Electronic Supplementary Information (ESI)

for

A phenanthroline-terpyridine hybrid as a chameleon-type ligand in a reversible metallosupramolecular rearrangement

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Abbreviations used:

TBAF: Tetra-*n*-butylammonium fluoride

DOSY: Diffusion-ordered spectroscopy

Synthesis

All commercial reagents were used without further purification. Solvents were dried with the appropriate desiccants and distilled prior to use. Silica gel (60-230 mesh) was used for column chromatography. Unless mentioned, ^{1}H NMR and ^{13}C NMR were recorded on a Bruker Avance 400 MHz, whereas DOSY NMR were recorded on a Varian VNMR-S 600 MHz spectrometer using the deuterated solvent as the lock and residual solvent as the internal reference. The following abbreviations were utilised to describe peak patterns: s = singlet, d = doublet, t = triplet, dd = doublet of doublets, td = triplet of doublets, dt = doublet of triplets, ddd = doublet of doublet of doublets, br = broad and m = multiplet. The numbering of carbon atoms in the molecular formulae is only used for assignment of NMR signals and thus is not necessarily in accordance with IUPAC nomenclature. Electrospray ionisation mass spectra (ESI-MS) were recorded on a Thermo-Quest LCQ Deca. Melting points were measured on a Büchi SMP-20 instrument. Infrared spectra were recorded using a Varian 1000 FT-IR instrument. Elemental analysis measurements were done using the EA 3000 CHNS. The numbering of the compounds follows the scheme in the publication. Complexes **C1-C3**[1], and compounds **2**[1], **3**[1] (precursors for **1**) were synthesised according to known procedures. The energy-minimised structures were computed using the semi-empirical method PM6 as implemented in Gaussian09. X-ray single-crystal diffraction data for complexes **C1** and **C2** were collected on a STOE IPDS one-circle image plate diffractometer and SIEMENS SMART CCD diffractometer, respectively. The structures were solved using SHELXS-97 and refined by full-matrix least-squares analysis.[2] Hydrogen atoms were generated theoretically onto the specific atoms and refined using a riding model. The non-hydrogen atoms were refined with aniosotropic thermal parameters. Further details are provided in the X-ray structure analysis section.

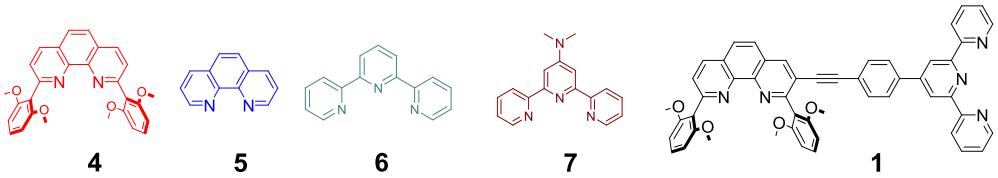


Chart 1: Ligands used in the present study.

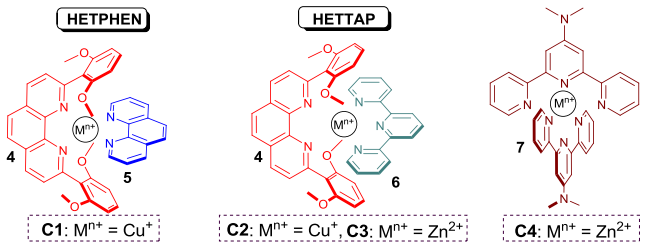
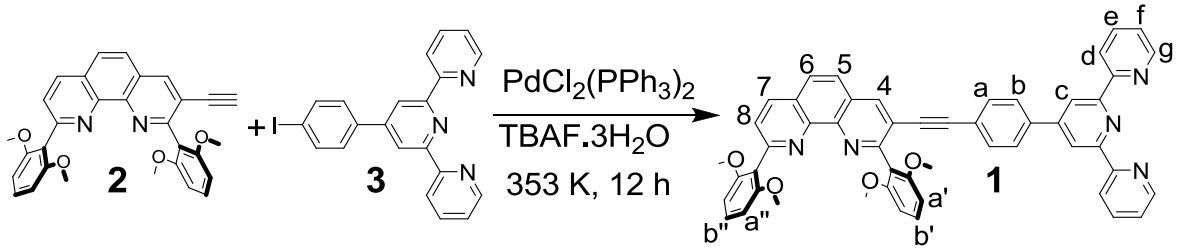


Chart 2: Mononuclear metal complexes used in the present study.

Synthesis and characterisation of 4'-{4-[2,9-bis(2,6-dimethoxyphenyl)-[1,10]phenanthrolin-3-ylethynyl]-phenyl}-[2,2';6',2'']terpyridine (1)



In an oven-dry Schlenk flask, 2,9-bis(2,6-dimethoxyphenyl)-3-ethynyl[1,10]phenanthroline (**2**, 150 mg, 315 µmol), 4'-(4-iodophenyl)-[2,2';6',2'']terpyridine, (**3**, 137 mg, 315 µmol), TBAF•3H_2O (795 mg, 2.52 mmol), and $PdCl_2(PPh_3)_2$ (11.5 mg, 16.4 µmol) were combined under nitrogen atmosphere. The solid mixture was then stirred at 353 K for 12 h. The reaction mixture was cooled, dissolved in dichloromethane (200 mL), and washed successively with aqueous KOH (200 mL) and water (6 × 200 mL). After drying over Na_2SO_4, the organic solvent was removed under reduced pressure. The crude product was purified using column chromatography (SiO_2; MeOH/CH_2Cl_2 = 1:49; R_f =0.25 [MeOH/CH_2Cl_2 = 1:9]) affording **1** as light yellow solid. Yield 55%. ^{1}H NMR (400 MHz, CD_2Cl_2) δ = 3.72 (s, 6 H, OCH_3), 3.75 (s, 6 H, OCH_3), 6.71 (d, ^3J = 8.4 Hz, 2 H, [a'/a'']-H), 6.78 (d, ^3J = 8.4 Hz, 2 H, [a'/a'']-H), 7.34 (d, ^3J = 8.4 Hz, 2 H, [a/b]-H), 7.37-7.41 (m, 3 H, [f, b'/b'']-H), 7.48 (t, ^3J = 8.4 Hz, 1 H, [b'/b'']-H), 7.59 (d, ^3J = 8.0 Hz, 1 H, 8-H), 7.84 (d, ^3J = 8.4 Hz, 2 H, [a/b]-H), 7.88-7.93 (m, 4 H, 5, 6, e-H), 8.31 (d, ^3J = 8.0 Hz, 1 H, 7-H), 8.50 (s, 1 H, 4-H), 8.68 (d, ^3J = 7.6 Hz, 2 H, d-H), 8.72 (d, ^3J = 4.8 Hz, 2 H, g-H), 8.75 (s, 2 H, c-H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ = 56.4, 56.6, 89.2, 94.5, 104.4, 118.9, 120.0, 121.0, 121.6, 124.2, 124.5, 126.4, 127.6, 127.7, 128.5, 129.0, 129.1, 130.3, 130.6, 132.4, 132.5, 132.7, 136.3, 137.4, 138.7, 139.0, 145.5, 146.5, 149.6, 149.7, 156.2, 156.5, 156.6, 157.7, 158.7, 158.9; IR (KBr) ν 3411, 3051, 3003, 2953, 2904, 2834, 1599, 1585, 1567, 1538, 1514, 1505, 1472, 1445, 1431, 1412, 1389, 1304, 1286, 1249, 1173, 1110, 1038, 1021, 991, 913, 891, 838, 790, 774, 739, 692, 660. ESI-MS *m/z* (%) 784.3 (100) $[M + H]^+$. Anal. Calcd for $C_{51}H_{37}N_5O_4$•2H_2O: C, 74.71; H, 5.04; N, 8.54. Found: C, 74.31; H, 4.60; N, 8.24.

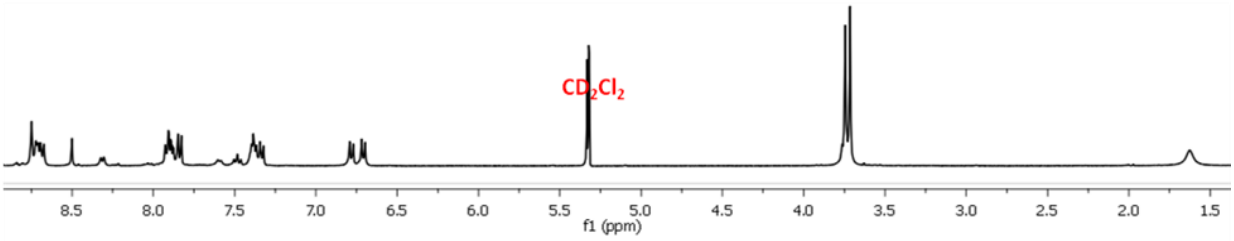


Figure S1. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2, 298 K) of **1**.

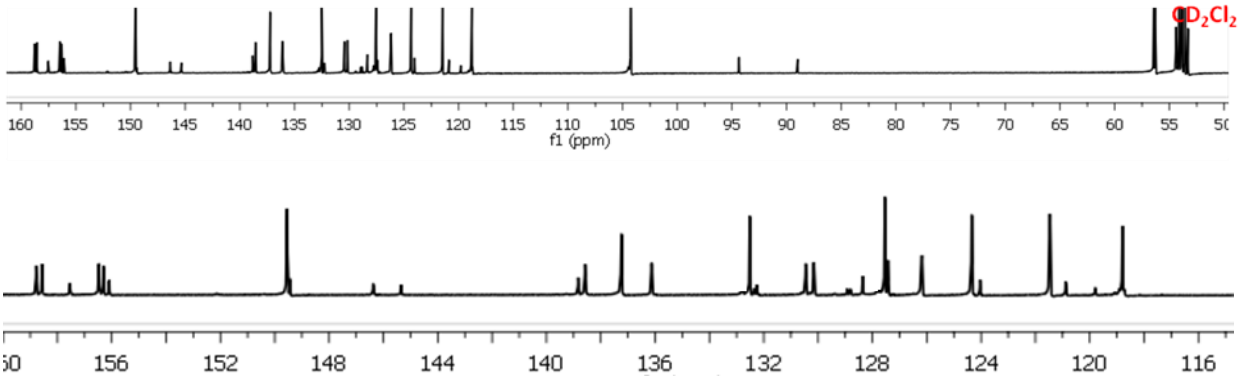


Figure S2. ^{13}C NMR spectrum (100 MHz, CD_2Cl_2, 298 K) of **1**. An expanded part of the spectrum is shown at the bottom.

