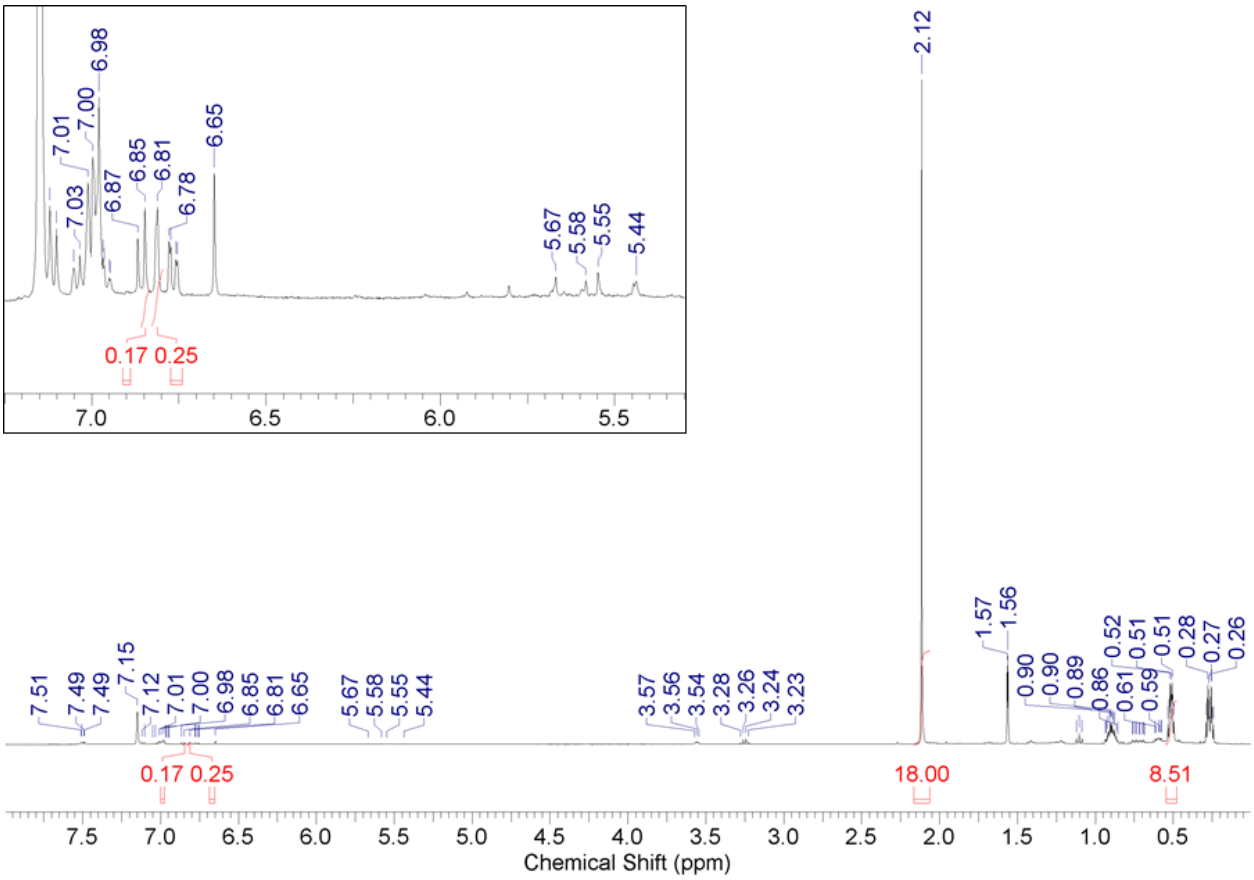

Figure S34. Reaction mixture of cyclopropylacetylene with 1 mol% catalyst at 50 °C for 24 hours (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 1.57 ppm, 0.90 ppm, 0.52 ppm, and 0.28 ppm correspond to the starting material (1H, 1H, 2H, and 2H respectively). The peak at 6.85 ppm corresponds to the 1,3,5-isomer (3H). The peak at 6.81 corresponds to the 1,2,4-isomer (1H). The peak at 2.12 corresponds to the internal integration standard hexamethylbenzene (18H, 0.20 mmol). The peaks at 7.50 and 6.98 correspond to diphenylacetylene. The peaks from 5.67 ppm to 5.44 ppm correspond to cyclooctatetraene products.

iv.

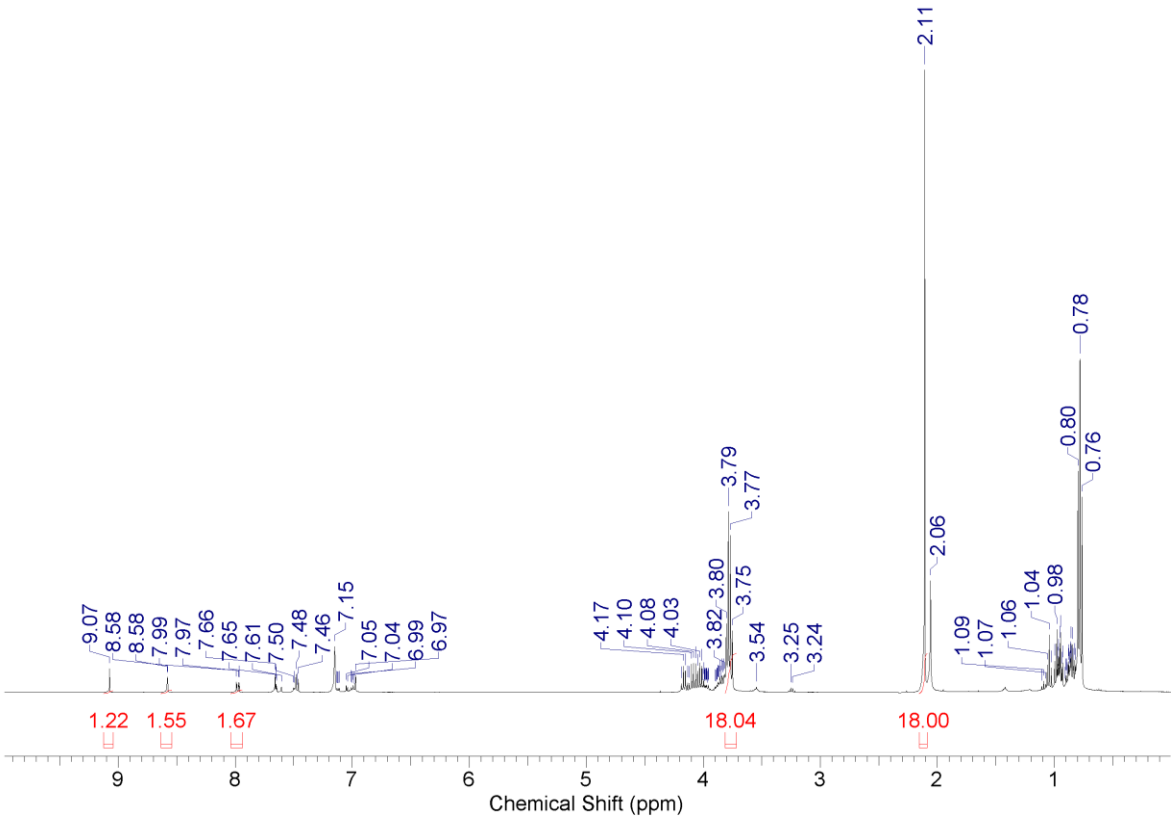

Figure S35. Reaction mixture of ethyl propiolate with 1 mol% catalyst at room temperature for 10 minutes (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.78 ppm, 2.06 ppm, and 0.78 ppm correspond to the starting material (2H, 1H, and 3H respectively). The peak at 9.07 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.58 ppm, 7.97 ppm, and 7.47 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.11 ppm corresponds to the internal integration standard hexamethylbenzene (18H, 0.06 mmol). The peaks at 3.54 ppm and 1.41 ppm correspond to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peak at 1.22 ppm corresponds to hexane. The peaks at 7.50 ppm and 6.98 ppm correspond to diphenylacetylene. All other peaks in the aromatic region correspond to cyclooctatetraenes.

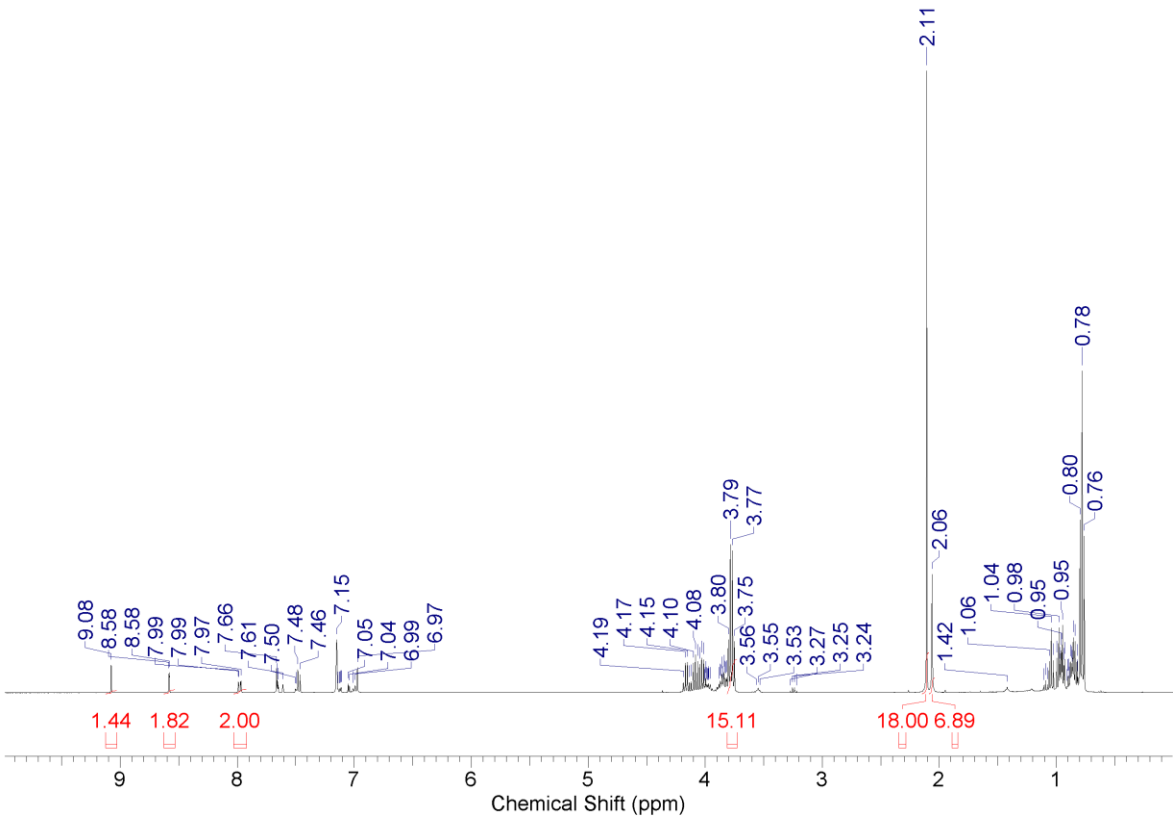

Figure S36. Reaction mixture of ethyl propiolate with 1 mol% catalyst at room temperature for 25 minutes (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.78 ppm, 2.06 ppm, and 0.78 ppm correspond to the starting material (2H, 1H, and 3H respectively). The peak at 9.07 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.58 ppm, 7.97 ppm, and 7.47 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.11 ppm corresponds to the internal integration standard hexamethylbenzene (18H, 0.06 mmol). The peaks at 3.54 ppm and 1.41 ppm correspond to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peak at 1.22 ppm corresponds to hexane. The peaks at 7.50 ppm and 6.98 ppm correspond to diphenylacetylene. All other peaks in the aromatic region correspond to cyclooctatetraenes.

