Electronic Supplementary Information

Cyclotrimerization of alkynes catalyzed by a self-supported cyclic tri-nuclear nickel(0) complex with α-diimine ligands

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S1. Experimental Section

S1.1 General considerations

All reactions and manipulations of air- and moisture-sensitive compounds were carried out under argon or nitrogen by using standard Schlenk or dry box techniques. The solvents Et_2O, DME, toluene and THF were dried by Na and were distilled under nitrogen. CH_2Cl_2, CH_3CN and DMF were dried using CaH_2 and were distilled under nitrogen. Benzene-d_6 was dried over Na/K alloy. Dimethoxyethane nickel dibromide [(DME)$NiBr_2$] [1a] and the ligand $\mathbf{L}^{\mathbf{Me\text{-}2,4}}$ [1b] were prepared according to literature procedures. Sodium metal, anhydrous nickel dibromide and alkynes were purchased from Alfa Aesar. NMR spectra were recorded on a Bruker Avance-400 MHz spectrometer in benzene-d_6 and $CDCl_3$.

Magnetic properties of complex 1, $[Ni_3(\mu_2\text{-}Br)_3(\mu_3\text{-}Br)_2(L^{Me\text{-}2,4})_3]\cdot Br$

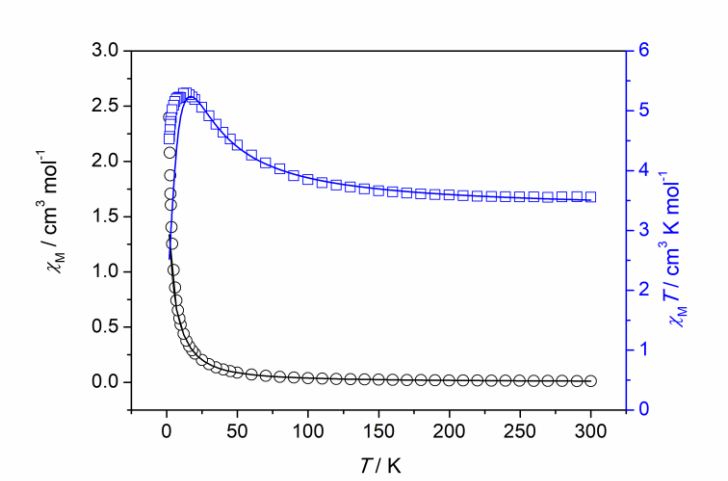


Fig. S1. Plots of χM *vs*. T and χMT *vs*. T for complex **1** in the temperature range of 2−300 K. The solid lines are the fitting results.

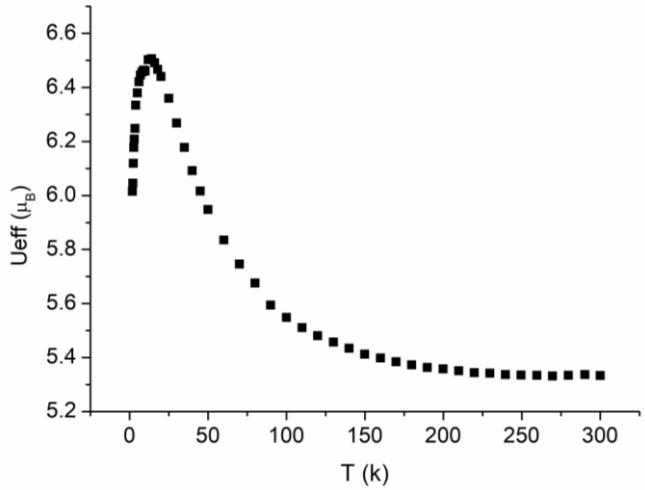


Fig. S2. Temperature dependence of the effective magnetic moment of **1**.

Variable-temperature magnetic susceptibilities for **1** were measured in the temperature range 2–300 K under a constant magnetic field of 1000 Oe. The plots of $\chi_M T$ versus T are shown in Fig. S2. Upon cooling, the $\chi_M T$ steadily increases from 3.56 cm^3 K mol^{-1} at 300 K to 4.02 cm^3 K mol^{-1} at 80 K. Below this

temperature, $\chi_M T$ sharply increases to reach a maximum of 5.29 cm^3 K mol^{-1} at 14 K, which indicates the presence of the intramolecular ferromagnetic coupling between adjacent Ni^{2+} centers.[2] The value of $\chi_M T$ drops sharply below 14 K, which might be attributed to the weak intermolecular antiferromagnetic interactions and/or the zero-field-splitting (ZFS) effects in the ground state.[3]

At such conditions, the magnetic interactions within the $\{Ni_3\}$ cluster can be defined according to the following isotropic spin Hamiltonian:

$$\hat{H} = -2J(\hat{S}_1\hat{S}_2 + \hat{S}_2\hat{S}_3 + \hat{S}_3\hat{S}_1) \quad (1)$$

where the *J* represents the coupling constant between adjacent Ni^{2+} centers. Taking the above isotropic spin Hamiltonian and molecular field approximation, we have fitted the magnetic susceptibility data with the following eq.

$$\chi_M = \frac{2Ng^2\beta^2}{kT} \times \frac{3e^{2J/kT} + 10e^{6J/kT} + 14e^{12J/kT}}{1 + 9e^{2J/kT} + 10e^{6J/kT} + 7e^{12J/kT}} \quad (2)$$

$$\chi = \chi_M / [1 - (2zJ / Ng^2\beta^2)\chi_M] \quad (3)$$

The above model gives a good fit of the magnetic properties of complex **1** in the whole temperature range: g = 2.11, J = 4.74 cm^{-1}, zJ = -0.27cm^{-1} and R = 7.7 × 10^{-4} (the error factor R is defined as $\sum[(\chi_M T)_{obsd} - (\chi_M T)_{calcd}]^2 / \sum[(\chi_M T)^2_{obsd}]$). The positive J value demonstrates the ferromagnetic coupling between Ni^{2+} ions through the bridging Br^- ions.

Moreover, plot of temperature dependence of the effective magnetic moment (μ_{eff}) is shown in Fig. S2. The effective magnetic moment increases slowly from 5.33 μ_B at 300 K to 6.50 μ_B at 14 K.

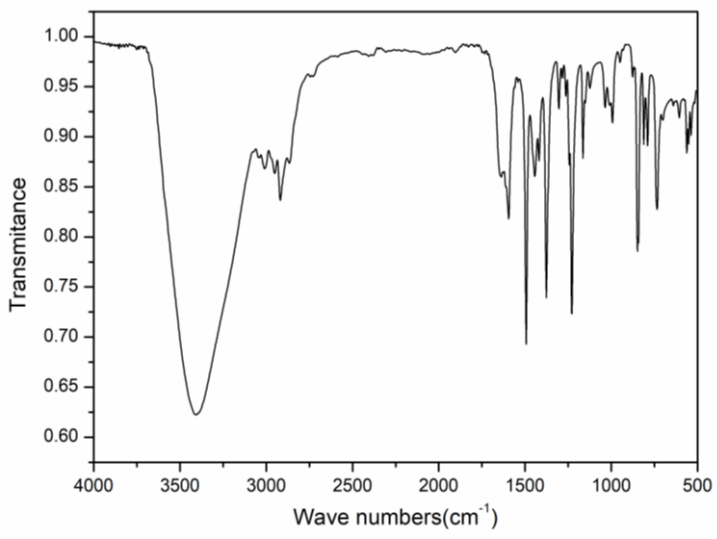


Fig. S3. IR spectrum of complex **1**.