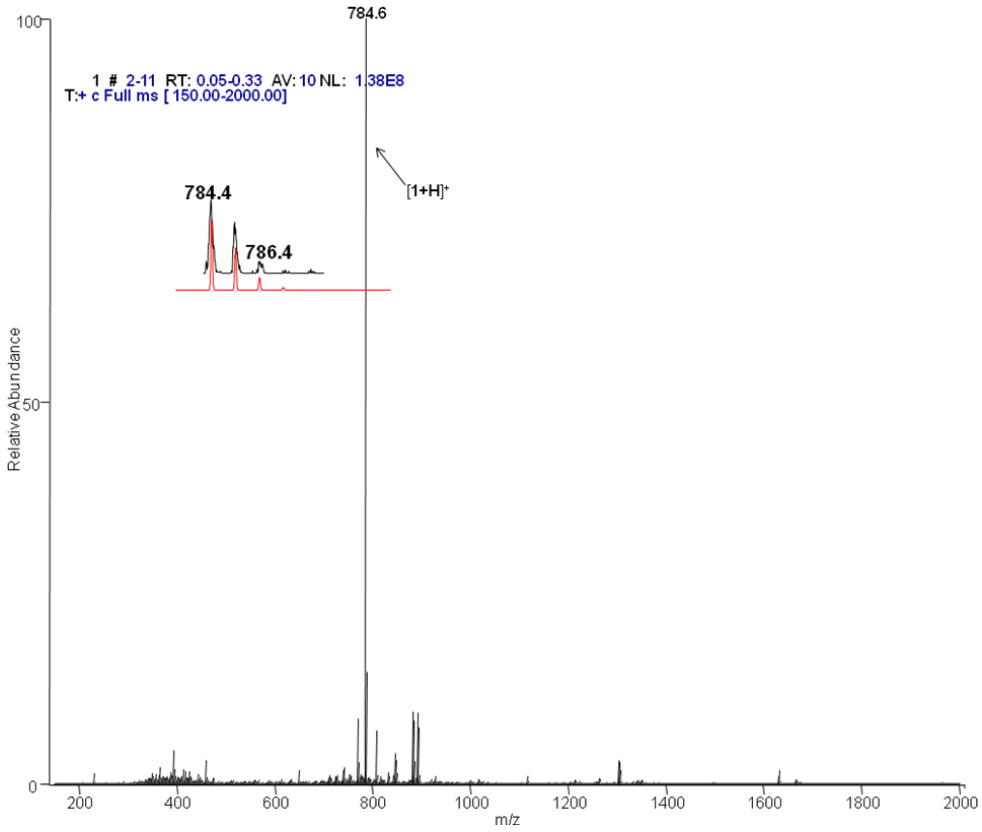
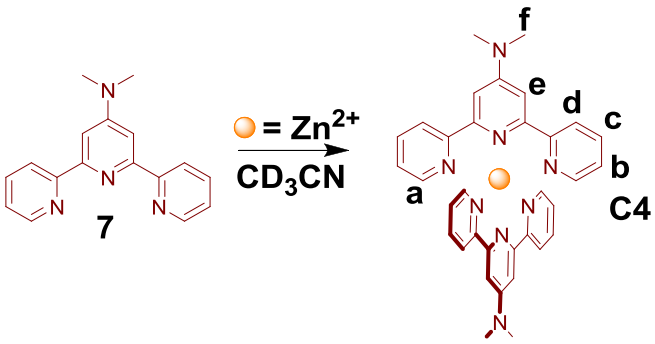


Figure S3. ESI-MS spectrum of ligand **1** in dichloromethane.

Synthesis and characterisation of complex C4



An NMR tube containing *N*,*N*-dimethylamino-[2,2';6',2"]terpyridine (**7**, 4.38 mg, 15.9 µmol) was loaded with a solution of $Zn(OTf)_2$ (2.88 mg, 7.93 µmol) in CD_2Cl_2:CD_3CN (1:5). The heterogeneous mixture was placed in an ultrasonic bath at room temperature for 2 h. Thereafter, the resultant solution was subjected to analytical characterisation without any further purification. Yield quantitative. ^{1}H NMR (400 MHz, CD_2Cl_2:CD_3CN (1:5)): δ = 3.42 (s, 12 H, f-H), 7.32 (ddd, ^3J = 8.0 Hz, ^3J = 5.1 Hz, ^4J = 0.8 Hz, 4 H, b-H), 7.71 (ddd, ^3J = 5.1 Hz, ^4J = 1.6 Hz, ^5J = 0.8 Hz, 4 H, a-H), 7.74 (s, 4 H, e-H), 8.06 (td, ^3J = 8.0 Hz, ^4J = 1.6 Hz, 4 H, c-H), 8.54 (ddd, ^3J = 8.0 Hz, ^4J = 0.8 Hz, ^5J = 0.8 Hz, 4H, d-H). ^{13}C NMR (100 MHz, CD_2Cl_2:CD_3CN = 1:5): δ = 40.8, 105.5, 123.0, 127.5, 141.4, 148.0, 149.7, 149.9, 159.7. ESI-MS: *m*/*z* (%) 308.0 (100) $[M-2OTf]^{2+}$, 765.4 (98) $[M-OTf]^+$. IR (KBr) ν 3398, 3093, 2927, 2362, 1619, 1571, 1535, 1473, 1436, 1389, 1269, 11756, 1025, 843, 796, 751, 638, 516. Anal. Calcd for $C_{36}H_{32}F_6N_8O_6S_2Zn$•5/4$CH_2Cl_2$: C, 43.76; H, 3.40; N, 10.96; S, 6.27. Found: C, 44.12; H, 3.68; N, 10.58; S, 5.92.

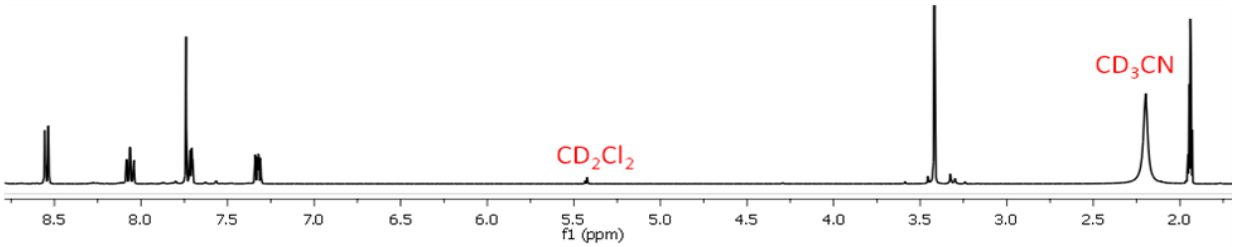


Figure S4. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2:CD_3CN (1:5), 298 K) of **C4**.

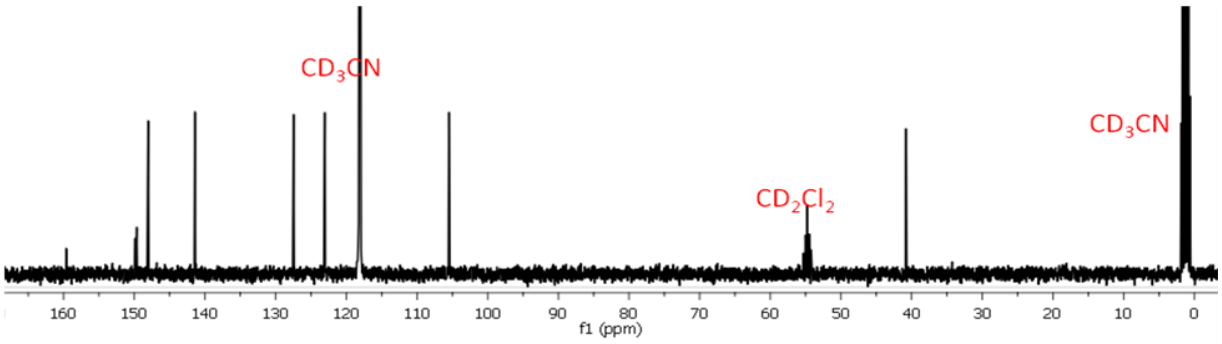


Figure S5. ^{13}C NMR spectrum (100 MHz, CD_2Cl_2:CD_3CN (1:5), 298 K) of **C4**.