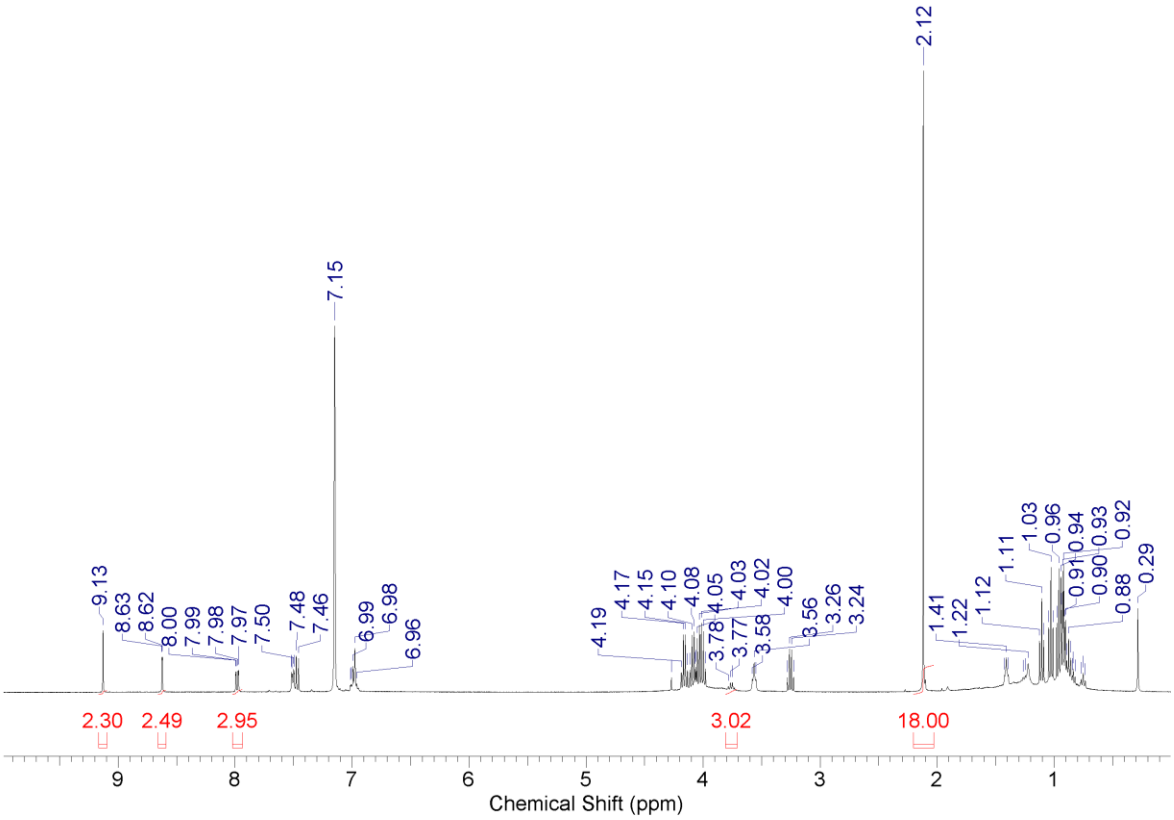

Figure S37. Reaction mixture of ethyl propiolate with 1 mol% catalyst at room temperature for 40 minutes (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.78 ppm, 2.06 ppm, and 0.78 ppm correspond to the starting material (2H, 1H, and 3H respectively). The peak at 9.07 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.58 ppm, 7.97 ppm, and 7.47 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.11 ppm corresponds to the internal integration standard hexamethylbenzene (18H, 0.06 mmol). The peaks at 3.54 ppm and 1.41 ppm correspond to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peak at 1.22 ppm corresponds to hexane. The peaks at 7.50 ppm and 6.98 ppm correspond to diphenylacetylene. All other peaks in the aromatic region correspond to cyclooctatetraenes.

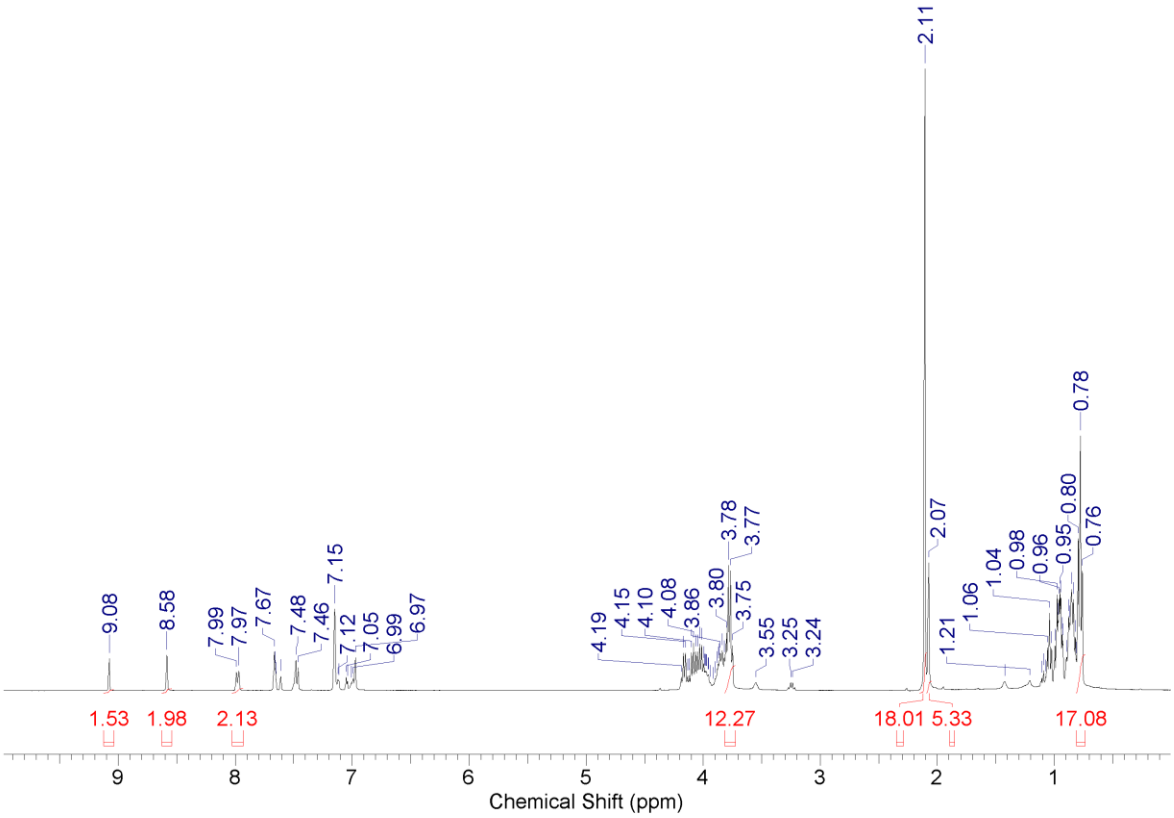

Figure S38. Reaction mixture of ethyl propiolate with 1 mol% catalyst at room temperature for 65 minutes (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.78 ppm, 2.06 ppm, and 0.78 ppm correspond to the starting material (2H, 1H, and 3H respectively). The peak at 9.07 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.58 ppm, 7.97 ppm, and 7.47 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.11 ppm corresponds to the internal integration standard hexamethylbenzene (18H, 0.06 mmol). The peaks at 3.54 ppm and 1.41 ppm correspond to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peak at 1.22 ppm corresponds to hexane. The peaks at 7.50 ppm and 6.98 ppm correspond to diphenylacetylene. All other peaks in the aromatic region correspond to cyclooctatetraenes.

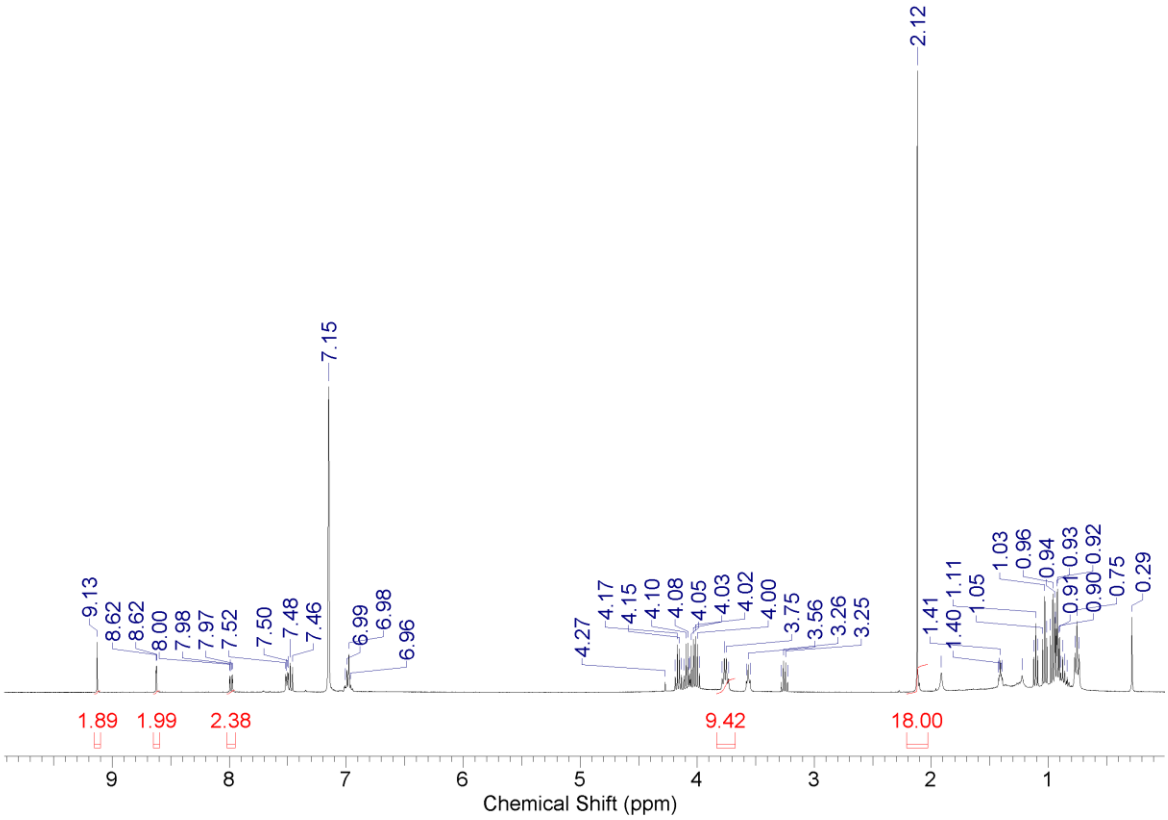

Figure S39. Reaction mixture of ethyl propiolate with 5 mol% catalyst at room temperature for 10 minutes (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.76 ppm, 1.91 ppm, and 0.75 ppm correspond to the starting material (2H, 1H, and 3H respectively). The peak at 9.13 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.62 ppm, 7.99 ppm, and 7.47 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.12 ppm corresponds to the internal integration standard hexamethylbenzene (18H, 0.016 mmol). The peaks at 3.56 ppm and 1.41 ppm correspond to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peak at 1.22 ppm corresponds to hexane. The peaks at 7.50 ppm and 6.98 ppm correspond to diphenylacetylene. The lack of other peaks in the aromatic region indicates the absence of cyclooctatetraene products.