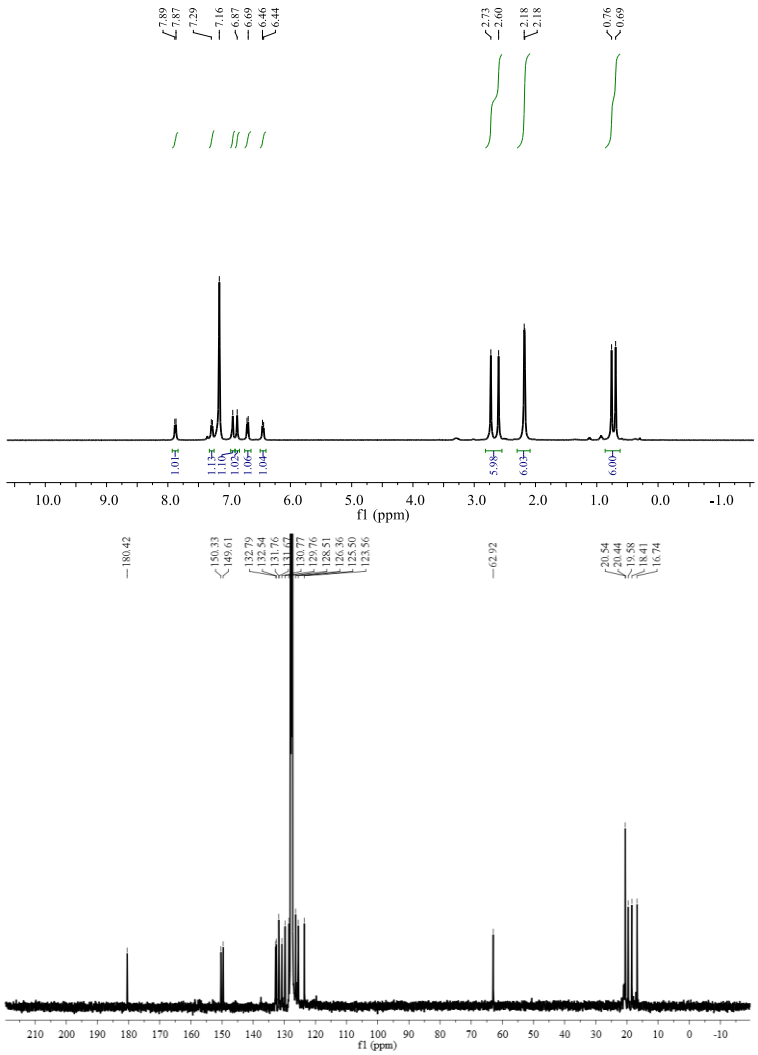


Fig. S4. ^{1}H and ^{13}C NMR spectra of complex **2**.

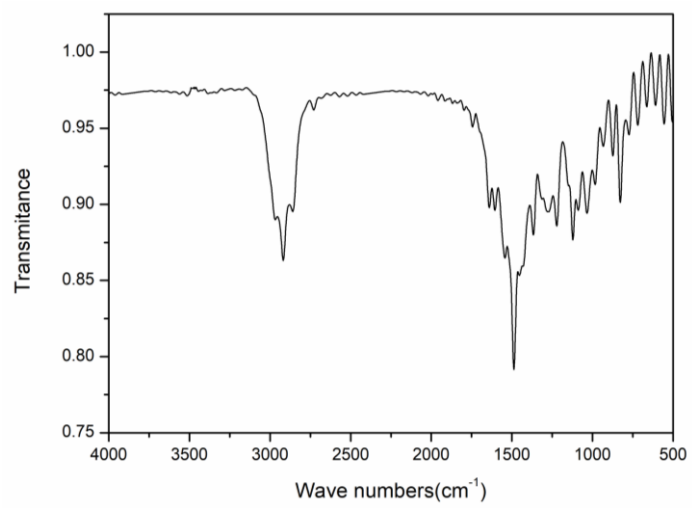


Fig. S5. IR spectrum of complex **2**.

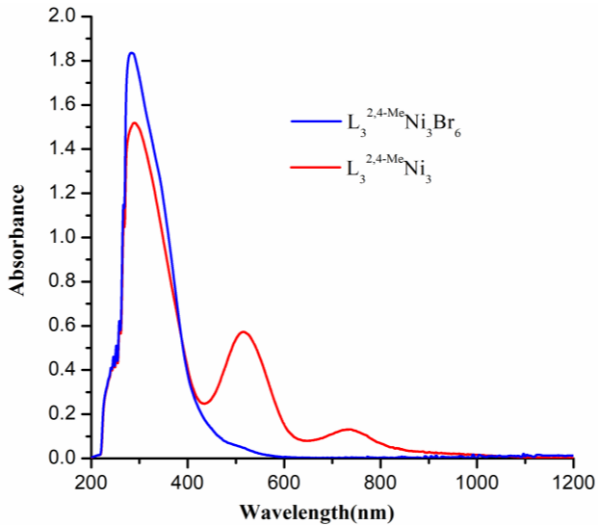


Fig. S6. UV-vis-NIR spectra of **1** (6.5×10^{-5} mol L^{-1}, red) and **2** (4.6×10^{-5} mol L^{-1}, blue) in THF.

UV-vis-near IR spectra of complexes **1** and **2** were recorded in THF at room temperature (Fig. S6). The spectra consist of absorptions across the UV, visible and near-IR regions. The absorption spectra of **1** and **2** are similar in the higher-energy region, with dominant peaks at about 289 nm. These absorptions are assigned to ligand-centered (π-π*) transitions.[4] However, complex **2** has two additional weak bands at 516 nm and 733 nm, which are expected to the metal-to-ligand charge-transfer (MLCT) bands.[5] TD-DFT computations were conducted at the bp86/6-311G* level on complex **2**. Both of the two theoretical bands at 543 and 497 nm correspond to the experimental 516 nm absorption and the lower energy band at 697 nm (experimental 733 nm) corresponds to an excitation from the nickel *d* orbital to the ligands (HOMO−4→LUMO+4, HOMO−3→LUMO+4, HOMO→LUMO+7 and HOMO−3→LUMO+2), indicating the facile transition of the metal-to-ligand charge-transfer under UV-Vis irradiation (Fig. S7).

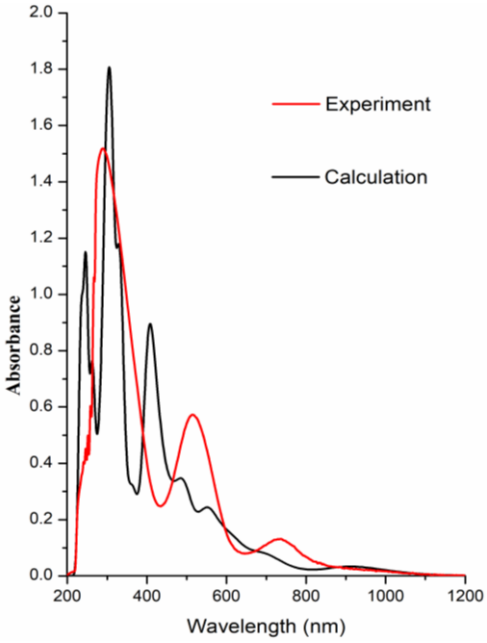


Fig. S7. Comparison of the experimental and computational (bp86/6-311G *) UV/Vis spectra of **2**. (the scale factor is 1.00 and the half-width is 2500 cm^{-1})

Table S1. Absorption wavelengths, oscillator strengths, main transition pairs and amplitudes for selected excited states of complex **2** at the bp86/6-311G * level of theory.

no.	transition (%)	Calculated transition energy/nm	Oscillator strength
1	HOMO-3=>LUMO+2 (72)	697	0.0084
2	HOMO=>LUMO+7 (51)	543	0.0101
3	HOMO-4=>LUMO+4 (39) HOMO-3=>LUMO+4 (39)	497	0.0187

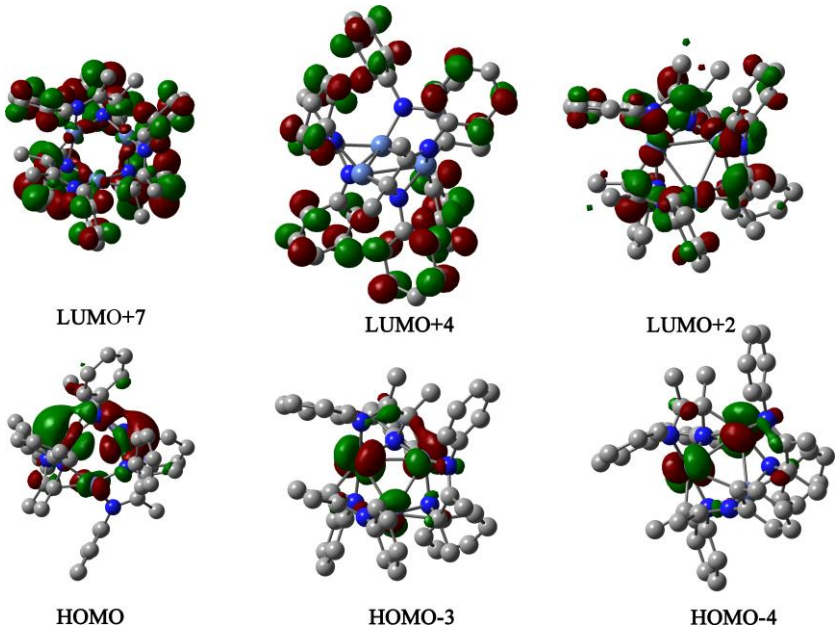


Fig. S8. Molecular orbitals of complex **2**.