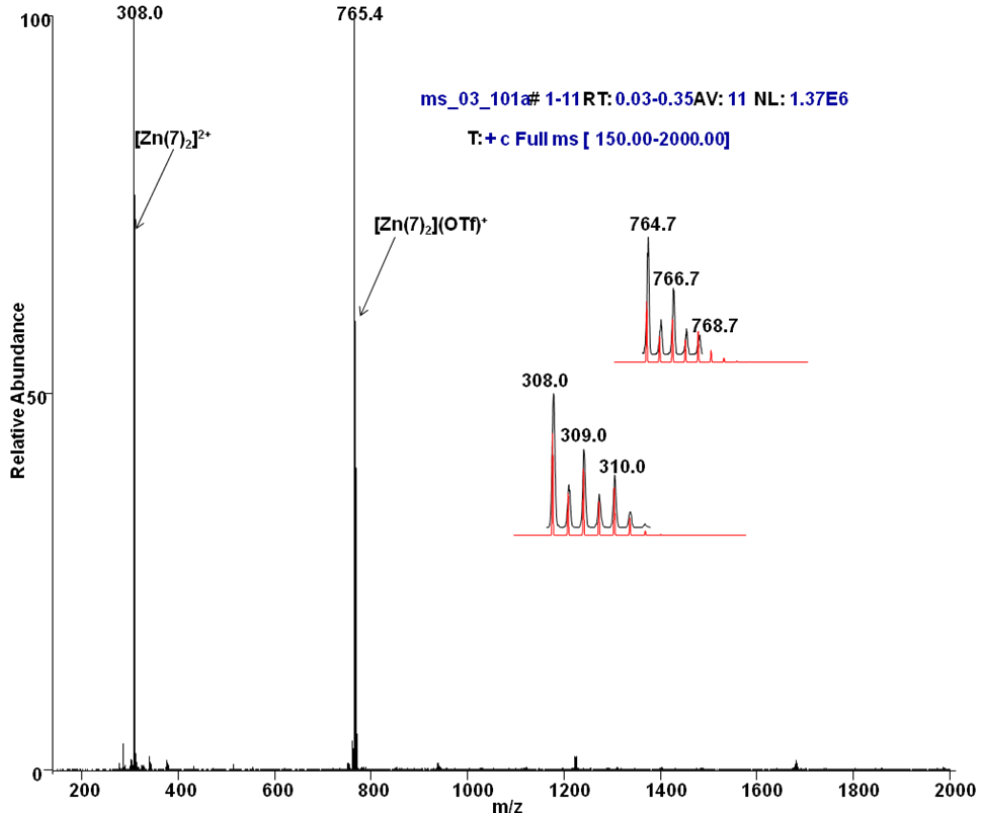


Figure S6. ESI-MS spectrum of **C4** = $[Zn(\mathbf{7})_2](OTf)_2$ (in acetonitrile) and experimental isotopic distributions (black lines) along with calculated isotopic distributions (red lines) for the peak associate with $[Zn(\mathbf{7})_2]^{2+}$ and$[Zn(\mathbf{7})_2](OTf)^{+}$.

Comparison of ^{1}H-NMR spectra of C2 and C3 with ligand 6.

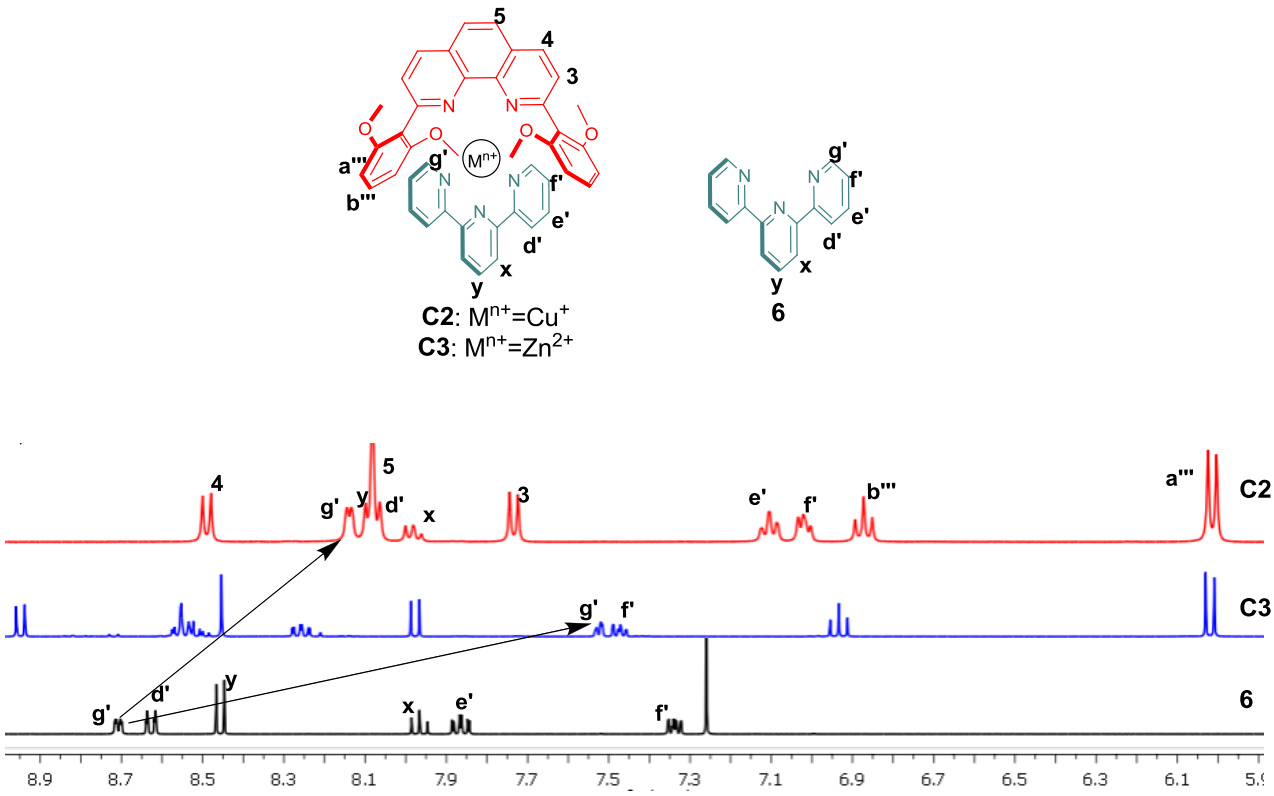


Figure S7. Comparison of partial ^{1}H NMR spectra (400 MHz, 298 K) recorded for **C2** (in CD_2Cl_2), **C3** (in CD_2Cl_2) and ligand **6** (in $CDCl_3$).

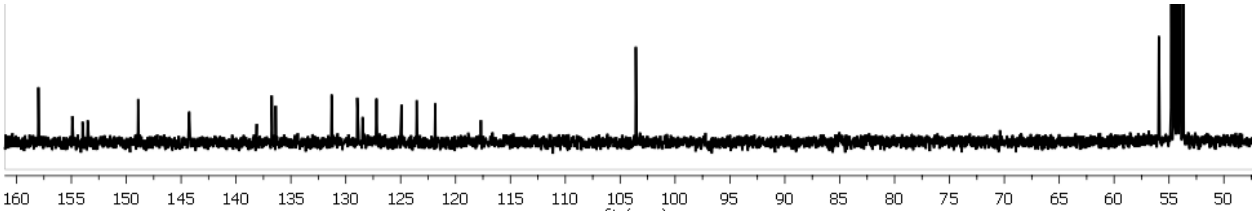
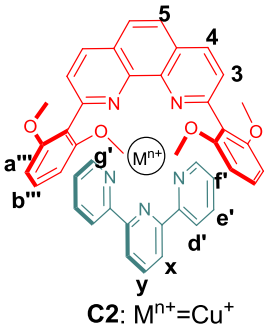


Figure S8. Partial ^{13}C NMR spectra (400 MHz, 298 K) of **C2**.

Variable temperature NMR (VT-NMR) experiment on C2.



C2: $M^{n+}=Cu^{+}$

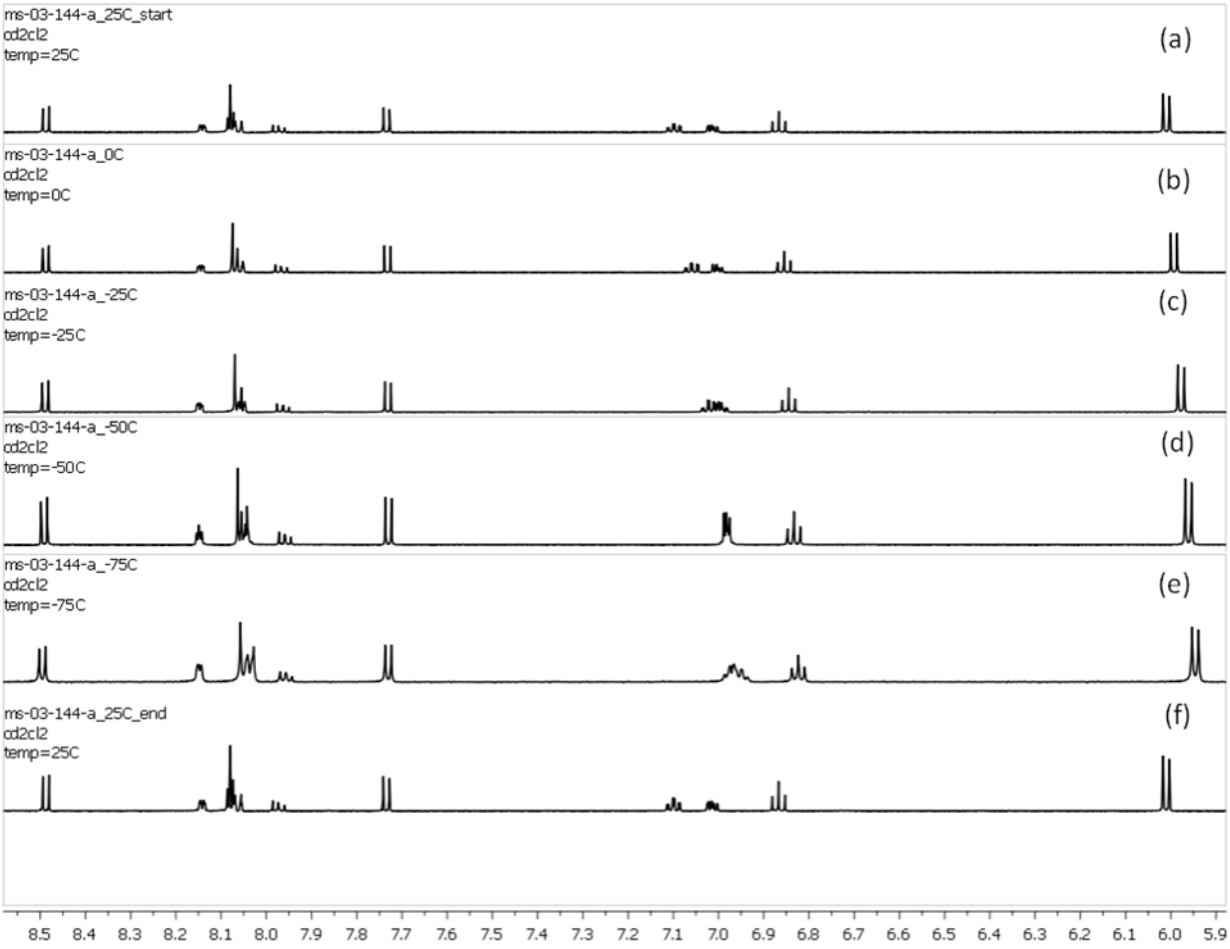
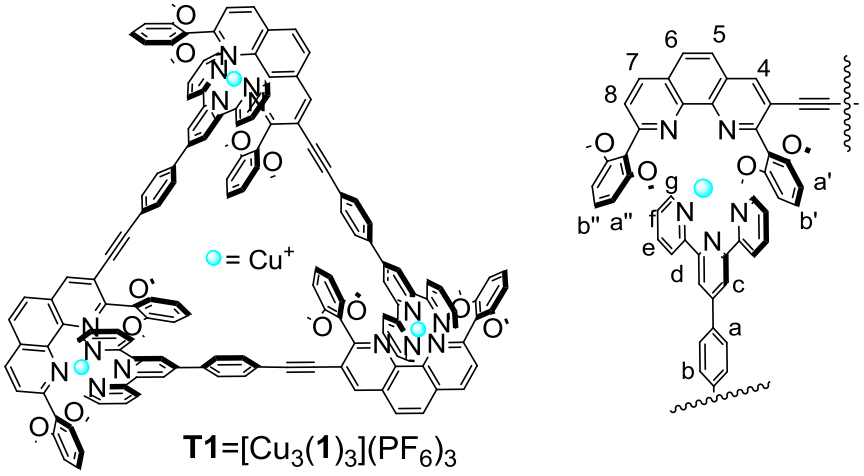