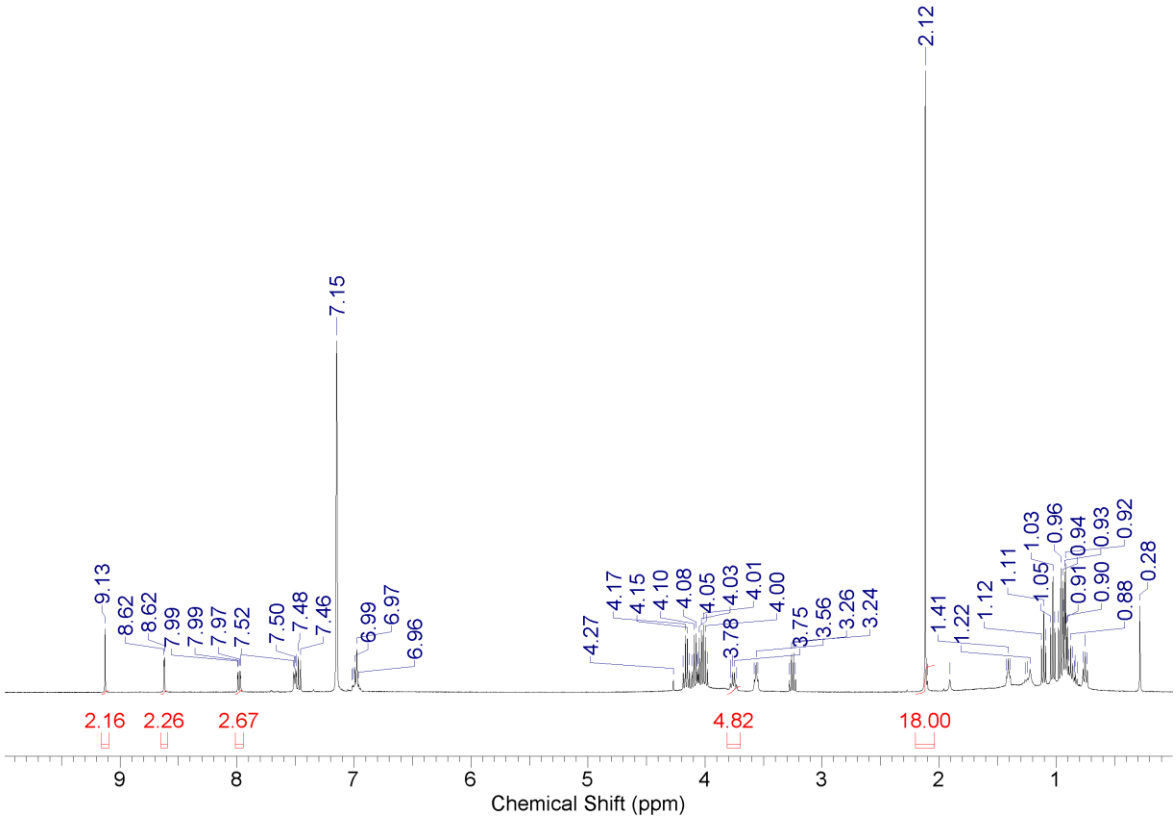

Figure S40. Reaction mixture of ethyl propiolate with 5 mol% catalyst at room temperature for 25 minutes (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.76 ppm, 1.91 ppm, and 0.75 ppm correspond to the starting material (2H, 1H, and 3H respectively). The peak at 9.13 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.62 ppm, 7.99 ppm, and 7.47 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.12 ppm corresponds to the internal integration standard hexamethylbenzene (18H, 0.016 mmol). The peaks at 3.56 ppm and 1.41 ppm correspond to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peak at 1.22 ppm corresponds to hexane. The peaks at 7.50 ppm and 6.98 ppm correspond to diphenylacetylene. The lack of other peaks in the aromatic region indicates the absence of cyclooctatetraene products.

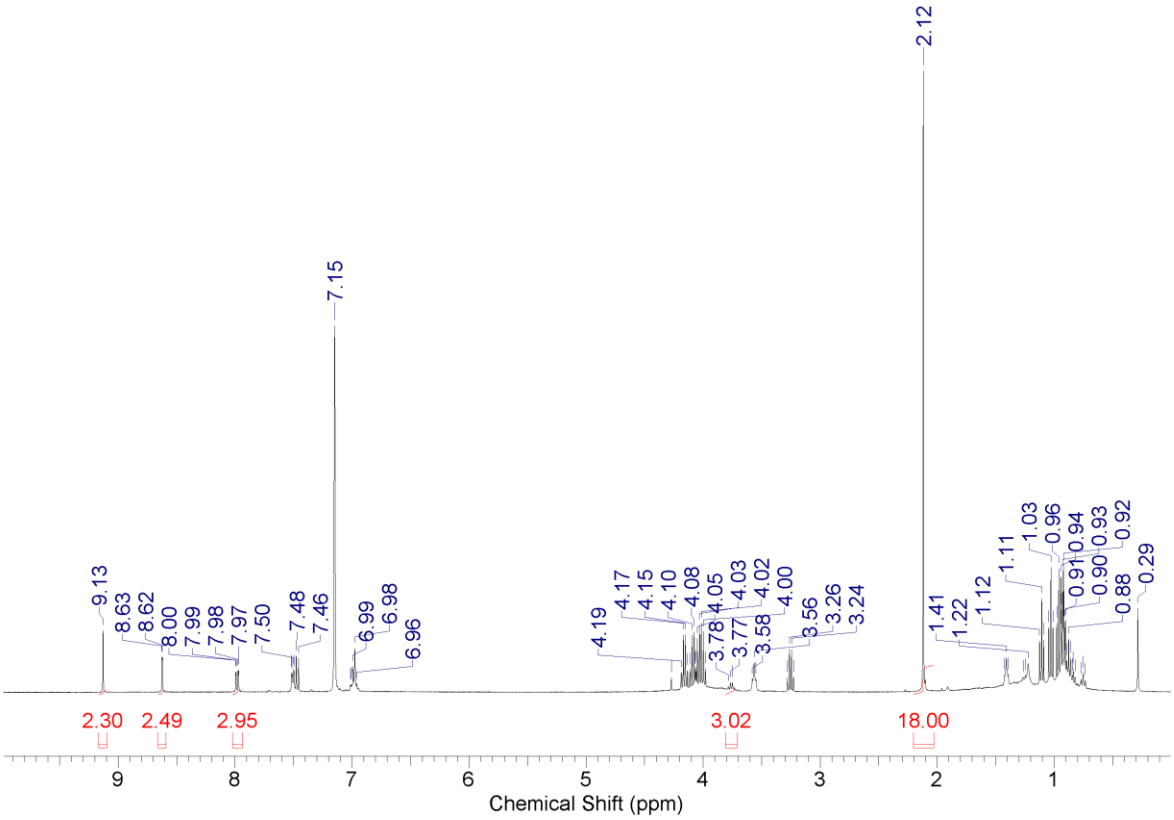

Figure S41. Reaction mixture of ethyl propiolate with 5 mol% catalyst at room temperature for 40 minutes (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.76 ppm and 0.75 ppm correspond to the starting material (2H, 1H, and 3H respectively). The peak at 9.13 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.62 ppm, 7.99 ppm, and 7.47 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.12 ppm corresponds to the internal integration standard hexamethylbenzene (18H, 0.016 mmol). The peaks at 3.56 ppm and 1.41 ppm correspond to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peak at 1.22 ppm corresponds to hexane. The peaks at 7.50 ppm and 6.98 ppm correspond to diphenylacetylene. The lack of other peaks in the aromatic region indicates the absence of cyclooctatetraene products.

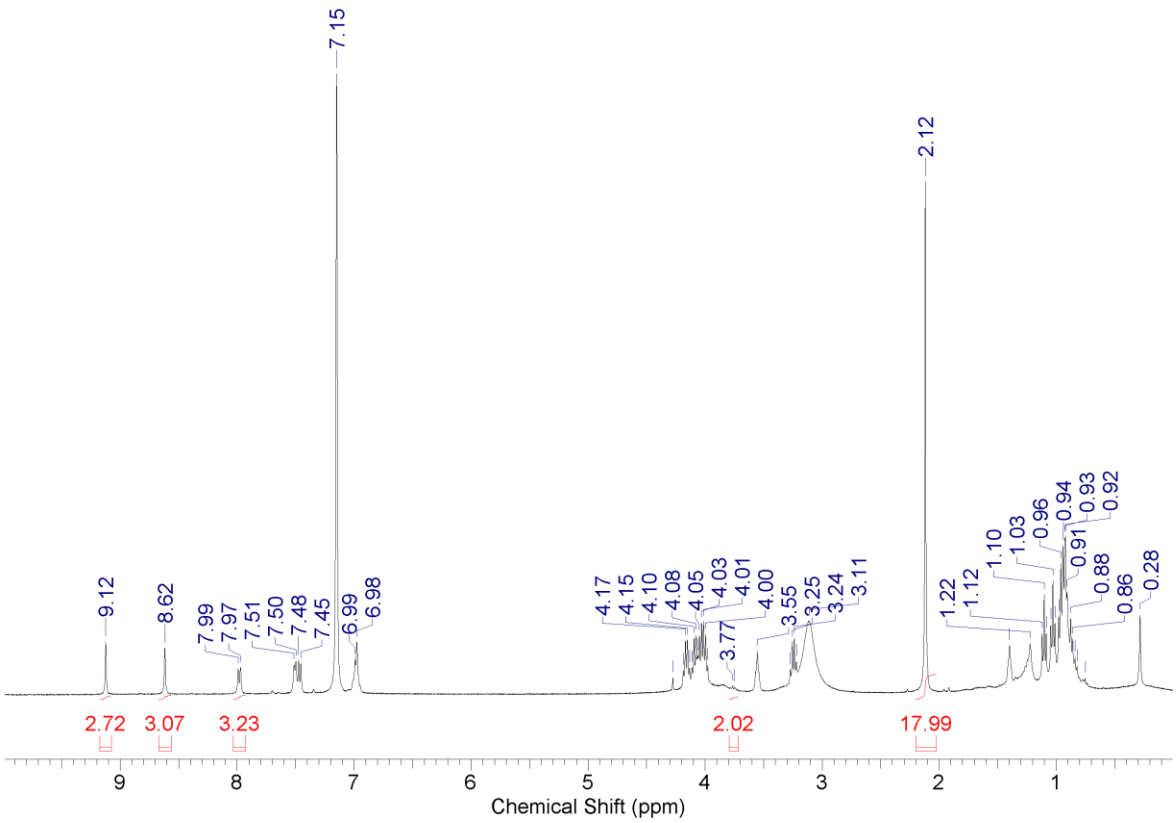

Figure S42. Reaction mixture of ethyl propiolate with 5 mol% catalyst at room temperature for 60 minutes (reaction in C_6D_6, NMR in C_6D_6).