S1.2 X-ray crystal structure determination

Diffraction data for the complexes **1** and **2** (sealed in thin glass tubes) and the cyclotrimerization product **4a** were collected on a Bruker SMART APEX II diffractometer at room temperature (298 K) with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). An empirical absorption correction using SADABS was applied for all data.[6] The structures were solved by direct methods using the SHELXS program.[7] All non-hydrogen atoms were refined anisotropically by full-matrix least squares on F^2 by the use of the program SHELXL.[7] Hydrogen atoms bonded to carbon were included in idealized geometric positions with thermal parameters equivalent to 1.2 times those of the atom to which they were attached. Crystallographic data and refinement details for **1**, **2** and **4a** are given in Table S2.

Table S2. Crystallographic data and refinement details for compounds **1**, **2**, **4a**.

	1	**2**	**4a**
formula	$C_{60}H_{72}Br_6N_6Ni_3$	$C_{60}H_{72}N_6Ni_3$	$C_{33}H_{30}O_6$
fw	1532.83	1053.37	522.57
crystal system	Trigonal	Monoclinic	Monoclinic
space group	*P*-3	*P*2(1)/*n*	*Cc*
a /Å	13.198(5)	13.1720(18)	22.007(7)
b /Å	13.198(5)	20.129(3)	12.847(7)
c /Å	23.606(9)	21.285(3)	11.149(5)
α /deg	90	90	90
β /deg	90	103.793(2)	112.394(8)
γ /deg	120	90	90
V /Å^3	3561(2)	5480.9(13)	2914(2)
Z	2	4	4
D_{calcd} /g cm^{-3}	1.492	1.277	1.191
F(000)	1536	2232	1104
μ /mm^{-1}	4.371	1.063	0.081
θ range	2.52−25.39	1.66−25.20	1.88−25.70
R_1, wR_2 (all data)	0.0866, 0.2385	0.0724, 0.1264	0.0912, 0.1401
GOF (F^2)	1.063	1.031	1.080

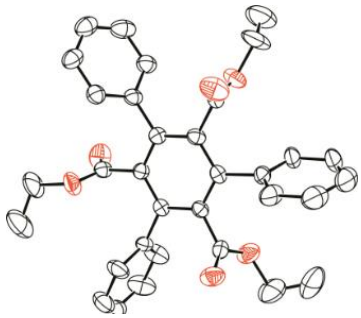


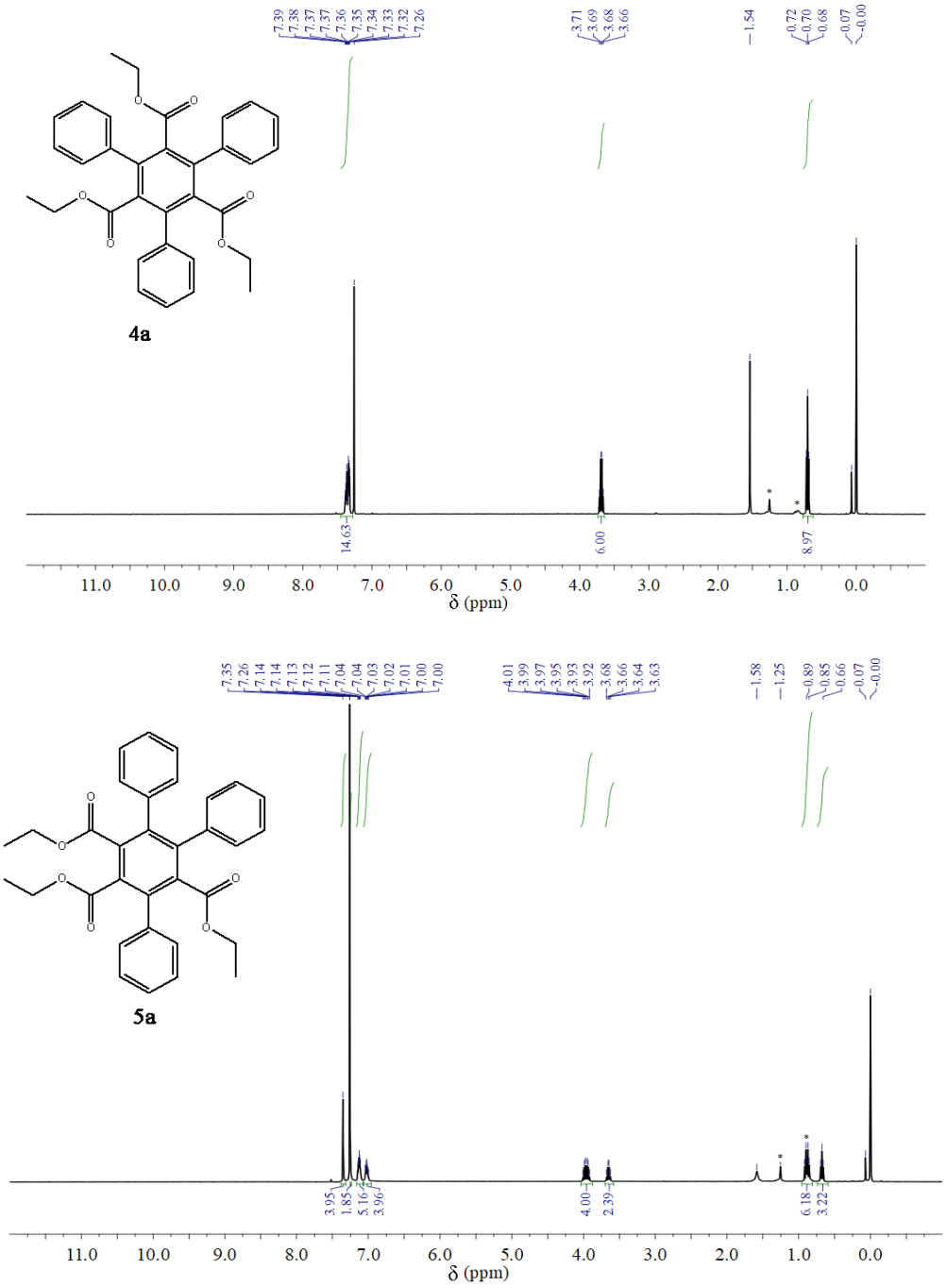
Fig. S9. X-ray structure of complex **4a** (30% probability level).

S1.3 Synthesis and characterization of the cyclotrimerization products

Synthesis and characterization of compounds 4a and 5a

In a 15 mL sealed pressure tube were added ethyl phenylpropiolate (2.5 mmol, 0.436 g) and complex **2** with 5 mL of *n*-hexane, and the mixture was stirred at 100 ℃ for 5 h under Ar. After cooling to room temperature, the mixture was filtered and the precipitate was dissolved in $CHCl_3$. The pure products **4a** and **5a** were obtained by flash chromatography on silica gel (gradient of ethyl acetate/ petroleum ether = 1/20