Figure S9. Comparison of partial ^{1}H NMR spectra (600 MHz, CD_2Cl_2) of **C2** at (a) 298 K, (b) 273 K, (c) 248 K, (d) 223 K, (e) 198 K and (f) after returning back to 298 K.

Synthesis and characterisation of equilateral triangle T1



In an oven-dried 10-mL single-neck round-bottom flask, a mixture of 4'-{4-[2,9-bis(2,6-dimethoxyphenyl)-[1,10]phenanthrolin-3-ylethynyl]-phenyl}-[2,2';6',2"]terpyridine (**1**, 3.30 mg, 4.20 µmol) and $[Cu(MeCN)_4]PF_6$ (1.57 mg, 4.20 µmol) was dissolved in 5 mL of acetonitrile and refluxed for 1 h. A clear red solution was obtained, the solvent evaporated and the solid subjected to analytical characterisation without any further purification. Yield quantitative. MP > 260°C. ^{1}H NMR (400 MHz, CD_3CN) δ = 3.14 (s, 18 H, OMe), 3.30 (s, 18 H, OMe), 5.91 (d, ^3J = 8.4 Hz, 6 H, a'-H), 6.27 (d, ^3J = 8.4 Hz, 6 H, a''-H), 6.84 (t, ^3J = 8.4 Hz, 3 H, b'-H), 6.97 (t, ^3J = 8.4 Hz, 3 H, b''-H), 7.12 (m, 6 H, f-H), 7.25 (m, 6 H, e-H), 7.30 (d, ^3J = 8.4 Hz, 6 H, b-H), 7.50-7.53 (m, 3 H, 5-H), 7.61-7.67 (m, 3 H, 6-H), 7.79 (d, ^3J = 8.4 Hz, 6 H, a-H), 7.96 (d, ^3J = 8.0 Hz, 3 H, 8-H), 8.09-8.28 (m, 18 H, c, d, g-H), 8.67 (s, 3 H, 4-H), 8.79 (d, ^3J = 8.0 Hz, 3 H, 7-H). IR (KBr) ν 3437, 2928, 2847, 1598, 1473, 1429, 1293, 1253, 1110, 1024, 844, 788, 736, 557; ESI-MS *m/z* (%) 847.3 (100) $[M - 3PF_6]^{3+}$, 1343.0 (10) $[M - 2PF_6]^{2+}$. Anal. Calcd for $C_{153}H_{111}Cu_3F_{18}N_{15}O_{12}P_3 \cdot 3H_2O$: C, 60.62; H, 3.89; N, 6.93. Found: C, 60.63; H, 4.29; N, 6.56.

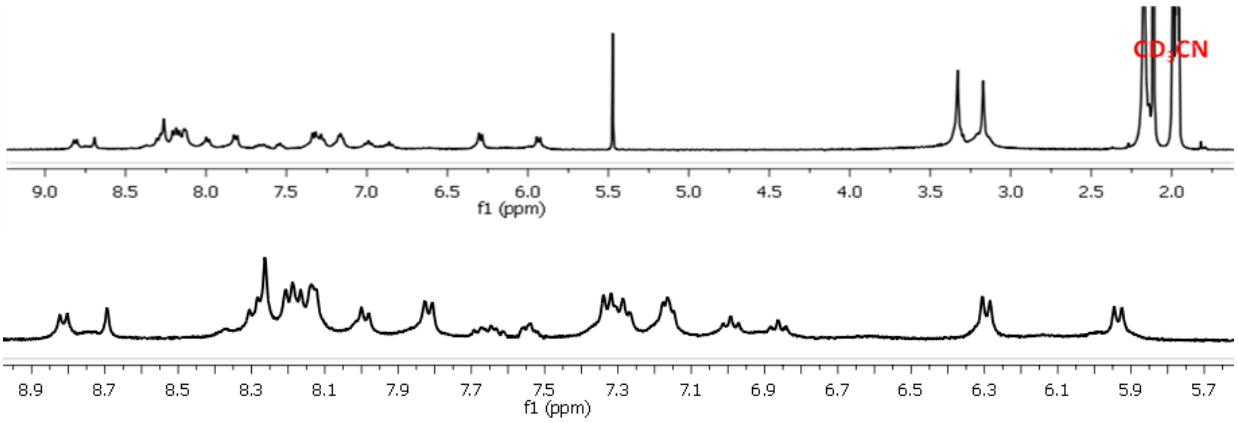


Figure S10. ^{1}H NMR spectrum (400 MHz, CD_3CN, 298 K) of triangle **T1** = $[Cu_3(\mathbf{1})_3](PF_6)_3$. An expanded part of the spectrum is shown at the bottom.

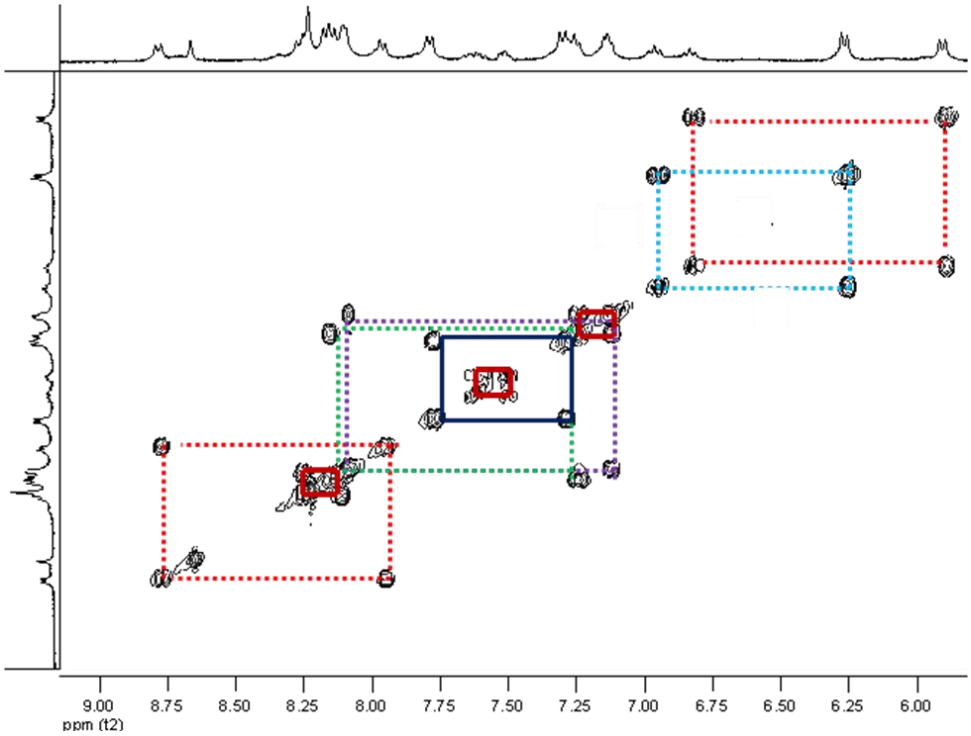


Figure S11. Partial ^{1}H-^{1}H COSY NMR spectrum (400 MHz, CD_3CN, 298 K) of triangle **T1** = $[Cu_3(\mathbf{1})_3](PF_6)_3$.