The peaks at 3.76 ppm and 0.75 ppm correspond to the starting material (2H, 1H, and 3H respectively). The peak at 9.13 ppm corresponds to the 1,3,5-isomer (3H). The peaks at 8.62 ppm, 7.99 ppm, and 7.47 ppm correspond to the 1,2,4-isomer (1H each). The peak at 2.12 ppm corresponds to the internal integration standard hexamethylbenzene (18H, 0.016 mmol). The peaks at 3.56 ppm and 1.41 ppm correspond to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peak at 3.11 ppm corresponds to methanol. The peak at 1.22 ppm corresponds to hexane. The peaks at 7.50 ppm and 6.98 ppm correspond to diphenylacetylene. The lack of other peaks in the aromatic region indicates the absence of cyclooctatetraene products.

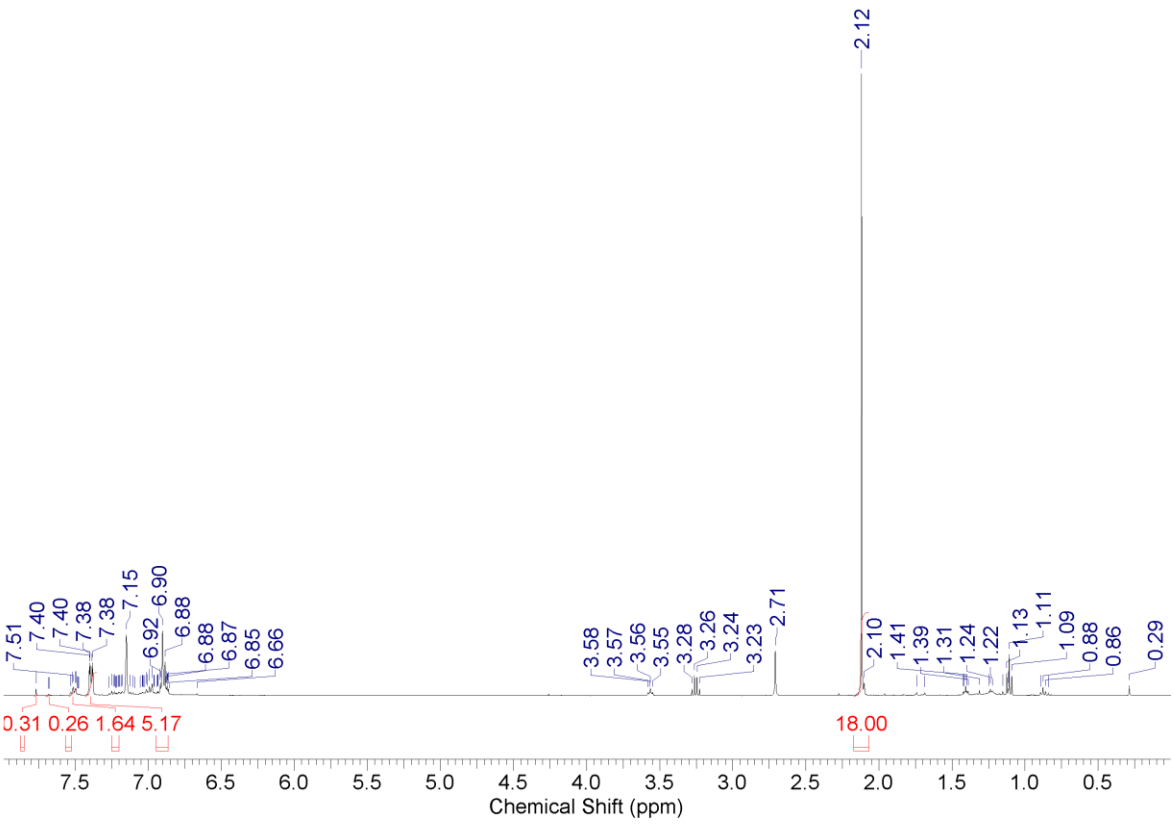

Figure S43. Reaction mixture of phenylacetylene with 5 mol% catalyst at 60 °C for 40 minutes (reaction in C_6D_6, NMR in C_6D_6).

The peak at 7.39 ppm corresponds to the starting material (2H). The peak at 7.77 ppm corresponds to the 1,3,5-isomer (3H). The peak at 7.51 corresponds to the 1,2,4-isomer (1H). The peak at 2.12 corresponds to the internal integration standard hexamethylbenzene (18H, 0.05 mmol). The peaks for diphenylacetylene (7.50 ppm and 6.99 ppm) are masked by the starting material and benzene products of the reaction. The lack of peaks in the vinylic region indicates the absence of cyclooctatetraene products. The peaks at 3.54 ppm and 1.41 ppm correspond to THF. The peaks at 3.25 ppm and 1.11 ppm correspond to ether. The peaks at 1.22 ppm and 0.88 ppm correspond to hexane.

iv. Reaction Profiles of Ethyl Propiolate Cyclotrimerization

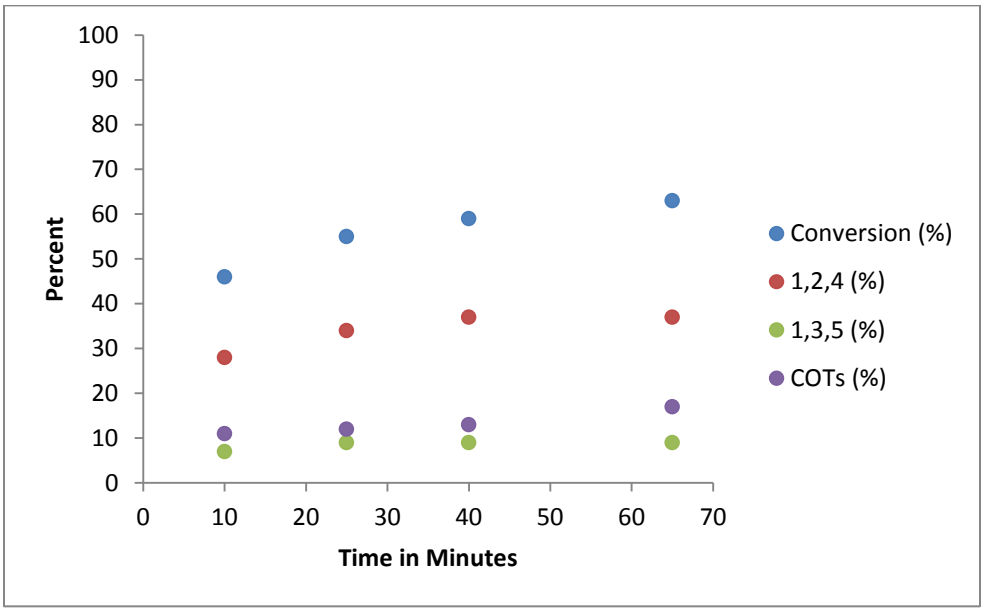

Figure S44. Reaction profile diagram of catalytic ethyl propiolate cyclotrimerization by *2* at room temperature in C_6D_6 (1 mol%).

Exact values are located in Table S1.

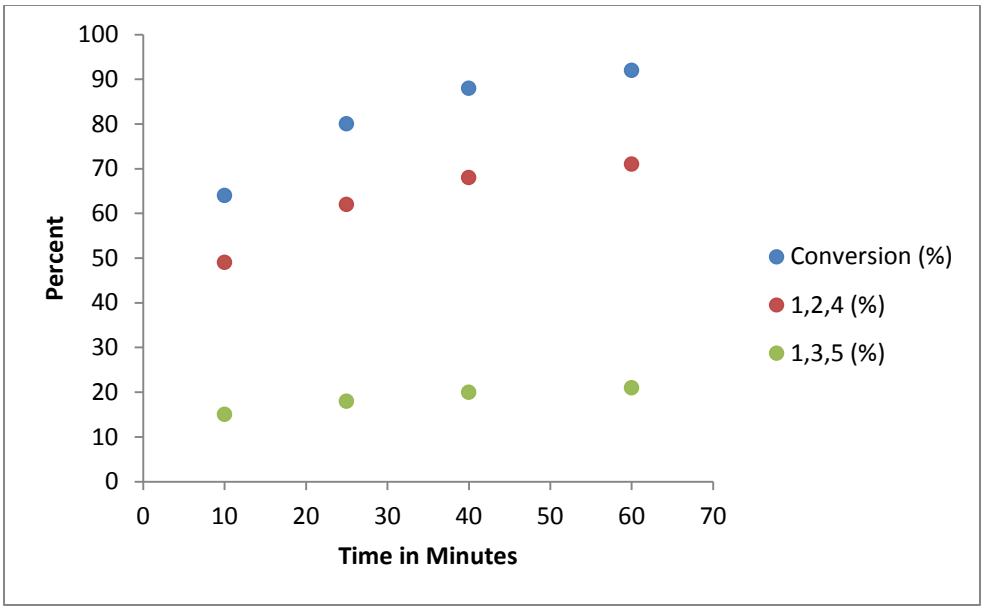

Figure S45. Reaction profile diagram of catalytic ethyl propiolate cyclotrimerization by *2* at room temperature in C_6D_6 (5 mol%).

Exact values are located in Table S1.

Table S1. Reaction profile of catalytic ethyl propiolate cyclotrimerization by *2* at room temperature in C_6D_6 (1 mol% and 5 mol%).

mol %	Time (min)	% conversion	Benzenes % 1,2,4 / % 1,3,5	Combined cyclotetraenes (%)
1	10	46	28 / 7	11
1	25	55	34 / 9	12
1	40	59	37 / 9	13
1	65	63	37 / 9	17
5	10	64	49 / 15	0
5	25	80	62 / 18	0
5	40	88	68 / 20	0
5	60	92	71 / 21	0

2. Computational Details

Electronic structure calculations were carried out using B3LYP/6-31G(d),[3] as implemented in Gaussian09.[4] Optimized structures were confirmed to be stable minima through analysis of the harmonic frequencies,[5] and the wavefunction at each minimum was confirmed to be stable.[6] Follow-up single point calculations were done at the B3LYP/6-311+G(d,p) for the acetylene complexes. Tables S2 and S3 contain the Cartesian coordinates and frequencies for the optimized species. Table S4 summarizes relevant thermodynamic values that were calculated as $G(gas)_{TZ} \approx G(gas)_{DZ} - E(SCF)_{DZ} + E(SCF)_{TZ}$, where DZ and TZ represent the 6-31G(d) and 6-311+G(d,p) basis sets, respectively.