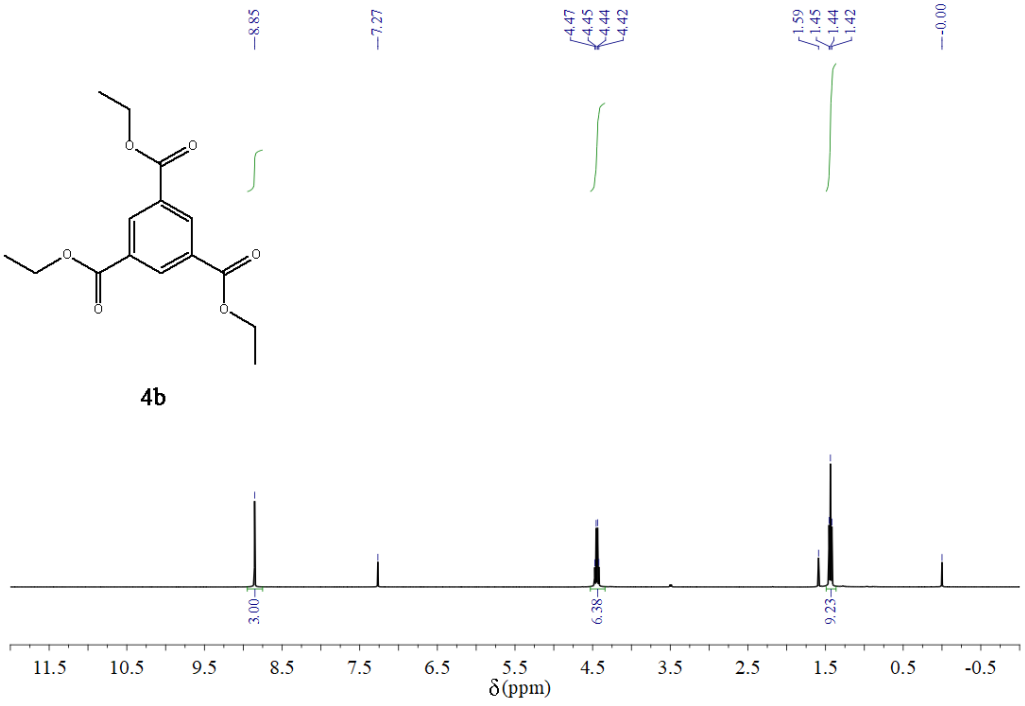
(v/v)). Compound **4a**:[8] white solid, yield: 64% (0.280 g). M.p.: 212−214 °C. ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 7.39−7.32 (15H, m, Ar-*H*), 3.68 (6H, q, *J* = 7.2 Hz, CH_2), 0.70 (9H, t, *J* = 7.2 Hz, CH_3); IR (KBr/cm^{-1}) 2984(m), 1730 (v, $\nu_{C=O}$), 1495(m), 1447(m), 1177(s), 1022(m), 760(m), 702(s). Compound **5a**:[8] white solid, yield: 29% (0.126 g). M.p.: 151−153 °C. ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 7.35 (4H, s, Ar-*H*), 7.26 (2H, m, Ar-*H*), 7.13 (5H, m, Ar-*H*), 7.02 (4H, m, Ar-*H*), 3.96 (4H, m, CH_2), 3.65 (2H, q, *J* = 7.2 Hz, CH_2), 0.88 (6H, m, CH_3), 0.68 (2H, t, *J* = 7.2 Hz, CH_3). IR (KBr/cm^{-1}): 2981(m), 1731 and 1728 (s, $\nu_{C=O}$), 1556(m), 1454(m), 1443(m), 1231(s), 1175(m), 1024(w), 764(w).

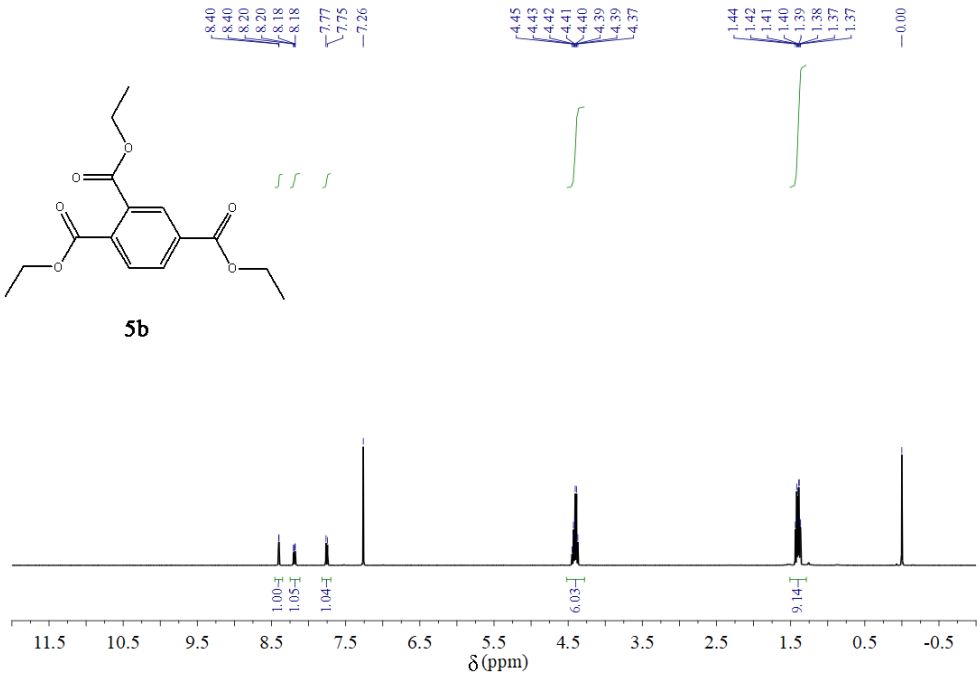


* peaks of solvent *n*-hexane

Synthesis and characterization of compounds 4b and 5b

In a 15 mL sealed pressure tube were added ethyl propiolate (2.5 mmol, 0.245 g) and complex **2** with 5 mL of *n*-hexane, and the mixture was stirred at room temperature for 0.5 h under Ar. After standing overnight, the mixture was filtered, the filtrate concentrated, and the precipitate was collected. The crude product was recrystallized from *n*-hexane/ethyl acetate to afford a white solid of compound **4b**. The other product **4b** and **5b** were obtained from the filtrate by flash chromatography on silica gel (gradient of ethyl acetate/ petroleum ether = 1/10 (v/v)). Compound **4b**:[9] white solid, yield: 55% (0.134 g). M.p.: 132−133 °C. ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 8.85 (1H, s, Ar-*H*), 4.45 (6H, m, C*H*$_2$), 1.44 (9H, t, *J* = 8.0 Hz, C*H*$_3$). IR (KBr/cm^{-1}): 2986(m), 1730(vs, $\nu_{C=O}$), 1389(m), 1306(s), 1283(s), 1242(vs), 1113(s), 1067(s), 1022(s), 866(w), 795(w), 752(m). Compound **5b**:[9,10] yellow oil, yield: 23% (0.056 g). ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 8.40 (1H, s, Ar-*H*), 8.19 (1H, d, *J* = 8.0 Hz, Ar-*H*), 7.76 (1H, d, *J* = 8.0 Hz, Ar-*H*), 4.40 (6H, m, C*H*$_2$), 1.39 (9H, m, C*H*$_3$). IR (KBr/cm^{-1}): 2993 (m), 2950(m), 1724 (vs, $\nu_{C=O}$), 1442(m), 1390(m), 1248(s), 1103(m), 1024(s), 839(m), 739(m), 719(m).