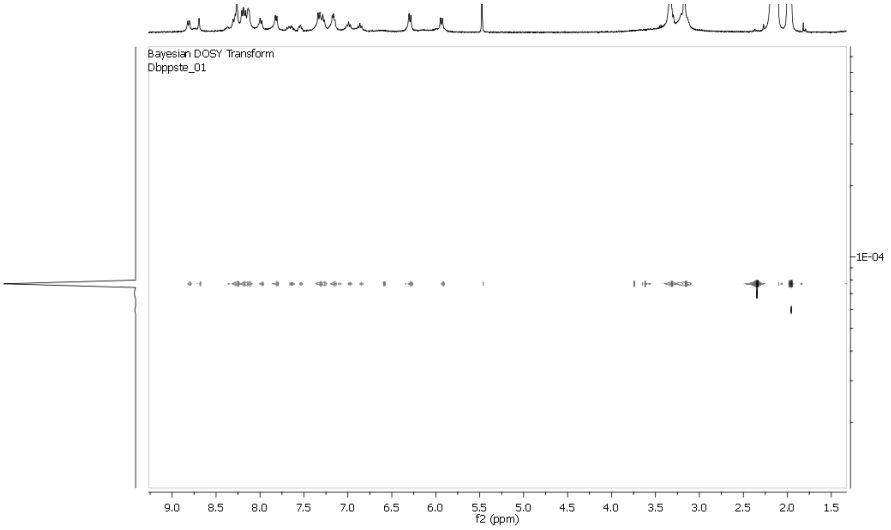


Figure S12. DOSY (600 MHz, CD_3CN, 298 K) plot of triangle **T1** = $[Cu_3(\mathbf{1})_3](PF_6)_3$.

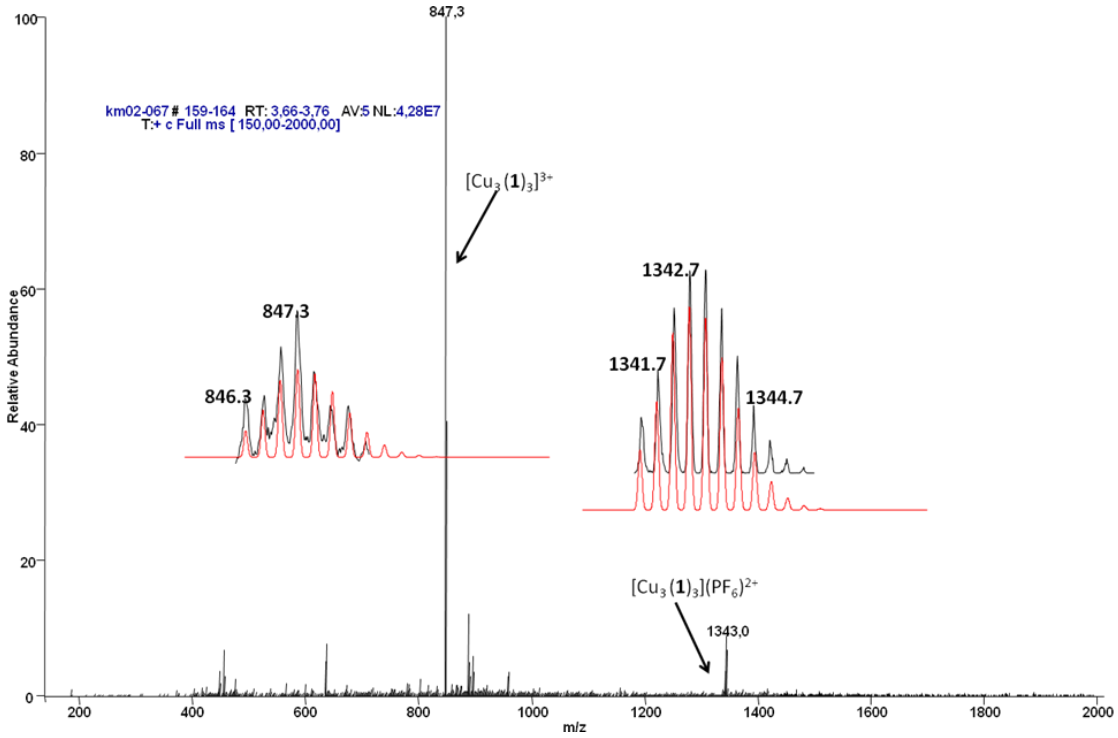
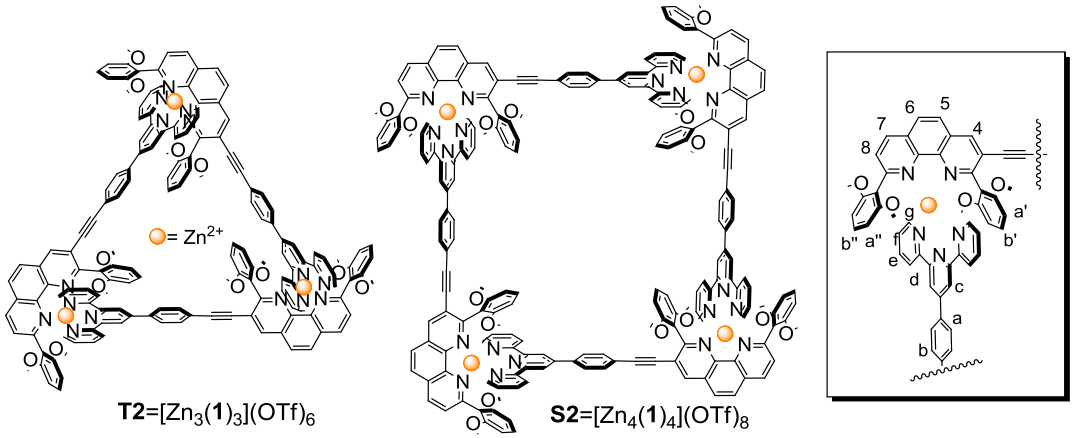


Figure S13. ESI-MS spectrum of **T1** = $[Cu_3(\mathbf{1})_3](PF_6)_3$ (in acetonitrile) and experimental isotopic distributions (black) along with calculated isotopic distributions (red) for the peaks associated with $[Cu_3(\mathbf{1})_3]^{3+}$ and $[Cu_3(\mathbf{1})_3](PF_6)^{2+}$.

Synthesis and characterisation of mixture containing triangle T2 and square S2



In an oven-dried 10-mL single-neck round-bottom flask, a mixture of 4'-{4-[2,9-bis(2,6-dimethoxyphenyl)-[1,10]phenanthrolin-3-ylethynyl]-phenyl}-[2,2';6',2"]terpyridine (**1**, 3.23 mg, 4.12 μmol) and $Zn(OTf)_2$ (1.50 mg, 4.12 μmol) was dissolved in acetonitrile and refluxed for 1 h. The solvent was evaporated from the light yellow solution and the solid was subjected to analytical characterisation without any further purification. ^{1}H NMR (600 MHz, CD_3CN:CD_2Cl_2 (4:1)) of two assemblies (**T2**/**S2**) in ratio of 2:1.

T2: δ = 2.82 (s, 9 H, OMe), 2.84 (s, 9 H, OMe), 2.88 (s, 9 H, OMe), 2.98 (s, 9 H, OMe), 6.05 (d, ^3J = 8.4 Hz, 3 H, a'-H), 6.07 (d, ^3J = 8.4 Hz, 3 H, a'-H), 6.10 (d, ^3J = 8.4 Hz, 3 H, a''-H), 6.16 (d, ^3J = 8.8 Hz, 3 H, a''-H), 6.78 (t, ^3J = 8.4 Hz, 3 H, b'-H), 6.99 (t, ^3J = 8.8 Hz, 3 H, b''-H), 7.40 (d, ^3J = 8.4 Hz, 6 H, b-H), 7.48-7.53 (m, 6 H, f-H), 7.68-7.70 (m, 6 H, g-H), 7.94 (d, ^3J = 8.4 Hz, 6 H, a-H), 8.05-8.24 (m, 9 H, [8, e]-H), 8.46-8.58 (m, 18 H, [5, 6, c, d]-H), 9.11 (d, ^3J = 8.8 Hz, 3 H, 7-H), 9.12 (s, 3 H, 4-H).

S2: δ = 2.85 (s, 12 H, OMe), 2.85 (s, 12 H, OMe), 2.88 (s, 24 H, OMe), 6.06 (d, ^3J = 8.4 Hz, 8 H, a'-H), 6.13 (d, ^3J = 8.4 Hz, 4 H, a''-H), 6.13 (d, ^3J = 8.4 Hz, 4 H, a''-H), 6.84-6.91 (m, 8 H, [b'/b'']-H), 7.38 (d, ^3J = 8.8 Hz, 8 H, b-H), 7.48-7.53 (m, 8 H, f-H), 7.68-7.70 (m, 8 H, g-H), 8.05-8.24 (m, 20 H, [8, a, e]-H), 8.46-8.58 (m, 24 H, 5, 6, c, d-H), 9.08 (d, ^3J = 8.4 Hz, 4 H, 7-H), 9.17 (s, 4 H, 4-H).

ESI-MS (**T2**) *m*/*z* (%) 539.1 (100) $[M - 5OTf]^{5+}$, 711.2 (35) $[M - 4OTf]^{4+}$, 1572.3 (5) $[M - 2OTf]^{2+}$.

ESI-MS (**S2**) *m*/*z* (%) 506.3 (20) $[M - 7OTf]^{7+}$, 615.7 (55) $[M - 6OTf]^{6+}$, 768.5 (18) $[M - 5OTf]^{5+}$, 1380.5 (5) $[M - 3OTf]^{3+}$.

ESI-MS signals shared by both **T2** and **S2**: *m*/*z* (%) 424.4 (**T2**/$[M - 6OTf]^{6+}$ + **S2**/$[M - 8OTf]^{8+}$) (43), 998.2 (**T2**/$[M - 3OTf]^{3+}$ +**S2**/$[M - 4OTf]^{4+}$) (60).