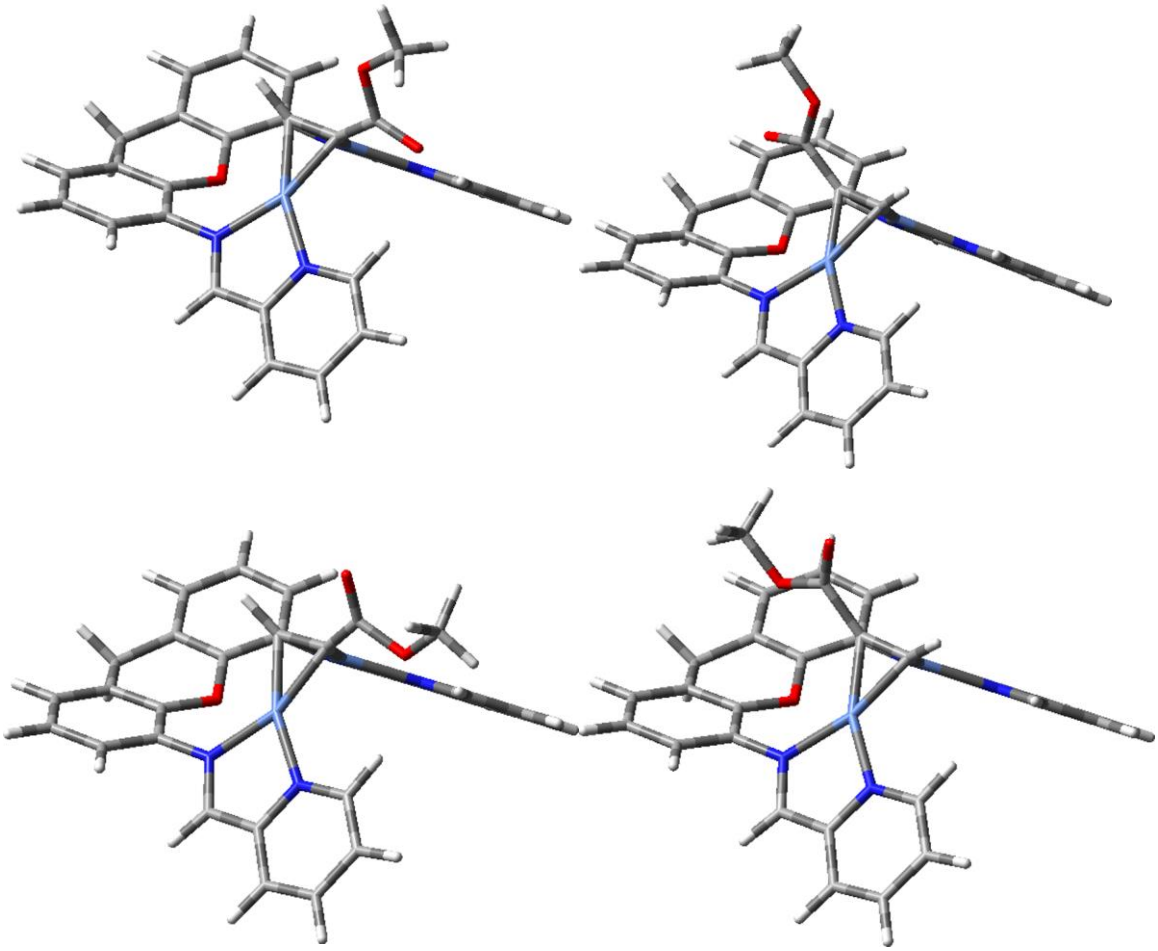

Figure S46. Comparison of the regioisomers of **5** (top left), **5a** (top right), **5b** (bottom left), and **5c** (bottom right).[7] Their relative free energies at the B3LYP/6-31G(d) level of theory are 0.00, 3.65, 1.72, and 3.13 kcal/mol, respectively.

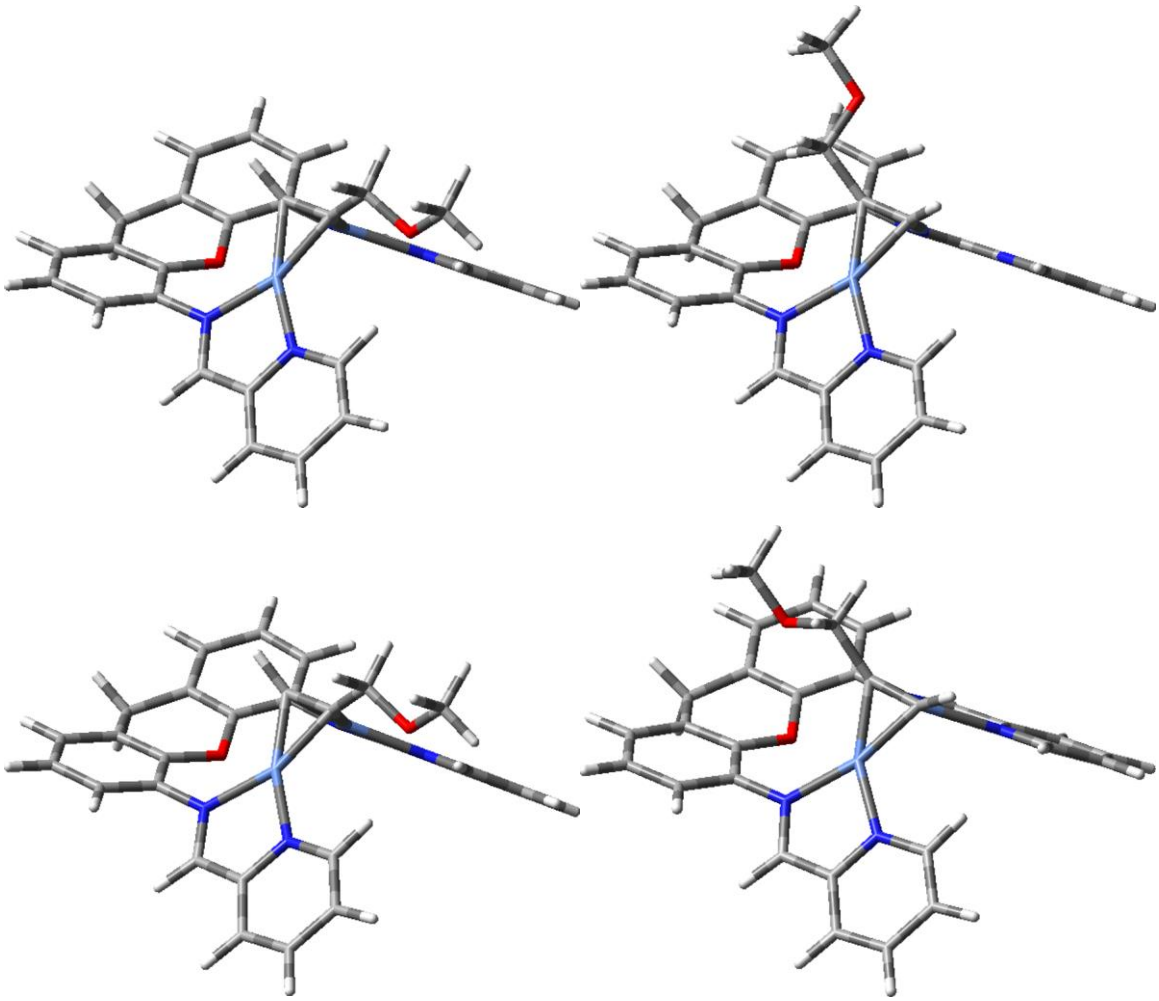

Figure S47. Comparison of the regioisomers of **6** (top left), **6a** (top right), **6b** (bottom left), and **6c** (bottom right).[7] Their relative free energies at the B3LYP/6-31G(d) level of theory are 0.00, 1.45, 0.01, and 3.06 kcal/mol, respectively.

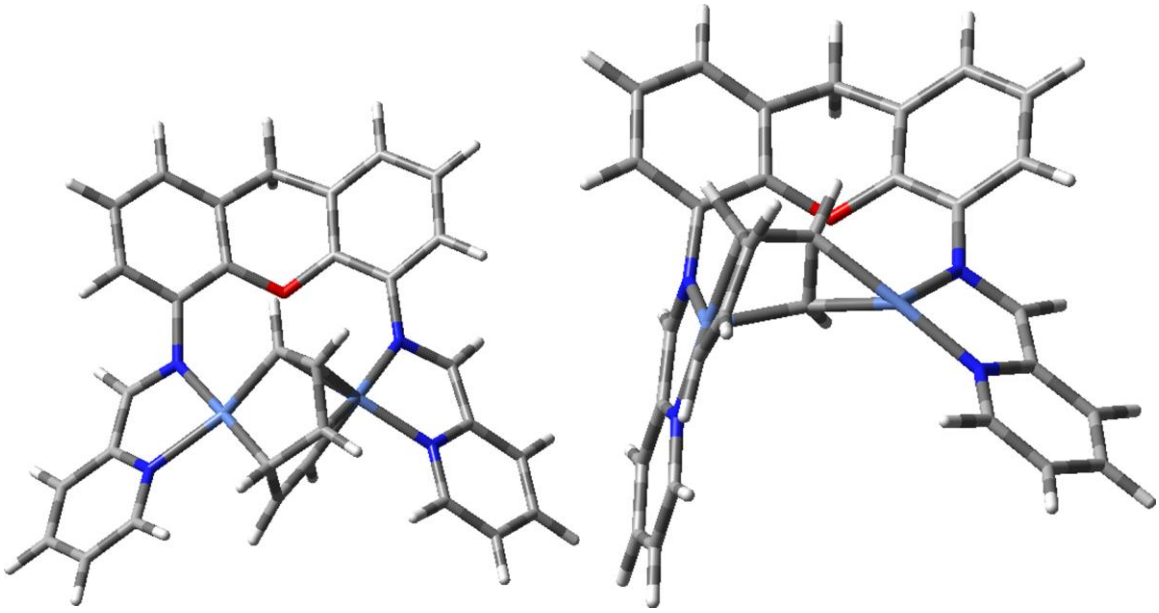

Figure S48. Images of the metallabicycles formed from approach of the alkyne from the bottom face **9c** (left) and **9d** (right) of the catalyst.[7] **9c** was so unfavorable that the newly added alkyne coordinated to the second nickel during geometry optimization. **9d** was similarly strained and preferred coordination of the nickelabutene to the second metal.