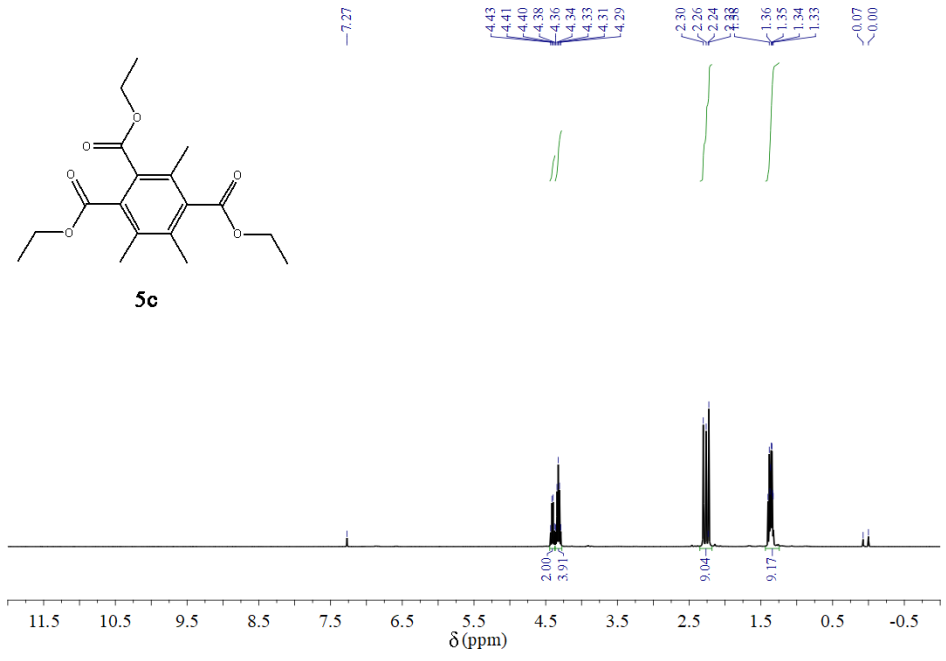




5b

Synthesis and characterization of compound 5c

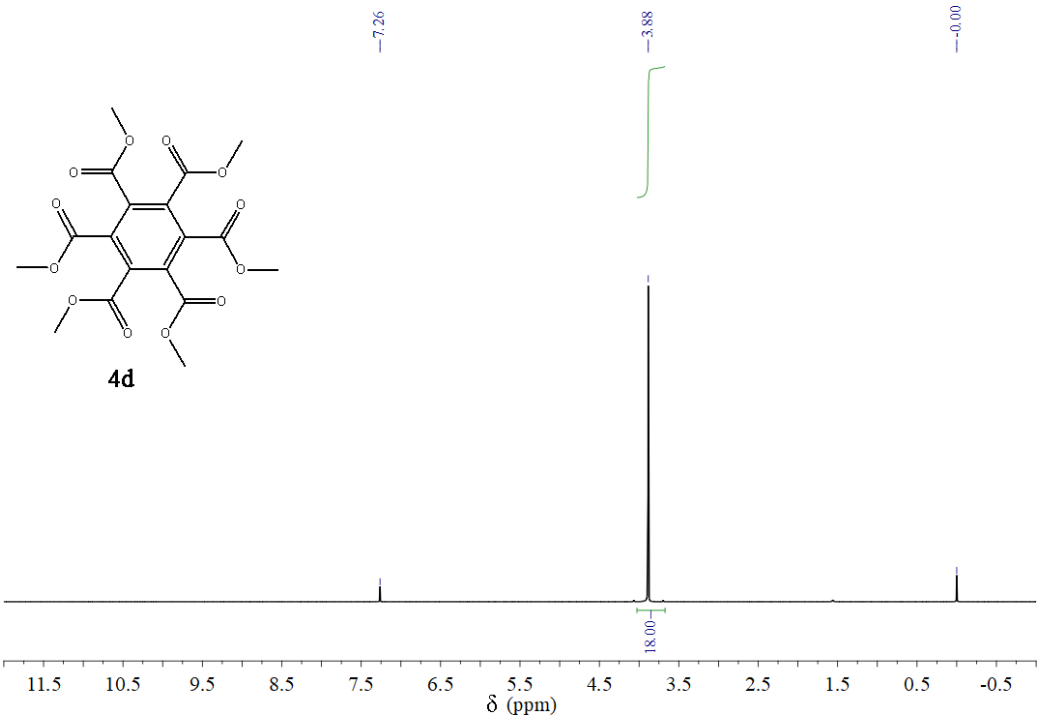
In a 15 mL sealed pressure tube were added ethyl 2-butynoate (2.5 mmol, 0.280 g) and complex **2** with 5 mL of *n*-hexane, and the mixture was stirred at 100 ℃ for 5 h under Ar. After cooling down, the volatiles were removed under reduced pressure and the pure product **5c** was obtained by flash chromatography on silica gel (gradient of ethyl acetate / petroleum ether = 1/10 (v/v)). Compound **5c**:[10] yellow oil, yield: 78% (0.219 g). ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 4.41 (2H, q, *J* = 8.0 Hz, CH_2,), 4.36−4.29 (4H, q, *J* = 8.0 Hz, CH_2), 2.30 (3H, s, ArCH_3), 2.26 (3H, s, ArCH_3), 2.23 (3H, s, ArCH_3), 1.40−1.33 (9H, m, CH_2CH_3); IR (KBr/cm^{-1}): 2986(m), 1729 (vs, $\nu_{C=O}$), 1448(m), 1418(m), 1374(m), 1320(s), 1294(s), 1214(s), 1152(s), 1037(s), 850(m), 797(w), 718(m).



5c

Synthesis and characterization of compounds 4d

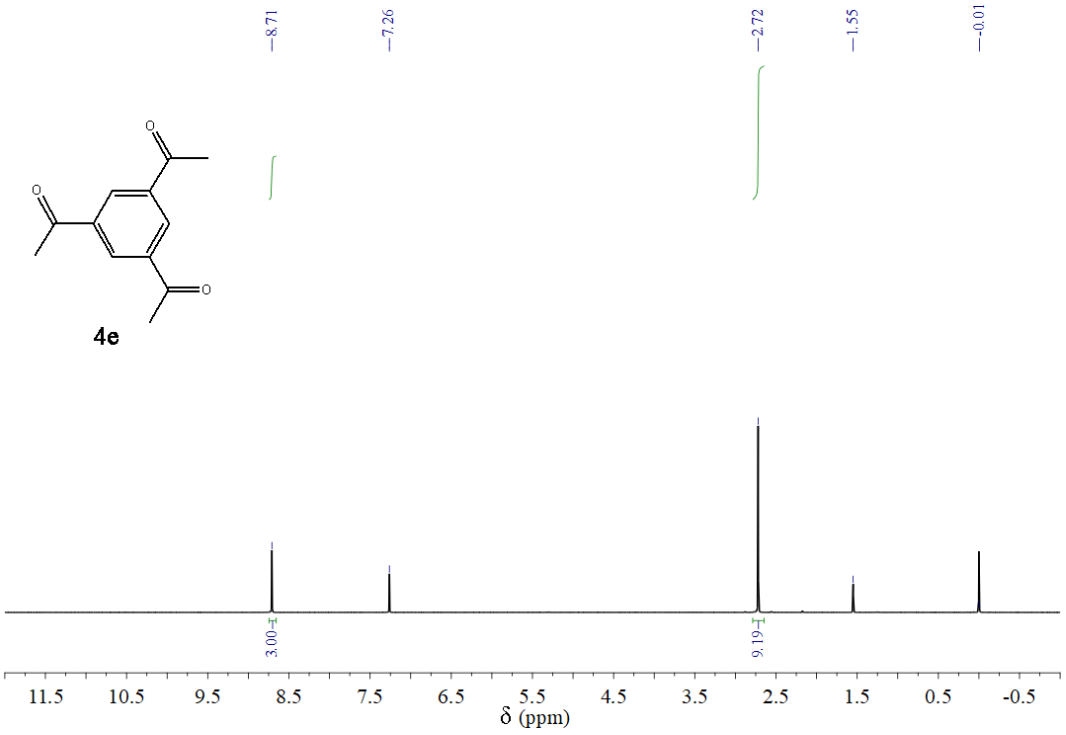
In a 15 mL sealed pressure tube were added dimethyl but-2-ynedioate (2.5 mmol, 0.355 g) and complex **2** with 5 mL of *n*-hexane, and the mixture was stirred at room temperature for 0.5 h under Ar. The volatiles were removed under reduced pressure and the pure products **4d** were obtained by flash chromatography on silica gel (gradient of ethyl acetate / petroleum ether = 1/8 (v/v)). Compound **4d**:[9] white solid, yield: 89% (0.316 g). M.p.: 189−190 °C. ^{1}H NMR (400 MHz, $CDCl_3$, TMS): 3.88 (18H, s, C*H*$_3$). IR (KBr/cm^{-1}): 3011(m), 2961(m), 1740(s, $\nu_{C=O}$), 1445(s), 1414(m), 1364(s), 982(s), 856(s), 754(m)