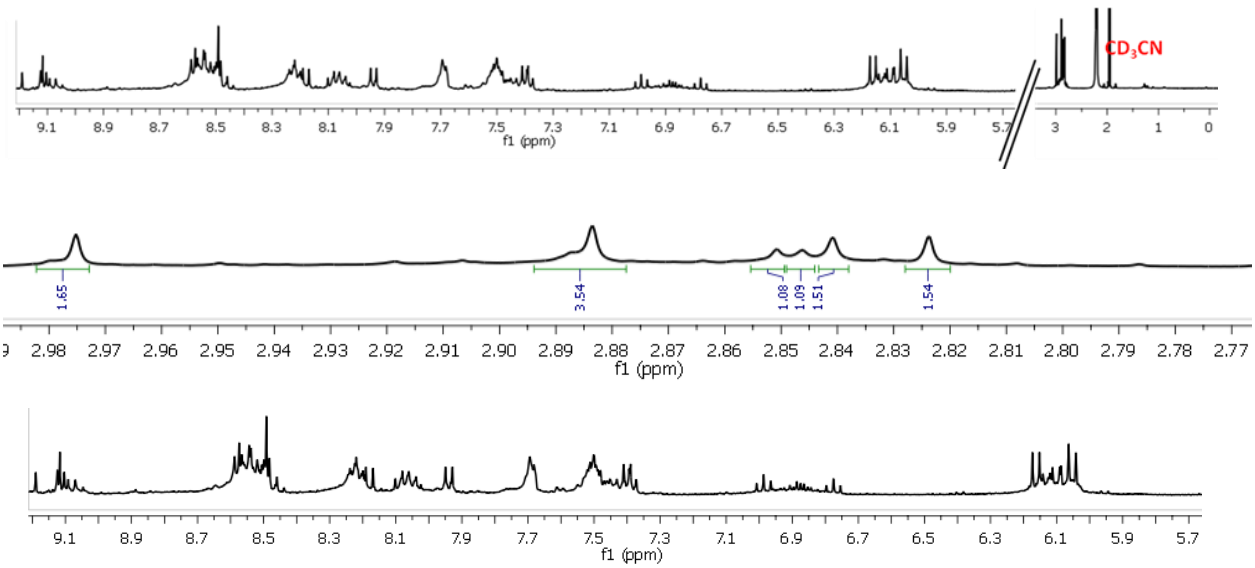


Figure S14. ^{1}H NMR spectrum (600 MHz, CD_3CN:CD_2Cl_2 (4:1), 298 K) of the triangle **T2** = $[Zn_3(\mathbf{1})_3](OTf)_6$ + **S2** = $[Zn_4(\mathbf{1})_4](OTf)_8$ mixture. Zoom in parts of the spectrum is shown at bottom.

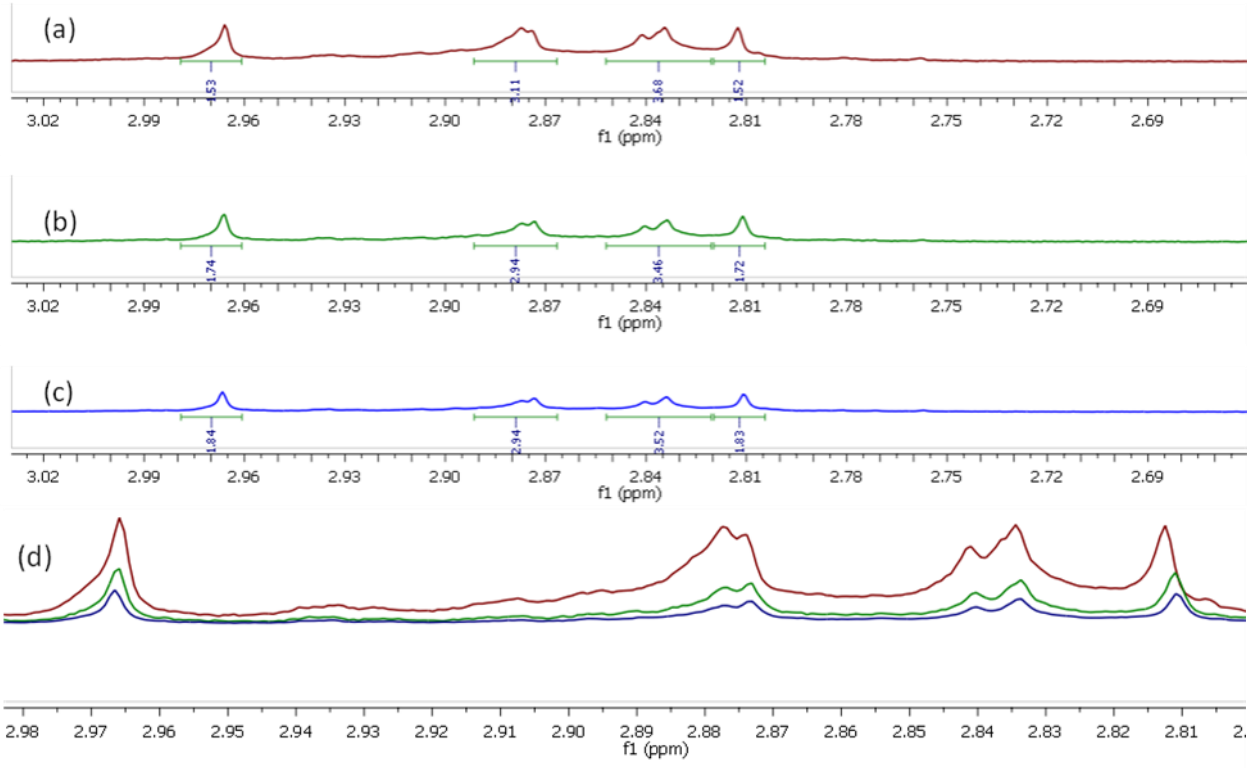


Figure S15. Partial ^{1}H NMR spectra (400 MHz, CD_3CN, 298 K) of pre-equilibrated **T2** = $[Zn_3(\mathbf{1})_3](OTf)_6$ + **S2** = $[Zn_4(\mathbf{1})_4](OTf)_8$ mixtures at ligand concentrations of (a) 3.68 mM, (b) 1.84 mM, (c) 1.23 mM, and (d) the superimposition of spectra a-c.

Analysis of the ^{1}H NMR spectra of T2 = $[Zn_3(1)_3](OTf)_6$ + S2 = $[Zn_4(1)_4](OTf)_8$ dependent on the concentration

Considering that **S2** and **T2** are composed of 8 and 6 pieces, respectively, one expects with decreasing concentration that the peaks assigned to **T2** increase in relative intensity while peaks for **S2** decrease. Thus, NMR spectra of mixtures were measured after full equilibration at three different concentrations (Figure S15 a-c).

Integrals were measured using the software MestRe-C. To make the intensity measurements reliable, we first put all recorded spectra (Figure S15 a-c) into the same window of MestRe-C, so that any area from one spectrum is automatically related to those of the other two. By using proton g-H (δ = 7.68-7.70 for both **T2** and **S2**) as an internal standard with an area value of 2H (corresponding to one ligand **1**) we probed the relative change in intensities for protons $OC\underline{H}_3$. For example, peaks at 2.82 and 2.98 ppm (attributed to protons $OC\underline{H}_3$ of **T2**) showed changes in relative integration from 1.53 to 1.84 on going from 3.68 mM to 1.23 mM concentration of ligand **1**. Based on these change in relative signal intensity, the assignment of both **S2** and **T2** as detailed on page S12 was double-checked.

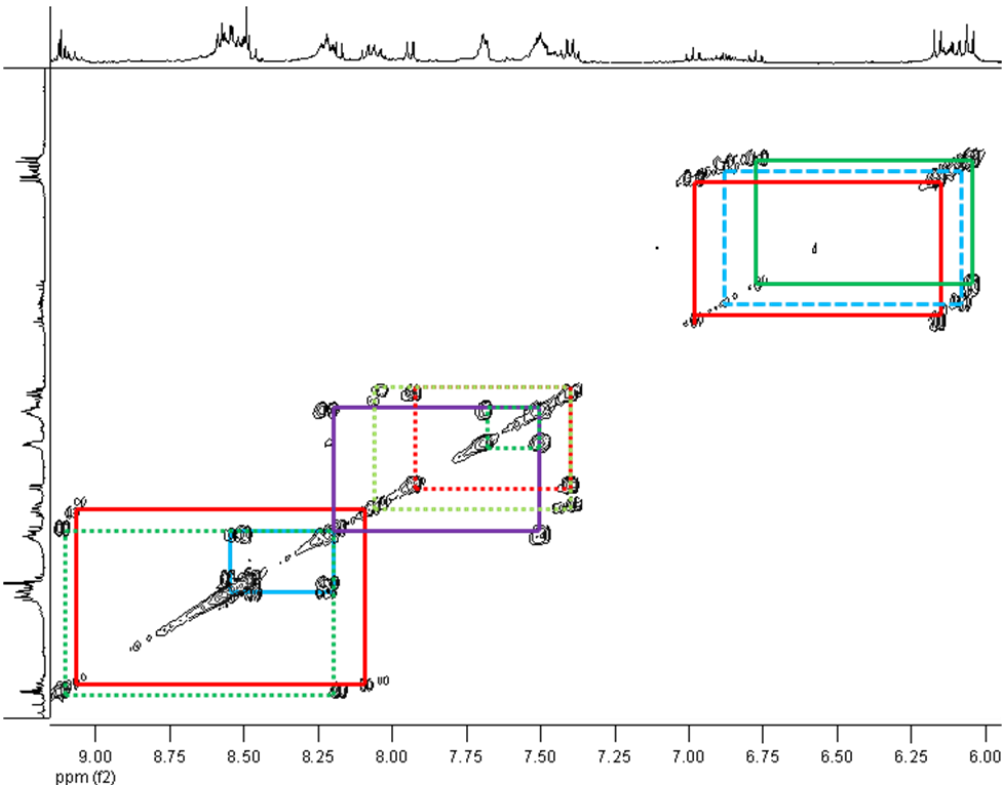


Figure S16. Partial ^{1}H-^{1}H COSY NMR spectrum (600 MHz, CD_3CN:CD_2Cl_2 = 4:1, 298 K) of the triangle **T2** = $[Zn_3(\mathbf{1})_3](OTf)_6$ + **S2** = $[Zn_4(\mathbf{1})_4](OTf)_8$ mixture.