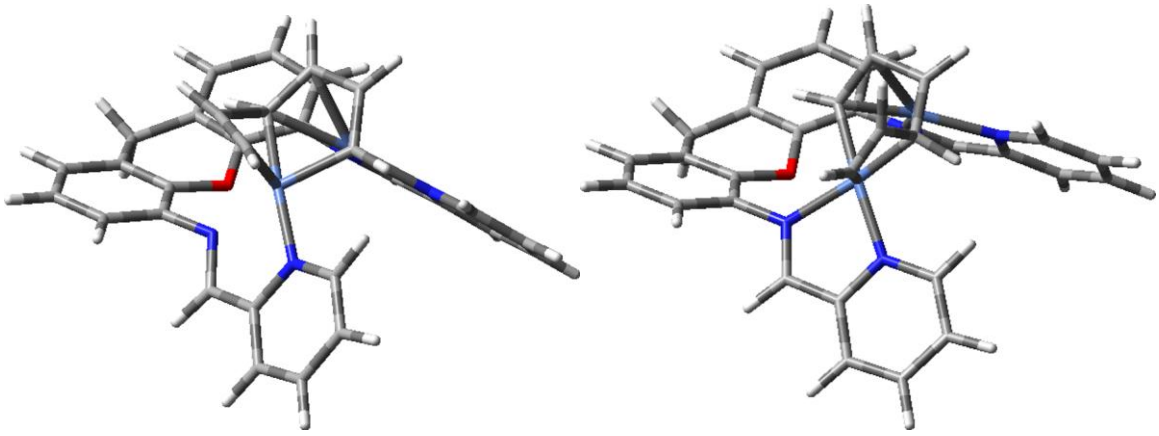

Figure S49. Images of [2 + 2] transition states **8–9a–TS** (left) and **8–9b–TS** (right).[7]

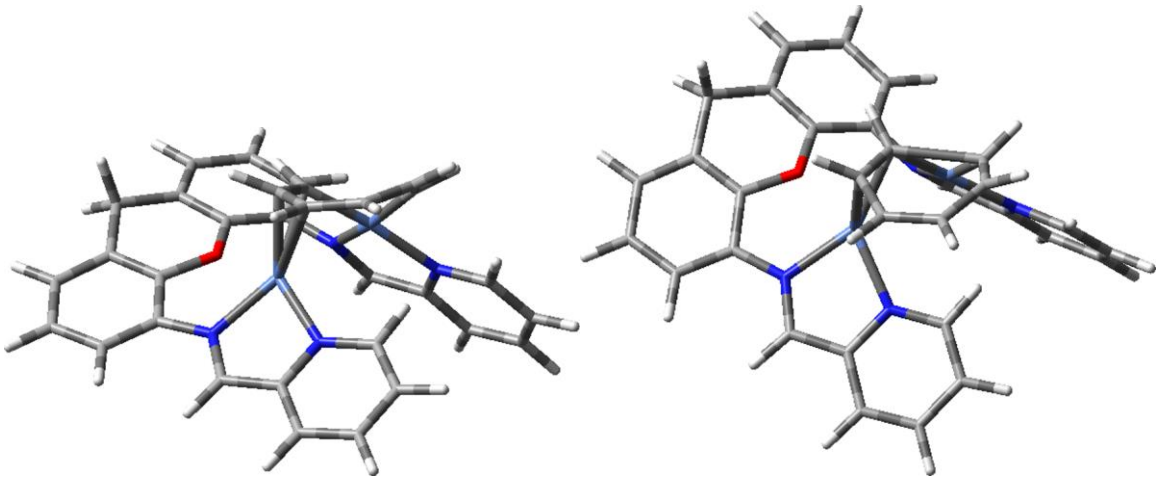

Figure S50. Image of isomer of nickelacycloheptatriene **10'** (left) and the transition state for reductive elimination of benzene from this intermediate (right).[7]

Table S2. Cartesian coordinates (Å) for all optimized structures.

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4
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C  -3.845697  3.637630  0.062929
C  -4.586180  2.477087 -0.137738
C  -3.945481  1.254938 -0.359438
C  -2.547861  1.192511 -0.352136
C  -1.776002  2.364027 -0.173607
C  -2.455866  3.575792  0.037219
C  -4.735782  0.007614 -0.667097
C  -2.552034 -1.184245 -0.349967
C  -3.949936 -1.241826 -0.356767
C  -4.594889 -2.461213 -0.132268
H  -5.681927 -2.488209 -0.125212
C  -3.858603 -3.624160  0.069822
C  -2.468558 -3.567433  0.042544
C  -1.784457 -2.358521 -0.170708
H  -5.680179  0.009903 -0.108846
H  -4.344368  4.584997  0.246845
H  -5.673113  2.508079 -0.131533
H  -1.865582  4.467527  0.223792
H  -4.360565 -4.569409  0.255612
H  -1.881191 -4.461051  0.229342
O  -1.878398  0.002678 -0.563096
H  -5.018611  0.006838 -1.732813
N  -0.367162  2.331690 -0.174127
N  -0.375467 -2.331222 -0.172966
C   0.275468  3.308120 -0.828139
H  -0.258682  4.020490 -1.453119
C   0.263326 -3.310282 -0.826775
H  -0.273958 -4.021988 -1.449845
C   1.690089  3.351199 -0.710701
C   2.527141  4.287239 -1.357071
N   2.216172  2.373250  0.108641
C   3.892927  4.223744 -1.166522
H   2.082051  5.045102 -1.995556
C   3.552027  2.329158  0.273947
C   4.424195  3.219734 -0.329563
H   4.550616  4.937298 -1.654719
H   3.913923  1.538474  0.924287
H   5.491696  3.136555 -0.155395
C   1.678060 -3.356924 -0.711863
C   2.511266 -4.295789 -1.359079
N   2.208497 -2.379417  0.105341
C   3.877644 -4.235512 -1.171790
H   2.062916 -5.053263 -1.995759
C   3.544757 -2.338939  0.267950
C   4.413313 -3.232204 -0.336895
H   4.532428 -4.951111 -1.660913
H   3.910116 -1.549147  0.917413
H   5.481399 -3.151707 -0.165081
Ni  0.809088  1.253956  0.876641
Ni  0.804896 -1.257284  0.875826
C   0.026703 -0.001203  2.025453
C   1.390933 -0.002757  2.155097
H   2.143272 -0.004307  2.937785
H  -0.867909 -0.000150  2.640172

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2'
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C   3.999194 -3.648647 -0.402223
C   4.767709 -2.494713 -0.519621
C   4.167425 -1.268197 -0.814649
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C   2.778797 -1.196586 -0.967202
C   1.981685 -2.357628 -0.872237
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6b

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6c

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7
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9a

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9b

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H   4.047992 -4.916099 -0.065450
H   5.592603 -2.978907 -0.317582
H   1.590700 -4.552193 -0.116291
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H   2.214289  4.200568  0.334908
O   2.076771 -0.132619 -0.889124
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9c

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H   4.670453  1.548073  0.577617
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H  -1.479167 -3.401480 -0.604486

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8-9a-TS
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C  -2.832361  0.921613 -0.519872
C  -2.226068  2.152389 -0.205342
C  -3.053792  3.219728  0.170321
C  -4.800865 -0.570358 -0.912311
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8-9b-TS

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H  -2.073218 -4.280380  0.437435
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9b-10-TS

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H  -2.270961 -4.253594  0.151256
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H  -5.233015  0.361615 -1.826225
N  -0.330413  2.229263 -0.396556
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H  -0.740031 -3.564118 -2.002848
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H   4.741606  4.238776 -2.220145
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C  -4.908498 -0.545221 -0.694604
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H  -5.788087 -0.588625 -0.039442
H  -4.926942  4.151743 -0.386968
H  -6.070631  1.947270 -0.437458
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H  -3.839279 -4.967472  0.486564
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O  -2.061720 -0.208758 -0.786769
H  -5.292426 -0.691033 -1.717352
N  -0.778670  2.137935 -0.580222
N  -0.240483 -2.200134 -0.274035
C  -0.123388  2.849406 -1.482003
H  -0.639069  3.390660 -2.274061
C   0.437498 -2.913731 -1.179296
H  -0.079056 -3.561378 -1.885295
C   1.301991  2.844829 -1.393307
C   2.159893  3.523387 -2.280726
N   1.796659  2.103965 -0.345631
C   3.527237  3.455134 -2.089434
H   1.732491  4.090508 -3.102717
C   3.132161  2.052139 -0.175848
C   4.027628  2.705496 -1.007580
H   4.204779  3.971808 -2.762978
H   3.470432  1.460283  0.669143
H   5.093276  2.629794 -0.819261
C   1.840670 -2.784585 -1.197667
C   2.701650 -3.420554 -2.123923
N   2.339163 -1.949043 -0.211993
C   4.058756 -3.196115 -2.060799
H   2.271586 -4.076582 -2.875617
C   3.672281 -1.746535 -0.177525
C   4.561707 -2.330034 -1.061715
H   4.732152 -3.675601 -2.765665
H   4.022261 -1.091154  0.613438
H   5.622854 -2.121199 -0.977211
Ni  0.375942  1.240711  0.715945
Ni  0.957063 -1.172991  0.924620
C  -0.414049 -0.355480  1.873758
C   1.837753  1.454965  3.219792
H   2.437321  2.271462  3.623904
C  -0.536425  0.823885  2.581328
H  -1.536906  1.158407  2.866116
C   0.522484  1.748680  2.958149
H   0.190575  2.758193  3.195219
```

```
H  -1.367544 -0.876314  1.764115
C   2.144336 -0.855051  2.299562
H   2.771884 -1.745737  2.434993
C   2.492017  0.178723  3.113639
H   3.369611  0.070347  3.757885

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10'
--------
C   2.767541 -4.346543  0.102889
C   3.842322 -3.468533  0.223158
C   3.634487 -2.085672  0.188133
C   2.331563 -1.613757  0.025551
C   1.221485 -2.469699 -0.120804
C   1.476878 -3.852174 -0.065230
C   4.790423 -1.114879  0.313458
C   3.109426  0.623970 -0.328957
C   4.443033  0.256616 -0.216430
C   5.410194  1.211544 -0.557401
H   6.462429  0.947982 -0.486907
C   5.034476  2.491071 -0.968382
C   3.688819  2.851434 -1.038333
C   2.694400  1.915926 -0.715166
H   5.088398 -1.030007  1.370743
H   2.932903 -5.419501  0.143728
H   4.853410 -3.848350  0.346523
H   0.632438 -4.529442 -0.146704
H   5.797618  3.222083 -1.219871
H   3.411968  3.861336 -1.323494
O   2.070857 -0.251257 -0.070116
H   5.667953 -1.512795 -0.211408
N  -0.083115 -1.983389 -0.331360
N   1.318565  2.118624 -0.684626
C  -0.742734 -2.547691 -1.365917
H  -0.205126 -3.116940 -2.121429
C   0.704255  3.177687 -1.197448
H   1.229341  3.983414 -1.706087
C  -2.135243 -2.375458 -1.441247
C  -2.954135 -2.846096 -2.499324
N  -2.680623 -1.691647 -0.367940
C  -4.311432 -2.620977 -2.463452
H  -2.491439 -3.380108 -3.324481
C  -4.012273 -1.484491 -0.363043
C  -4.861599 -1.919216 -1.366075
H  -4.951260 -2.977324 -3.266040
H  -4.394769 -0.946874  0.499192
H  -5.925669 -1.720121 -1.297828
C  -0.716150  3.185557 -1.089301
C  -1.534387  4.216998 -1.596269
N  -1.257363  2.086009 -0.460884
C  -2.906524  4.125087 -1.461826
H  -1.070269  5.069600 -2.083985
C  -2.594420  2.028760 -0.324762
C  -3.452411  3.005271 -0.809763
H  -3.551907  4.908145 -1.849921
H  -2.969932  1.161569  0.204773
H  -4.523264  2.895809 -0.675650
Ni -1.336402 -1.072055  0.896843
Ni  0.175699  0.873935  0.304091
C  -0.055929 -0.310854  1.994315
C  -2.566620 -0.676288  2.219859
H  -3.214128 -1.552137  2.371745
C   0.079128  0.947598  2.560730
H   1.061204  1.204193  2.972132
C  -2.934297  0.400130  2.964480
H  -3.848391  0.325968  3.562148
H   0.831875 -0.937641  2.138917
C  -2.263544  1.672257  3.082055
H  -2.866553  2.498150  3.460768
C  -0.941155  1.924793  2.880119
H  -0.579716  2.928980  3.097872