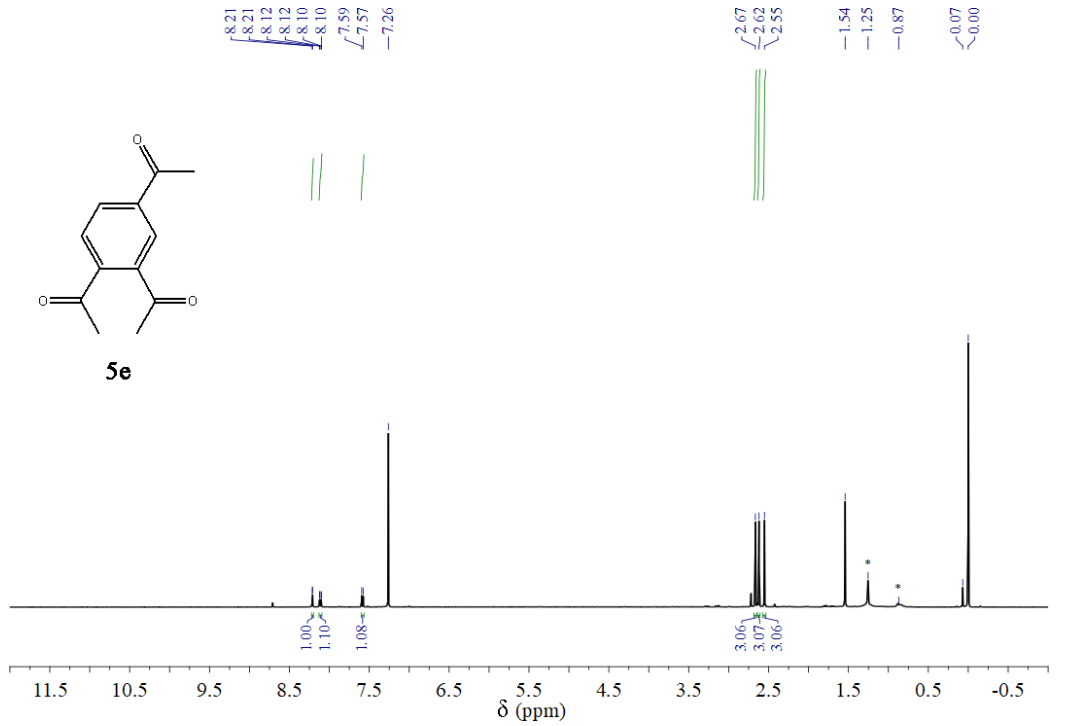


4d

Synthesis and characterization of compounds 4e and 5e

In a 15 mL sealed pressure tube were added dimethyl but-2-ynedioate (2.5 mmol, 0.170 g) and complex **2** with 5 mL of *n*-hexane, and the mixture was stirred at room temperature for 0.5 h under Ar. The volatiles were then removed under reduced pressure and the pure products **4e** and **5e** were obtained by flash chromatography on silica gel (gradient ethyl acetate / petroleum ether = 1/8 (v/v)). Compound **4e**:[9] white solid, yield: 59% (0.101 g). M.p.: 156−157 °C. ^{1}H NMR (400 MHz, $CDCl_3$, TMS): 8.71 (3H, s, Ar-*H*), 2.72 (9H, s, C*H*$_3$). IR (KBr/cm^{-1}): 3086(w), 3062(m), 3003(m), 1690(vs, $\nu_{C=O}$), 1585(m), 1420(m), 1362(s), 1227(s), 907(m), 687(m), 586(s). Compound **5e**:[10] yellow oil, yield: 20% (0.034 g). ^{1}H NMR (400 MHz, $CDCl_3$): 8.21 (1H, s, Ar-*H*), 8.12 (1H, d, *J* = 8.0 Hz, Ar-*H*), 7.58 (1H, d, *J* = 8.0 Hz, Ar-*H*), 2.67 (3H, s, C*H*$_3$), 2.62 (3H, s, C*H*$_3$), 2.55 (3H, s, C*H*$_3$). IR (KBr/cm^{-1}): 3083(w), 3059(m), 1697 and 1700 (s, $\nu_{C=O}$), 1601(m), 1424(m), 1355(s), 1235(s), 875(m), 867(m).



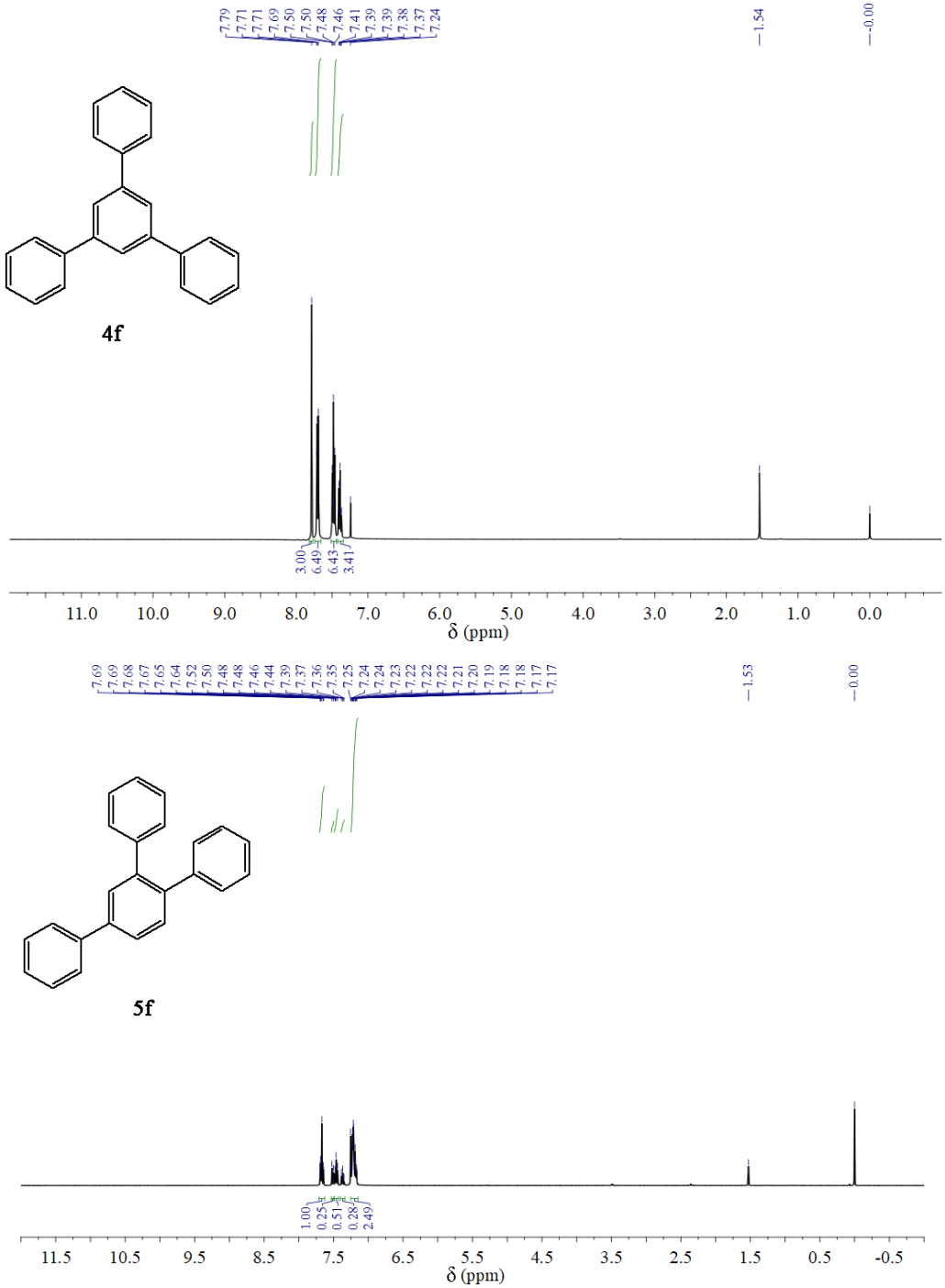


* peaks of solvent *n*-hexane.

Synthesis and characterization of compounds 4f and 5f

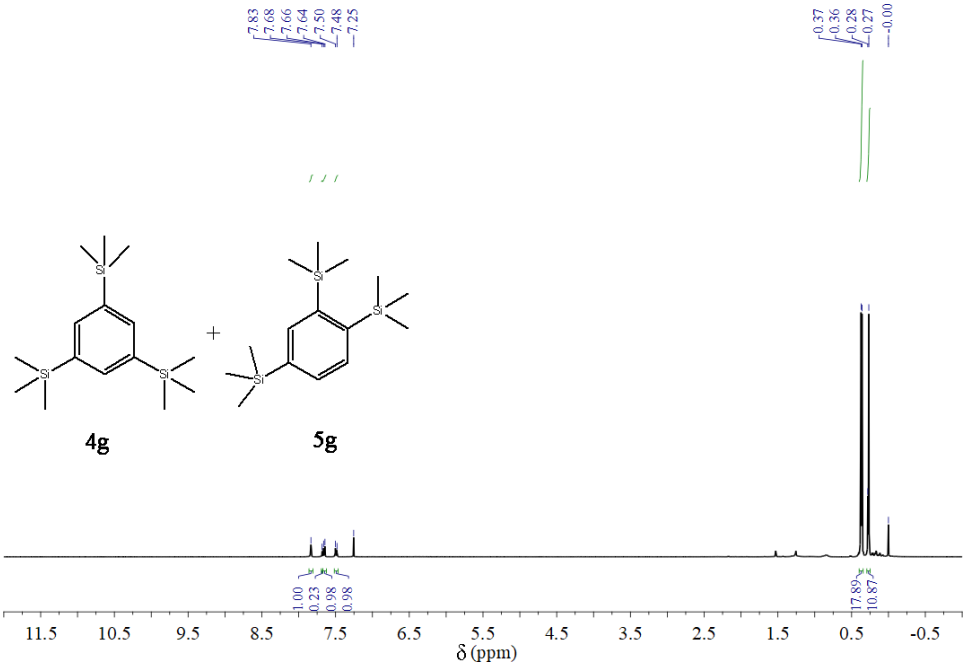
In a 15 mL sealed pressure tube were added phenylacetylene (2.5 mmol, 0.255 g) and complex **2** with 5 mL of *n*-hexane, and the mixture was stirred at 100 ℃ for 5 h under Ar. After cooling down, the volatiles