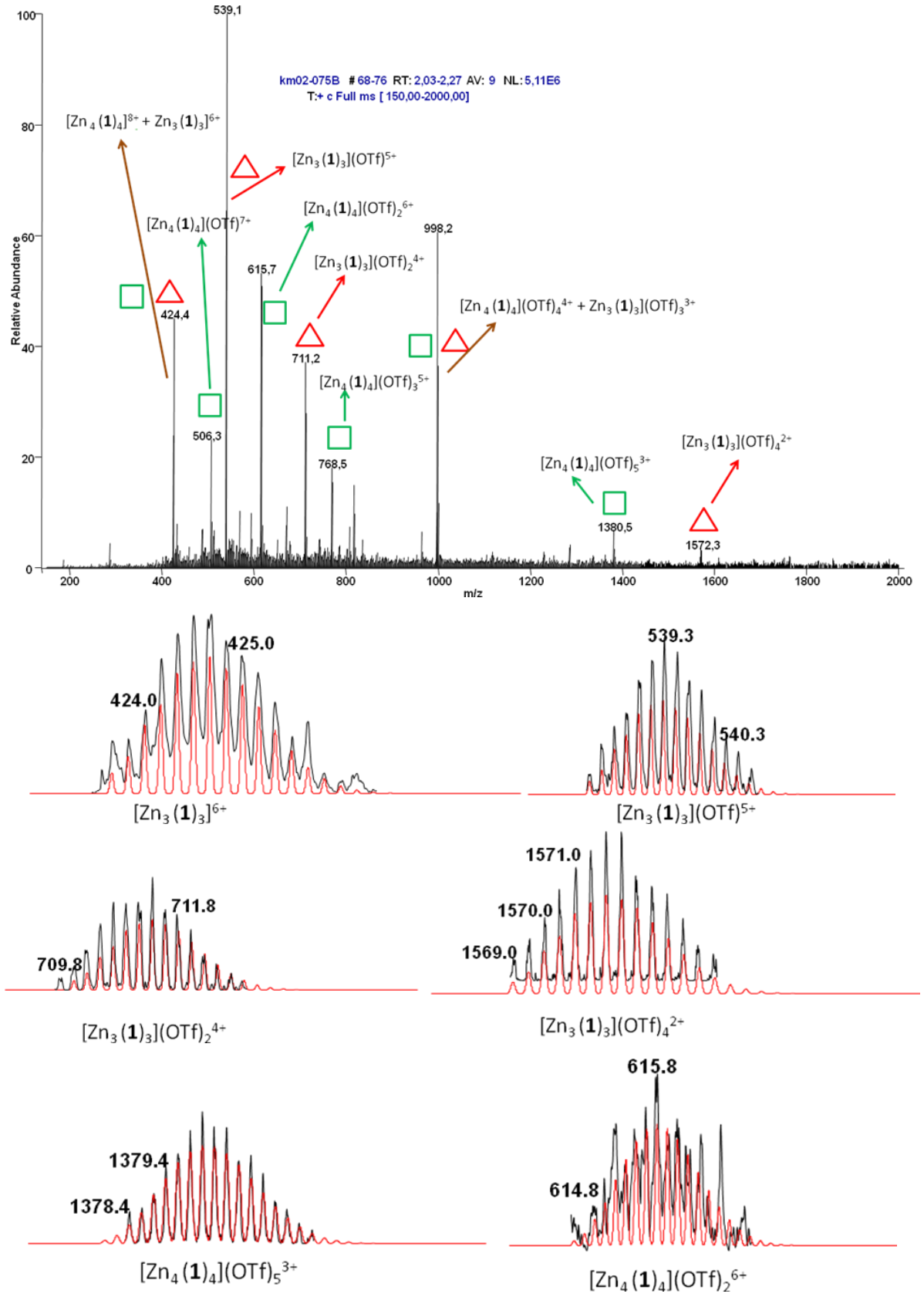
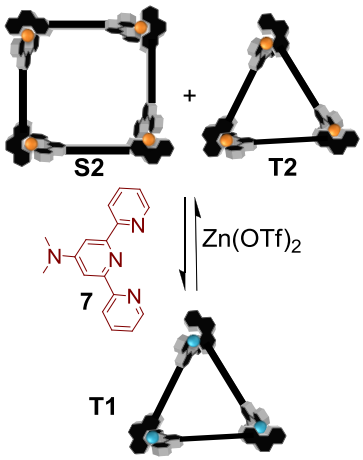


Figure S17. ESI-MS spectrum of **1** in presence of Zn^{2+} (in acetontrile) and experimental isotopic distributions (black) along with calculated isotopic distributions (red) for the different charged species obtained after the loss of counter anion(s). The peaks for triangle and square are marked as Δ and □ respectively.

Interconversion of T1 and (T2+S2) states



$Zn(OTf)_2$ (520 µg, 1.44 µmol) was added to a NMR tube loaded with a solution of **T1** (1.43 mg, 0.480 µmol) in CD_3CN. The solution was degassed through three evacuation/argon fill cycles and then kept in a thermostat at 333 K for 1 h. ^{1}H-NMR characterisation of the resultant mixture was done without any further purification. Thereafter, *N,N*-dimethylamino-[2,2';6',2'']terpyridine (**7**, 797 µg, 2.88 µmol) was added to this mixture. The solution was again degassed by three evacuation/argon fill cycles and kept in a thermostat at 333 K for 1 h. Analytical characterisation of the mixture was done without any further purification.

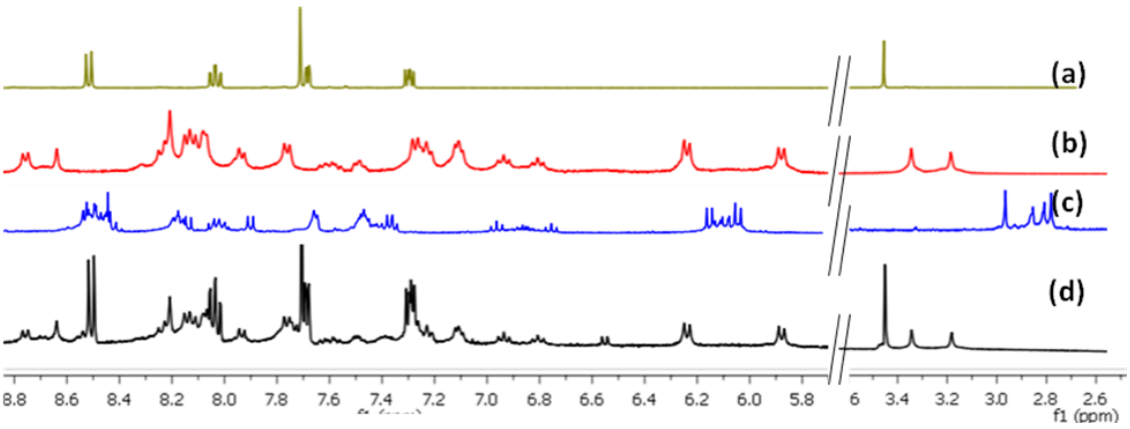


Figure S18. Comparison of partial ^{1}H NMR spectra (400 MHz, CD_3CN, 298 K) of (a) **C4**; (b) **T1**; (c) reaction mixture of **T1** + $Zn(OTf)_2$ (1:3) after 1 h at 333K; (d) the above mixture in presence of 6 equiv **7** (related to the initial amount of **T1**) after additional 1 h at 333 K.

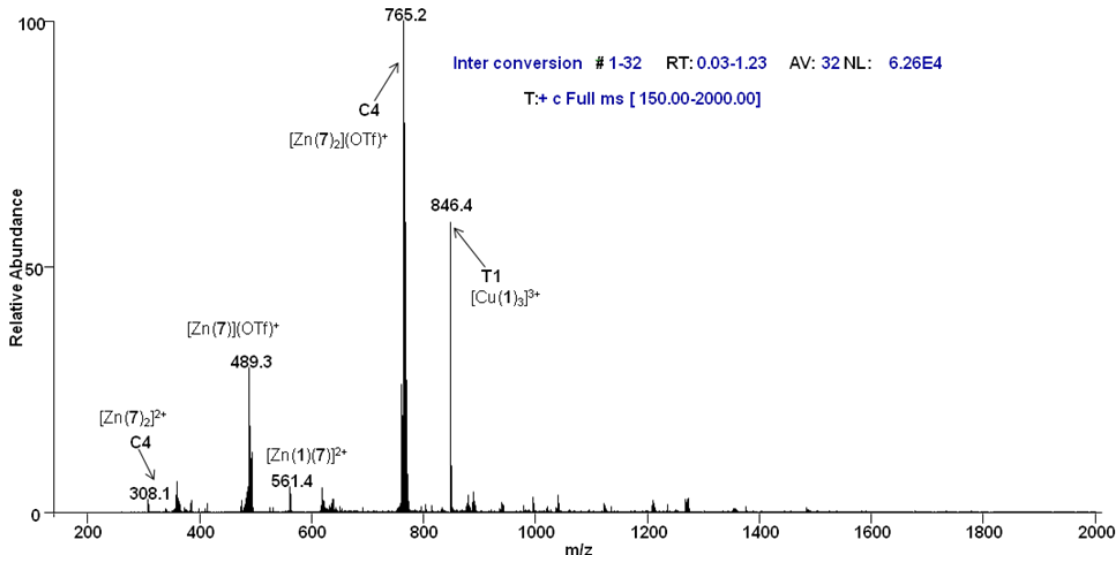


Figure S19. ESI-MS of the crude reaction mixture after performing the following two steps: (1.) **T1** + $Zn(OTf)_2$ (1:3) after 1 h at 333 K, and (2.) then react the mixture in presence of 6 equiv of **7** (related to the initial amount of **T1**) at 333 K for 1 h.