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10' red el
--------
C   2.618534 -4.395782 -0.198751
C   3.715968 -3.576014  0.059216
C   3.543247 -2.193801  0.183086
C   2.261752 -1.665329  0.030803
C   1.128785 -2.455277 -0.253246
C   1.348927 -3.845515 -0.347798
C   4.705311 -1.261236  0.460888
C   3.132809  0.544348 -0.219754
C   4.447377  0.119453 -0.097713
C   5.456172  1.016713 -0.470923
H   6.496238  0.710451 -0.395056
C   5.132400  2.297313 -0.924739
C   3.803656  2.711780 -1.016625
C   2.767909  1.831207 -0.664696
H   4.871236 -1.189081  1.547947
H   2.749578 -5.471571 -0.276850
H   4.710514 -4.000195  0.169597
H   0.491436 -4.487131 -0.523758
H   5.925963  2.986185 -1.200332
H   3.570908  3.718266 -1.349769
O   2.066832 -0.286631  0.089312
H   5.628877 -1.677459  0.041831
N  -0.149041 -1.903738 -0.429545
N   1.400299  2.072422 -0.674968
C  -0.892744 -2.447320 -1.422796
H  -0.418142 -3.009565 -2.224489
C   0.815335  3.130744 -1.226089
H   1.366480  3.921887 -1.730363
C  -2.287903 -2.276860 -1.384468
C  -3.192998 -2.734144 -2.377123
N  -2.750698 -1.621606 -0.255497
C  -4.544949 -2.532766 -2.211995
H  -2.801201 -3.241031 -3.254439
```

```
C  -4.077713 -1.438058 -0.120972
C  -5.008039 -1.867784 -1.052928
H  -5.248695 -2.881777 -2.962762
H  -4.383418 -0.921294  0.784530
H  -6.065258 -1.692553 -0.885321
C  -0.607073  3.153624 -1.168101
C  -1.397653  4.185200 -1.719708
N  -1.184722  2.068752 -0.543674
C  -2.774128  4.106838 -1.638497
H  -0.907634  5.027156 -2.200613
C  -2.527021  2.024803 -0.461962
C  -3.357000  2.999650 -0.994826
H  -3.396335  4.890124 -2.062404
H  -2.932590  1.165489  0.058675
H  -4.433355  2.899391 -0.905338
Ni -1.311912 -0.996382  0.872392
Ni  0.213521  0.866207  0.308228
C  -0.150059 -0.260064  2.096071
C  -2.270654 -0.620414  2.407412
H  -2.694769 -1.568463  2.769419
C   0.081546  1.063380  2.496896
H   1.073547  1.299789  2.893258
C  -2.774343  0.493994  3.026292
H  -3.641152  0.372524  3.682126
H   0.658858 -0.947360  2.376672
C  -2.226953  1.811707  2.983187
H  -2.855959  2.633522  3.322581
C  -0.905688  2.078508  2.731836
H  -0.544567  3.096440  2.866930

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11
--------
C   4.631352 -2.555339  1.390714
C   5.244383 -1.422417  0.862251
C   4.493440 -0.503265  0.127475
C   3.119968 -0.699119 -0.050507
C   2.507728 -1.903256  0.359088
C   3.287025 -2.792762  1.125370
C   5.107589  0.692623 -0.550758
C   2.783542  1.582562 -0.539275
C   4.156486  1.856348 -0.459976
C   4.612393  3.161283 -0.277735
H   5.681159  3.344006 -0.202385
C   3.700611  4.205413 -0.169169
C   2.342259  3.934415 -0.257040
C   1.837345  2.631845 -0.474253
H   6.072592  0.947186 -0.099712
H   5.198261 -3.259500  1.993121
H   6.305853 -1.242286  1.012059
H   2.802790 -3.679286  1.522316
H   4.039337  5.221516  0.011242
H   1.634180  4.738136 -0.091446
O   2.352193  0.272486 -0.688350
H   5.309941  0.451478 -1.607194
N   1.208946 -2.253878 -0.053081
N   0.436251  2.445830 -0.530358
C   1.054211 -3.529848 -0.422276
H   1.902206 -4.207995 -0.477327
C  -0.257087  3.471818 -1.012894
H   0.221072  4.260711 -1.589818
C  -0.228903 -3.963314 -0.812928
C  -0.519934 -5.276254 -1.251063
N  -1.211790 -2.999111 -0.718924
C  -1.818355 -5.618378 -1.560405
H   0.290171 -5.995817 -1.328322
C  -2.473022 -3.363315 -1.019775
C  -2.825379 -4.640029 -1.428938
H  -2.061692 -6.623379 -1.893784
H  -3.219355 -2.585706 -0.924999
H  -3.864564 -4.865210 -1.643587
C  -1.639749  3.576308 -0.690466
C  -2.472981  4.634256 -1.104910
N  -2.093166  2.589370  0.145929
C  -3.761448  4.711367 -0.608574
H  -2.086002  5.379535 -1.793920
C  -3.348388  2.685245  0.627094
C  -4.202819  3.725451  0.293404
H  -4.417936  5.525600 -0.901343
H  -3.662523  1.890239  1.293143
H  -5.197099  3.763216  0.725784
Ni -0.503646 -1.275407 -0.076840
Ni -0.836119  1.066409  0.179990
C  -2.060221 -0.616107  3.042081
C  -1.767488 -0.230245 -0.989018
H  -1.346003 -0.086609 -1.995237
C  -3.340477 -0.860791  2.533250
H  -3.987569 -1.144236  3.364345
C  -3.154635 -0.190791 -0.995910
H  -3.620921  0.058633 -1.953788
H  -2.089610 -0.707678  4.128870
C  -4.117368 -0.452185  0.007574
H  -5.128638 -0.419000 -0.401764
C  -4.150539 -0.786114  1.365154
H  -5.179208 -1.010712  1.650617
C  -0.730334 -0.300096  2.642257
H  -0.097851 -0.144019  3.521585
C  -0.044422 -0.220914  1.435139
H   1.026886 -0.078618  1.585312

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12
--------
C   2.721179 -4.133386 -0.826054
C   3.839579 -3.416570 -0.393616
C   3.707167 -2.084526  0.009149
C   2.434996 -1.519964 -0.043933
C   1.294677 -2.190010 -0.500461
```

```
C   1.464008 -3.529818 -0.883933
C   4.858173 -1.207719  0.474016
C   3.296345  0.678729  0.045470
C   4.609512  0.244567  0.106180
C   5.607711  1.183196 -0.189768
H   6.652856  0.887060 -0.160328
C   5.254643  2.494964 -0.520105
C   3.919511  2.897854 -0.590346
C   2.889710  1.976226 -0.321763
H   4.971128 -1.297486  1.566278
H   2.829914 -5.171138 -1.128376
H   4.818014 -3.889495 -0.369633
H   0.597479 -4.083399 -1.233231
H   6.036046  3.218297 -0.737144
H   3.679005  3.919378 -0.867174
O   2.253664 -0.199238  0.317355
H   5.801493 -1.556853  0.039294
N   0.046533 -1.512611 -0.615705
N   1.517747  2.154193 -0.406800
C  -0.504777 -1.596217 -1.867953
H   0.133108 -1.740491 -2.736124
C   0.922737  3.277002 -0.820408
H   1.472232  4.176383 -1.091100
C  -1.899165 -1.527052 -1.978726
C  -2.616253 -1.526500 -3.204812
N  -2.567823 -1.485245 -0.763030
C  -3.991042 -1.509265 -3.191787
H  -2.058833 -1.544933 -4.136597
C  -3.918083 -1.464920 -0.785360
C  -4.665324 -1.482829 -1.949701
H  -4.551773 -1.514020 -4.122215
H  -4.400012 -1.417963  0.183185
H  -5.748324 -1.471795 -1.893767
C  -0.492661  3.247823 -0.899922
C  -1.270856  4.365505 -1.285308
N  -1.093000  2.047309 -0.561641
C  -2.645985  4.268717 -1.311416
H  -0.765634  5.291200 -1.546913
C  -2.437448  1.992908 -0.566842
C  -3.250846  3.052939 -0.936721
H  -3.252939  5.120474 -1.606119
H  -2.870031  1.050741 -0.251938
H  -4.328922  2.934241 -0.929183
Ni -1.364325 -1.446470  0.715653
Ni  0.269024  0.714931  0.149294
C   0.017282  0.400098  2.216772
C  -2.637645 -1.595730  2.268761
H  -3.229582 -2.511929  2.219757
C  -0.789955  1.468600  2.765821
H  -0.187288  2.362165  2.935926
C  -3.503281 -0.446401  2.502388
H  -4.556967 -0.700771  2.382696
H   1.068758  0.610706  2.424683
C  -3.286349  0.854660  2.852979
H  -4.206804  1.419414  3.006005
C  -2.114667  1.658324  3.052313
H  -2.346176  2.652224  3.432729
C  -0.187892 -1.048713  2.322171
H   0.758359 -1.589742  2.347453
C  -1.284669 -1.878177  2.641860
H  -1.042186 -2.926648  2.811081

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C2H2
--------
C   0.000000  0.000000  0.602487
H   0.000000  0.000000  1.669139
C   0.000000  0.000000 -0.602487
H   0.000000  0.000000 -1.669139

--------
C2Ph2
--------
C  -0.000002  0.608237 -0.000004
C   0.000002 -0.608237 -0.000004
C   0.000006 -2.033193 -0.000010
C  -0.000046 -2.750701 -1.213329
C   0.000048 -2.750690  1.213323
C  -0.000046 -4.142732 -1.208461
H  -0.000084 -2.202974 -2.150723
C   0.000048 -4.142717  1.208472
H   0.000082 -2.202945  2.150707
C   0.000002 -4.843983  0.000007
H  -0.000084 -4.683049 -2.151343
H   0.000083 -4.683028  2.151357
H   0.000001 -5.930536  0.000015
C  -0.000006  2.033193 -0.000010
C   0.000046  2.750701 -1.213329
C  -0.000048  2.750690  1.213323
C   0.000046  4.142732 -1.208461
H   0.000084  2.202974 -2.150723
C  -0.000048  4.142717  1.208472
H  -0.000082  2.202945  2.150707
C  -0.000002  4.843983  0.000007
H   0.000084  4.683049 -2.151343
H  -0.000083  4.683028  2.151357
H  -0.000001  5.930536  0.000015

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HC2CO2Me
--------
C  -2.633531 -0.410023 -0.000118
H  -3.668255 -0.671555  0.000414
C  -1.463397 -0.113782 -0.000102
C  -0.076262  0.307843  0.000061
O   0.286057  1.464804  0.000031
O   0.750655 -0.756426  0.000146
C   2.153239 -0.433061 -0.000075
```