were removed under reduced pressure and the pure products **4f** and **5f** were obtained by flash chromatography on silica gel (eluent petroleum ether). Compound **4f**:[9] white solid, yield: 42% (0.106 g). M.p.: 170−171 °C. ^{1}H NMR (400 MHz, $CDCl_3$, TMS): 7.79 (3H, s, C_6H_3, 1,3,5-$(C_6H_5)_3C_6H_3$), 7.70 (6H, d, J = 8.0 Hz, *o*-C_6H_5,1,3,5-$(C_6H_5)_3C_6H_3$), 7.49 (6H, t, J = 8.0 Hz, *m*-C_6H_5, 1,3,5-$(C_6H_5)_3C_6H_3$), 7.40 (3H, t, J = 8.0 Hz, *p*-C_6H_5, 1,3,5-$(C_6H_5)_3C_6H_3$); IR (KBr/cm^{-1}): 3057(m), 1590(m), 1497(m), 1410(m), 872(m), 750(s), 690(s), 609(m). Compound **5f**:[9] yellow solid, yield: 42% (0.106 g). M.p.: 115−117 °C. ^{1}H NMR (400 MHz, $CDCl_3$, TMS): 7.64−7.69 (4H, m, Ar-*H*), 7.51 (1H, d, J = 8.0 Hz, Ar-*H*), 7.48−7.44 (2H, m, Ar-*H*), 7.37 (1H, t, J = 8.0 Hz, Ar-*H*), 7.17−7.24 (10H, m, Ar-*H*). IR (KBr/cm^{-1}): 3061(m), 1600(m), 1477(s), 1439(s), 839(m), 764(s), 690(s), 573(m).



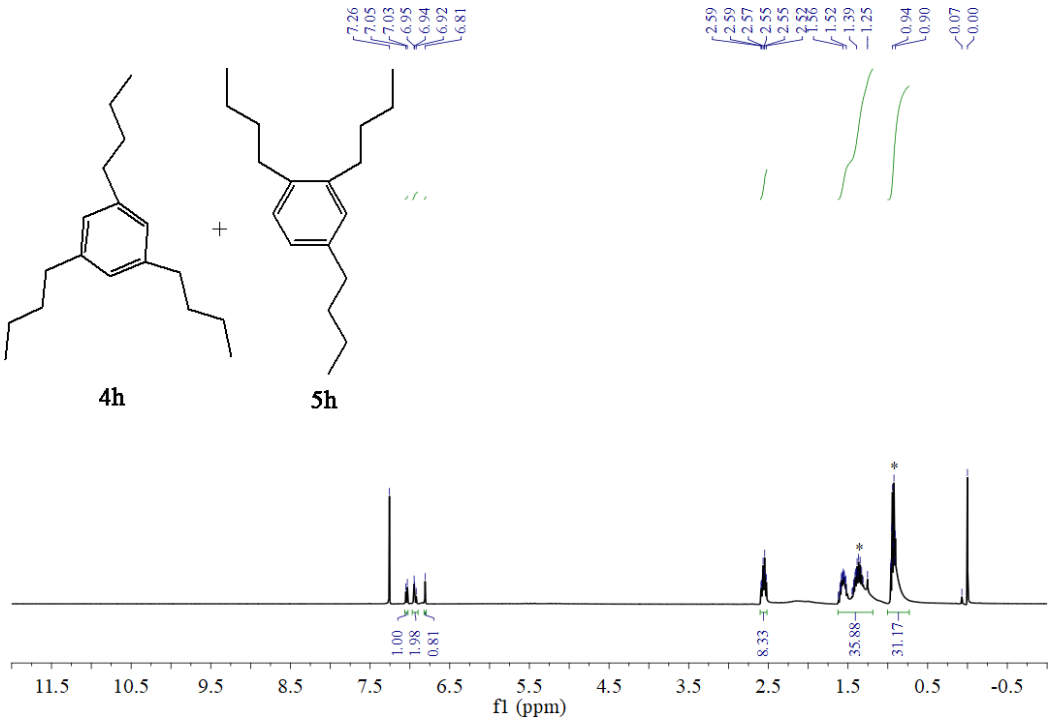
Synthesis and characterization of compounds 4g and 5g

In a 15 mL sealed pressure tube were added trimethylsilyl acetylene (2.5 mmol, 0.245 g) and complex **2** with 5 mL of *n*-hexane, and the mixture was stirred at 100 ℃ for 5 h under Ar. After cooling down, the volatiles were removed under reduced pressure and the products **4g** and **5g** were obtained by flash chromatography on silica gel (eluent petroleum ether). **4g** + **5g**:[11] yellow oil, yield: 52% (0.127 g). ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 7.68 (3H, s, Ar-*H*, **4g**), 0.28 (27H, s, *Me*$_3$Si, **4g**), 7.83 (1H, s, Ar-*H*, **5g**), 7.65 (1H, d, *J* = 8.0 Hz, Ar-*H*, **5g**), 7.49 (1H, d, *J* = 8.0 Hz, Ar-*H*, **5g**), 0.37 (9H, s, *Me*$_3$Si, **5g**), 0.36 (9H, s, *Me*$_3$Si, **5g**), 0.27 (9H, s, *Me*$_3$Si, **5g**).



Synthesis and characterization of compounds 4h and 5h

In a 15 mL sealed pressure tube were added 1-hexyne (2.5 mmol, 0.205 g) and complex **2** with 5 mL of *n*-hexane, and the mixture was stirred at 100 ℃ for 5 h under Ar. After cooling down, the volatiles were removed under reduced pressure and the products **4h** and **5h** were obtained by flash chromatography on silica gel (eluent petroleum ether). Compounds **4h** + **5h**:[9] yellow oil, yield: 38% (0.078 g). ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 7.05−7.03 (1H, d, J = 7.6 Hz Ar-*H*, **5h**), 6.95−6.92 (2H, m, Ar-*H*, **5h**), 6.81 (1H, s, Ar-*H*, **4h**), 2.56 (8H, m, C*H*$_2$, **4h**+**5h**), 1.56 (8H, m, C*H*$_2$, **4h**+**5h**), 1.37 (8H, m, C*H*$_2$, **4h**+**5h**), 0.94 (11H, s, C*H*$_3$, **4h**+**5h**).



* peaks of solvent *n*-hexane.

S1.4 Kinetics studies

5 mM of complex 2: Complex **2** (21.0 mg, 0.020 mmol, 1 mol%) was placed in a Schlenk tube under an argon atmosphere and dissolved in dry *n*-hexane (4 mL). Portions (0.5 mL) of this solution were transferred to six sealed pressure tubes (10 mL) and ethyl phenylpropiolate (500 mM, 41 μL, 0.25 mmol) was added to each tube and the mixture was stirred for 10, 20, 30, 40, 50 and 60 min, respectively, at 100 ℃. The resulting solution was filtered and washed with chloroform (10 mL). After evaporating solvent, the crude residue was analyzed by ^{1}H NMR to determine the chemical yield, by the integration value of peaks at 4.27–4.32 ppm (**3a**: O***CH*$_2$**CH$_3$) and peaks at 3.92–4.01 and 3.63–3.72 ppm (**4a + 5a**: O***CH*$_2$**CH$_3$).

10 mM complex 2: Following a same procedure, complex **2** (42.2 mg, 0.040 mmol, 2 mol%) and ethyl phenylpropiolate (500 m*M*, 41 μL, 0.25 mmol) were used.

15 mM complex 2: Complex **2** (63.1 mg, 0.060 mmol, 3 mol%) and ethyl phenylpropiolate (500 m*M*, 41 μL, 0.25 mmol) were used.

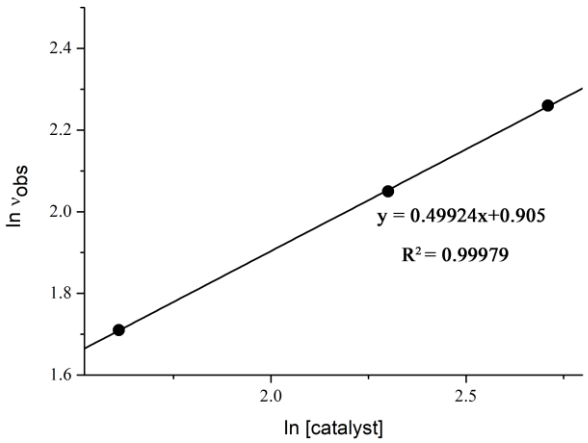
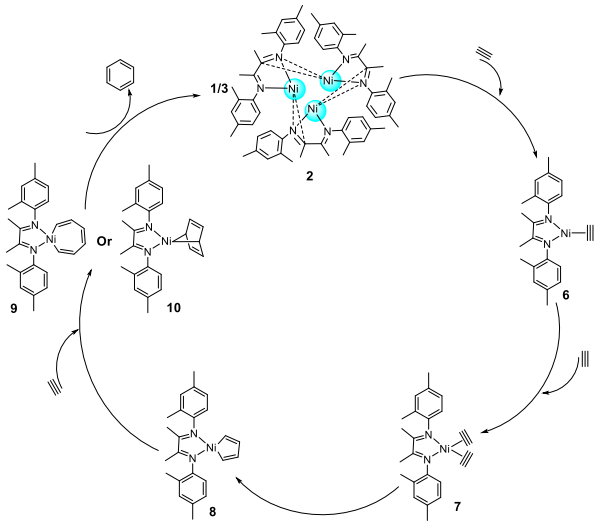


Fig. S10. Ln-Ln plot of observed rate constant vs. [catalyst] at 100 ℃. By assuming pseudo first-order consumption of **3a** to give **4a** and **5a**, ln v_{obs} is plotted versus ln[catalyst], showing half-order dependency in concentration of the catalyst component.



Scheme S1. Proposed mechanism for the alkyne cyclotrimerization catalytic cycle of the complex **2**.

S2. DFT Computations

Computations for **2** were conducted using the bp86/6-311G(d) method[12] of the Gaussian 03 software package.[13] Geometry optimization gave bond distances that are in good agreement with the X-ray structure.

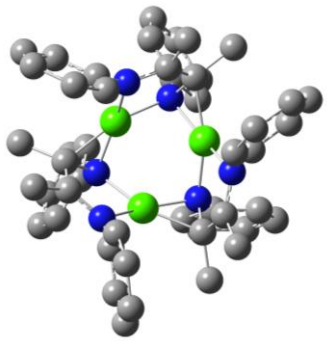


Fig. S11. Optimized structure of **2** (hydrogen atoms have been omitted for clarity).

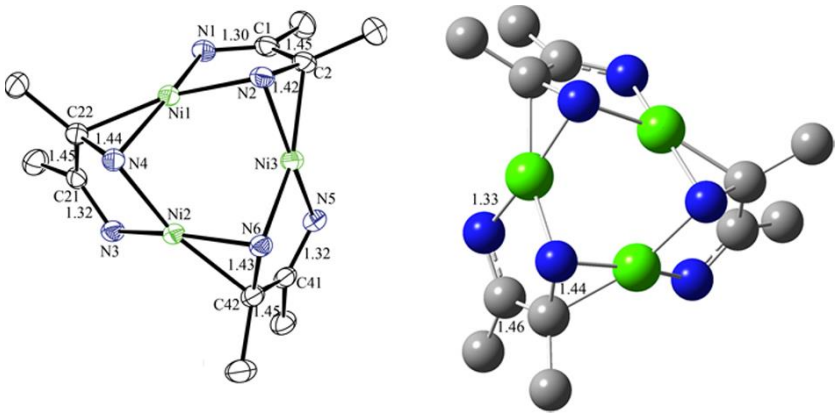


Fig. S12. Selected bond lengths of **2 (**hydrogen atoms and the aryl rings are omitted for clarity).

Table S3. Cartesian coordinates of the optimized geometry of **2** in the singlet state.

Ni	1.53307500	0.42318300	0.25127600	H	-1.23629800	1.49207000	3.20543300
Ni	-0.40005100	-1.53927300	0.25127600	C	2.64304600	1.42004000	-2.22979800
Ni	-1.13302400	1.11609100	0.25127600	C	4.02498900	1.34531600	-1.96293800
N	0.39676100	1.79078600	1.07214200	C	4.93564600	1.08659700	-2.99170900
N	1.76110300	1.65685700	-1.14442400	H	6.00647600	1.04764500	-2.76782500
N	1.35248600	-1.23899900	1.07214200	C	4.48362600	0.87679800	-4.30422200
N	0.55432900	-2.35358800	-1.14442400	C	3.10954100	0.93013500	-4.57376200
N	-1.74924700	-0.55178800	1.07214200	H	2.74405700	0.75974500	-5.59170900
N	-2.31543100	0.69673100	-1.14442400	C	2.19286800	1.20048400	-3.54841200
C	-0.62935700	4.04002400	0.39575200	H	1.11945400	1.22942000	-3.75672800
H	0.12359700	4.82282400	0.61034000	C	3.81344200	-1.47497300	0.39575200
H	-1.26168500	3.94385500	1.28966900	H	4.11489000	-2.51845000	0.61034000
H	-1.26733000	4.40268400	-0.42513600	H	4.04632100	-0.87927600	1.28966900
C	0.00000000	2.70561800	0.03567000	H	4.44650100	-1.10380200	-0.42513600
C	0.84605500	2.62515000	-1.15286200	C	2.34313400	-1.35280900	0.03567000
C	0.69391700	3.64297200	-2.25095800	C	1.85042000	-2.04528000	-1.15286200
H	1.50044100	3.57986000	-2.99262600	C	2.80794800	-2.42243600	-2.25095800
H	0.69028400	4.66153000	-1.82930400	H	2.35002900	-3.08935000	-2.99262600
H	-0.26786200	3.51478700	-2.77687200	H	3.69186200	-2.92856800	-1.82930400
C	0.57950200	2.31853000	2.39026800	H	3.17782600	-1.52541800	-2.77687200
C	1.73190700	3.08451300	2.66463700	C	1.71815500	-1.66112900	2.39026800
C	1.94947300	3.60474500	3.94420300	C	1.80531300	-3.04213200	2.66463700
H	2.84835300	4.19830400	4.14144100	C	2.14706400	-3.49066500	3.94420300
C	1.02542100	3.36274300	4.97291100	H	2.21166100	-4.56589800	4.14144100
C	-0.11904000	2.60056800	4.70381900	C	2.39951000	-2.56941200	4.97291100
H	-0.84906600	2.40377500	5.49511000	C	2.31167700	-1.19719200	4.70381900
C	-0.34719100	2.08828400	3.41986300	H	2.50626300	-0.46657500	5.49511000

C	1.98210200	-0.74346600	3.41986300	C	-2.19263800	-1.40337500	4.70381900
H	1.91031900	0.32463000	3.20543300	H	-1.65719700	-1.93720000	5.49511000
C	-0.09173200	-2.99896500	-2.22979800	C	-1.63491200	-1.34481800	3.41986300
C	-0.84741700	-4.15840000	-1.96293800	H	-0.67402100	-1.81670000	3.20543300
C	-1.52680300	-4.81769300	-2.99170900	C	-2.55131400	1.57892500	-2.22979800
H	-2.09595000	-5.72558300	-2.76782500	C	-3.17757200	2.81308400	-1.96293800
C	-1.48248400	-4.32133300	-4.30422200	C	-3.40884300	3.73109600	-2.99170900
C	-0.74925000	-3.15800900	-4.57376200	H	-3.91052500	4.67793800	-2.76782500
H	-0.71407000	-2.75629500	-5.59170900	C	-3.00114200	3.44453600	-4.30422200
C	-0.05678400	-2.49932100	-3.54841200	C	-2.36029100	2.22787400	-4.57376200
H	0.50498200	-1.58418500	-3.75672800	H	-2.02998700	1.99655000	-5.59170900
C	-3.18408500	-2.56505100	0.39575200	C	-2.13608400	1.29883700	-3.54841200
H	-4.23848600	-2.30437400	0.61034000	H	-1.62443600	0.35476500	-3.75672800
H	-2.78463600	-3.06457800	1.28966900	H	-4.04158600	0.50358700	1.86098300
H	-3.17917100	-3.29888200	-0.42513600	H	-3.86055500	-0.84484200	5.97558200
C	-2.34313400	-1.35280900	0.03567000	H	1.58467400	-3.75191000	1.86098300
C	-2.69647400	-0.57987000	-1.15286200	H	2.66193200	-2.92091700	5.97558200
C	-3.50186500	-1.22053600	-2.25095800	H	-0.87711600	-4.53143700	-0.93526600
H	-3.85047000	-0.49051000	-2.99262600	H	-2.01930200	-4.83434000	-5.10763800
H	-4.38214500	-1.73296200	-1.82930400	H	-3.48578200	3.02532300	-0.93526600
H	-2.90996400	-1.98936900	-2.77687200	H	-3.17701000	4.16593700	-5.10763800
C	-2.29765700	-0.65740100	2.39026800	H	4.36289800	1.50611400	-0.93526600
C	-3.53722000	-0.04238100	2.66463700	H	5.19631200	0.66840300	-5.10763800
C	-4.09653700	-0.11408000	3.94420300	H	2.45691200	3.24832200	1.86098300
H	-5.06001500	0.36759400	4.14144100	H	1.19862200	3.76576000	5.97558200
C	-3.42493100	-0.79333100	4.97291100				

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