```
H    2.669656 -1.392829  0.003462
H    2.412883  0.142652 -0.892259
H    2.411726  0.148848  0.888365

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HC2CH2OMe
--------
C    2.579074 -0.244520 -0.000531
H    3.592696 -0.575881  0.001176
C    1.427620  0.114830  0.000234
C    0.045014  0.589578  0.000090
H   -0.128691  1.226490 -0.885459
H   -0.128834  1.226801  0.885388
C   -2.196535 -0.092700 -0.000158
H   -2.809498 -0.997069  0.000050
H   -2.439494  0.505837  0.893023
H   -2.439152  0.505202 -0.893852
O   -0.847259 -0.511813  0.000233
```

Table S3. Harmonic frequencies (cm^{-1}) for all optimized structures. A small imaginary frequency (< 6 cm–1) was ignored for one of the regioisomers of species **6**.

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--------
4
--------
   20.1557    25.9074    47.1567
   51.6312    55.0049    59.8288
   68.2238    92.1375    98.3059
  129.6583   133.1565   151.5127
  162.3884   181.7906   195.8049
  208.2302   220.0748   227.3906
  249.1610   252.4325   266.2105
  276.6038   301.8350   304.6204
  315.9423   324.0295   340.1788
  388.8423   390.0785   408.8518
  423.4729   431.0035   439.2451
  458.5823   518.0171   522.3093
  523.3047   533.0861   542.6653
  543.6832   547.0749   551.1609
  567.7208   572.2700   588.3239
  598.6177   613.7063   634.5825
  651.2237   655.7022   662.6086
  673.8426   683.1431   722.6890
  723.4525   733.2698   738.6278
  751.8784   753.7424   766.5936
  779.5016   785.7809   793.0255
  801.9267   804.8243   808.4275
  842.3080   849.6465   854.5281
  869.2095   869.6036   890.4410
  890.5772   896.9756   920.7668
  924.4545   956.4153   956.5462
  956.5798   959.4556   973.3152
  979.0786   979.2794   982.8414
 1017.2101  1024.1564  1029.0495
 1054.2256  1056.1280  1060.4241
 1118.5397  1120.4035  1142.5337
 1143.3098  1181.5911  1182.5747
 1199.4999  1199.7462  1216.6924
 1216.7750  1229.1720  1257.5608
 1266.0272  1272.6179  1274.1426
 1283.5467  1288.6183  1317.4059
 1318.7157  1329.3661  1331.7947
 1338.1780  1341.4626  1345.1496
 1359.5797  1374.2192  1379.4935
 1457.0465  1460.7127  1491.4370
 1497.7476  1501.0658  1502.7495
 1505.9704  1515.1097  1516.5945
 1520.5779  1523.5801  1585.4669
 1587.3186  1627.1785  1630.1522
 1631.1707  1640.0405  1644.5959
 1661.7729  2989.1949  3062.3429
 3179.2795  3179.4279  3180.9928
 3181.2964  3189.2606  3192.7429
 3192.8003  3198.1575  3198.2954
 3203.6523  3204.2687  3209.9082
 3210.2061  3213.1766  3213.3407
 3215.5455  3225.8342  3226.1869

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2'
--------
   10.1504    19.0005    23.2937
   29.7364    32.4213    41.7552
   42.9263    49.7983    58.5613
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  272.6077   281.2342   286.5939
  298.1944   304.0929   320.2751
  321.9754   326.0523   344.3507
  353.0306   373.3451   383.6845
  388.0073   426.3367   432.2201
  433.7549   443.8127   461.4438
  468.9855   503.0781   507.9909
  515.1434   527.3081   546.0369
  546.7776   558.4350   559.6776
  574.9905   580.7116   591.9941
  617.9697   636.5908   646.5735
  654.7451   662.7131   673.6086
  675.4946   701.6457   704.0013
  719.3986   727.8951   733.1378
  734.3650   740.2177   744.6256
  757.2033   757.7899   764.7110
  769.4058   770.5253   774.2545
  790.5064   799.5690   823.8567
  844.8605   853.6814   854.5317
  860.3208   862.7947   863.6508
  892.7640   895.4815   905.0575
  906.0858   912.9685   933.4043
  949.0474   953.9745   956.9602
  961.8086   969.9460   970.3123
  977.9971   978.8085   984.4684
  997.7560   999.4725  1005.5847
 1014.4478  1027.1819  1043.8162
 1046.2833  1057.9718  1063.2137
 1097.2206  1103.3235  1143.9197
 1148.5300  1161.9821  1183.6473
 1184.3373  1194.4225  1200.1627
 1200.7905  1206.0556  1214.0822
 1223.3054  1252.0112  1260.3217
 1267.1158  1274.2646  1275.3362
 1290.3737  1315.7201  1318.5549
 1323.6085  1323.8918  1334.0378
 1336.8590  1339.7636  1354.1918
 1358.8037  1363.2439  1366.5393
 1383.0511  1436.0035  1442.4918
 1446.1565  1465.8367  1477.7828
 1495.1301  1500.0460  1501.5511
 1506.2874  1510.4543  1512.8791
 1515.4604  1519.9374  1522.9568
 1533.8164  1542.4356  1548.5693
 1581.4201  1587.7491  1596.1752
 1614.3866  1633.7889  1639.6032
 1642.5107  1649.3339  1671.3155
 1672.8597  3004.0302  3084.7873
 3089.1729  3102.5222  3118.5475
 3125.7506  3135.2800  3141.9778
 3156.5928  3160.4692  3170.4895
 3184.9401  3186.3334  3188.5451
 3189.3782  3195.1774  3199.6467
 3200.0497  3204.7530  3211.0636
 3213.1165  3213.8507  3220.7234
 3223.1196  3244.4086  3251.3749

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C2H2
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  534.9410   534.9410   775.2658
  775.2658  2088.1210  3441.4891
 3541.6634

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C2Ph2
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   27.7733    47.3471    52.7584
  142.6735   144.0622   260.6102
  290.3758   406.5911   412.2370
  413.5488   473.9243   529.5221
  538.6556   547.4142   561.2301
  635.4701   637.9195   703.9053
  704.7634   716.5652   771.3453
  774.2036   854.7304   855.0124
  859.5337   925.8991   927.4216
  966.8254   966.9346   996.0411
  996.0564  1016.0504  1016.3397
 1054.7563  1057.3871  1108.7801
 1110.0524  1167.8101  1193.5161
 1193.5358  1211.3171  1213.0453
 1326.7120  1330.5725  1351.2807
 1364.7933  1365.2921  1487.5196
 1490.0150  1533.8250  1551.9548
 1624.9876  1626.5262  1654.4898
 1662.8949  2315.2187  3184.5462
 3184.6168  3193.1615  3193.2045
 3204.7637  3204.8645  3212.7136
 3212.9159  3216.7557  3217.0188

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HC2CO2Me
--------
  121.1394   144.5200   166.3308
  311.7706   312.0028   548.0674
  596.6715   632.8605   667.4927
  764.2792   874.4998  1033.9996
 1182.8367  1217.4774  1273.8847
 1489.8119  1511.7565  1522.4511
 1801.3910  2239.6269  3077.5842
 3153.2844  3188.7329  3490.7321

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HC2CH2OMe
--------
   92.2223   174.4938   229.4454
  343.9008   376.4844   528.4652
  590.8895   654.3390   968.8487
  998.8345  1044.7801  1156.3759
 1190.6732  1228.3307  1268.7341
 1427.4302  1499.5426  1512.9864
 1525.9172  1544.8644  2251.7276
 2963.8872  2983.0905  2989.2736
 3031.4784  3145.2115  3495.2312
```

Table S4. Thermodynamics (E_h) for all computed species.

Species	$E(SCF)_{DZ}$	$G(gas)_{DZ}$	$E(SCF)_{TZ}$	$G(gas)_{TZ}$
4	-4351.483352	-4351.133836	-4352.110975	-4351.761459
2'	-4813.610239	-4813.110908	–	–
5	-4579.376753	-4578.987752	–	–
5a	-4579.369299	-4578.981929	–	–
5b	-4579.373699	-4578.985014	–	–
5c	-4579.369702	-4578.982763	–	–
6	-4505.323292	-4504.915695	–	–
6a	-4505.318557	-4504.913379	–	–
6b	-4505.323288	-4504.915675	–	–
6c	-4505.317612	-4504.910818	–	–
7	-4428.819437	-4428.436847	-4429.455115	-4429.072525
7-8-TS	-4428.810707	-4428.430379	-4429.447287	-4429.066959
8	-4428.912347	-4428.524994	-4429.541657	-4429.154304
9a	-4506.264864	-4505.847961	-4506.910052	-4506.493149
9b	-4506.261654	-4505.845175	-4506.907982	-4506.491503
9c	-4506.188086	-4505.773764	-4506.841679	-4506.427357
9d	-4506.255077	-4505.836900	-4506.895607	-4506.477430
8-9a-TS	-4506.212844	-4505.803509	-4506.866774	-4506.457439

8-9b-TS	-4506.229103	-4505.814890	-4506.881570	-4506.467357
9b-10-TS	-4506.253728	-4505.840055	-4506.904522	-4506.490849
10	-4506.307458	-4505.890987	-4506.963325	-4506.546854
10'	-4506.307668	-4505.891349	-4506.964177	-4506.547858
10' red el	-4506.304542	-4505.888579	-4506.960200	-4506.544237
11	-4583.672599	-4583.224526	-4584.342556	-4583.894483
12	-4583.725669	-4583.276436	-4584.403958	-4583.954725
C_2H_2	-77.325646	-77.318036	-77.356567	-77.348957
C_2Ph_2	-539.462244	-539.308841	–	–
$HCCCO_2Me$	-305.200930	-305.159666	–	–
$HCCCH_2OMe$	-231.159534	-231.099164	–	–

3. X-ray crystallographic details

Structures of compound **2** was confirmed by X-ray structure determination. The crystal was mounted on a Bruker APEXII/Kappa three circle goniometer platform diffractometer equipped with an APEX-2 detector. A graphic monochromator was employed for wavelength selection of the Mo Kα radiation (λ = 0.71073 Å). The data were processed and refined using the APEX2 software. Structures were solved by direct methods in SHELXS and refined by standard difference Fourier techniques in the SHELXTL program suite (6.10 v., Sheldrick G. M., and Siemens Industrial Automation, 2000). Hydrogen atoms were placed in calculated positions using the standard riding model and refined isotropically; all other atoms were refined anisotropically. The structure contains one molecule of ether and half molecule of hexane (on special position) per asymmetric unit. Detailed crystal and structure refinement data are given in **Table S5**.

Table S5. X-ray crystallographic details for compound **2**.

complex	**HOR'**
formula	$C_{49}H_{48}N_4Ni_2O_2 \times C_4H_{10}O \times 0.5C_6H_{14}$
fw	943.54
crystal system	monoclinic
space group	*P* $2_1/c$
a (Å)	12.397(1)
b (Å)	15.322(2)
c (Å)	25.014(3)
α (deg)	90.00
β (deg)	100.198(5)
γ (deg)	90.00
V (Å^3)	4676.3(8)
D_c (g cm^{-3})	1.340
Z	4
μ (mm^{-1})	0.853
T (K)	100(2)
R_1	5.26
GOF	1.030

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