X-ray structure analysis

Table 1. Crystal data for compound **C1** = [Cu(**4**)(**5**)]PF_6 and **C2** = [Cu(**4**)(**6**)]PF_6

Compound name	**C1** (CCDC 931595)	**C2** (CCDC 931141)
Empirical formula	$C_{80}\ H_{68}Cu_2F_{12}N_8O_{10}P_2$	$C_{43}\ H_{35}\ Cu\ F_6\ N_5\ O_4\ P$
Formula weight	1718.44	894.27
Temperature/ K	153(2)	170(2)
Wavelength/ Å	0.71073	0.71073
Crystal system	Orthorhombic	Triclinic
Space group	*Cmca*	$P\bar{1}$
a/ Å	24.1554(12)	10.6732(5)
b/ Å	14.3528(7)	13.5845(6)
c/ Å	21.3467(9)	14.7036(7)
α/ deg	90.00	96.960(10)
β/ deg	90.00	107.775(10)
γ/ deg	90.00	103.619(10)
Volume/ $Å^3$	7400.9(6)	1929.62(15)
Z	4	2
Density (calculated) (g/cm^3)	1.542	1.539
Absorption coefficient (mm^{-1})	0.716	0.689
F(000)	3520	916
Reflections collected	29361	23103
Independent reflections	3435 [*R*(int) = 0.0666]	9038 [*R*(int) = 0.0275]
Reflections with I > 2sigma(I)	2351	7880
Absorption correction type	Empirical	Multi-scan
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.000	1.066
Final R indices	[>2sigma(I)] *R*1 = 0.0563, *wR*2 = 0.1551	[I>2sigma(I)] *R*1 = 0.0359, *wR*2 = 0.0844
R indices (all data)	*R*1 = 0.0829, *wR*2 = 0.1692	*R*1 = 0.0440, *wR*2 = 0.0884

Table 2. Selected bond lengths (Å) and angles (deg) for **C1** and **C2**

C1 = [Cu(**4**)(**5**)]PF_6

Cu1–N1	2.027(2)	N1–Cu1–N2	133.5(3)
		N1–Cu1–N3	128.3(3)
Cu1–N2	2.046(13)		
Cu1–N3	1.993(12)	N2–Cu1–N3	82.7(3)

C2 = [Cu(**4**)(**6**)]PF_6

Cu1–N1	2.0133(13)	N1–Cu1–N2	82.28(5)
		N1–Cu1–N3	125.07(6)
Cu1–N2	2.0805(13)	N1–Cu1–N4	138.25(6)
		N2–Cu1–N3	116.78(6)
Cu1–N3	2.0058(15)	N2–Cu1–N4	115.06(5)
Cu1–N4	2.0804(14)	N3–Cu1–N4	82.54(6)

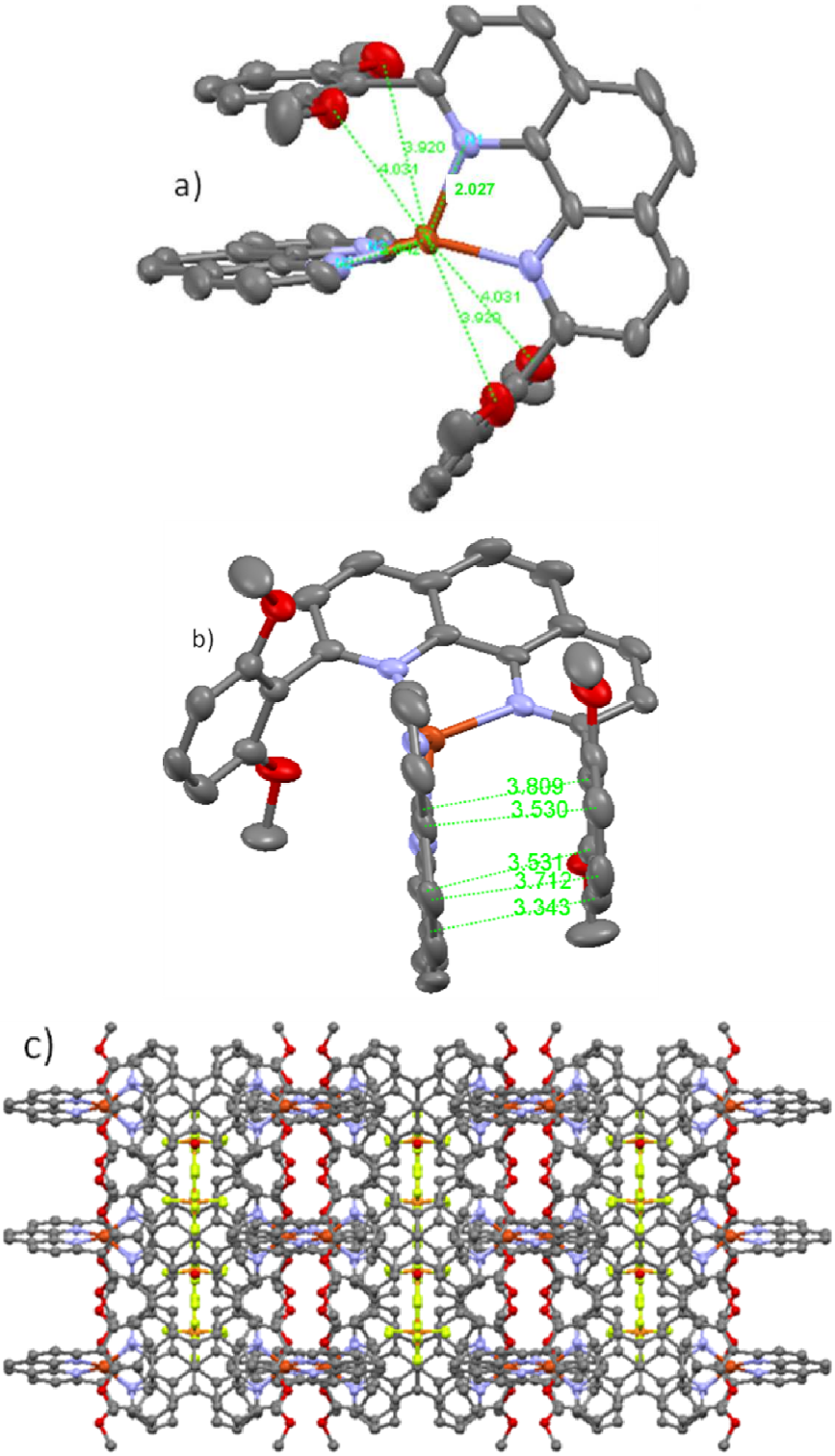


Figure S20: Solid state structure of **C1** = [Cu(**4**)(**5**)]PF_6 (thermal ellipsoids were drawn at the 50% probability level) showing (a) the Cu–N and Cu–O distances; (b) the distances between 2,6-dimethoxyphenyl ring and the 1,10-phenanthroline moiety Hydrogen atoms and counter ions are omitted for clarity. (c) Ball and stick representation of the packing diagram of **C1**. Hydrogen atoms are omitted for clarity.

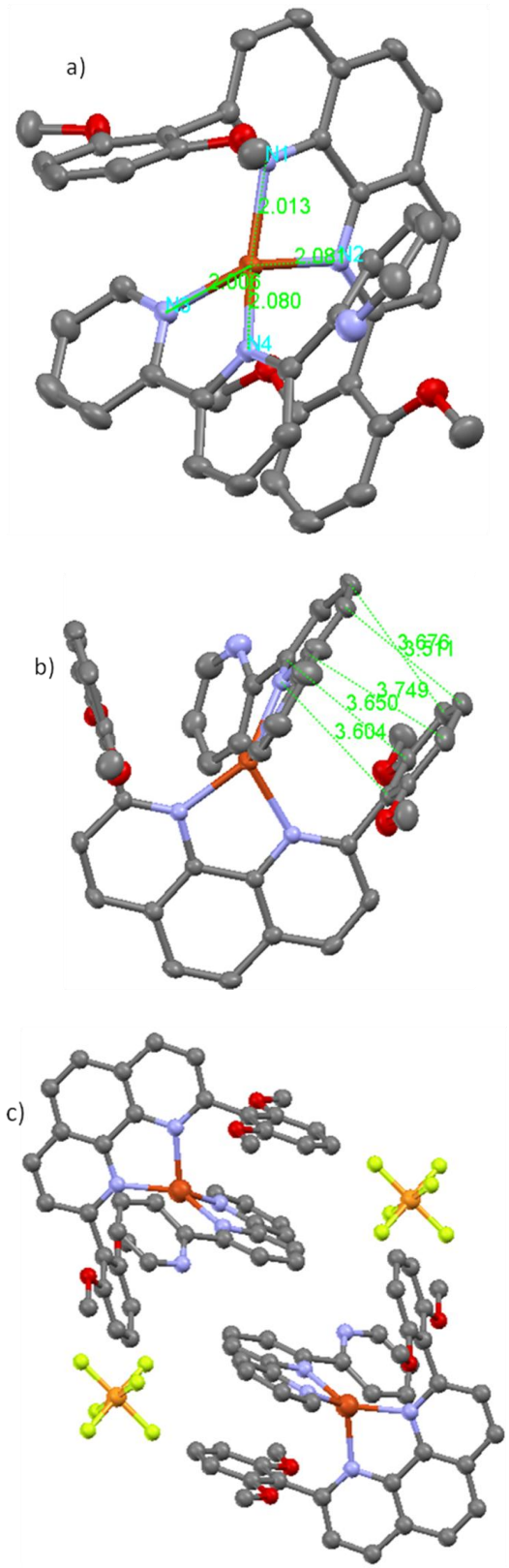


Figure S21: Solid state structure of **C2** = [Cu(**4**)(**6**)]PF_6 (thermal ellipsoids were drawn at the 50% probability level) showing (a) the Cu–N distances; (b) the distances between 2,6-dimethoxyphenyl ring and the terpyridine moiety Hydrogen atoms and counter ion are omitted for clarity. (c) Ball and stick representation of the packing diagram of **C2**. Hydrogen atoms are omitted for clarity.

Energy minimised structures using PM6 method

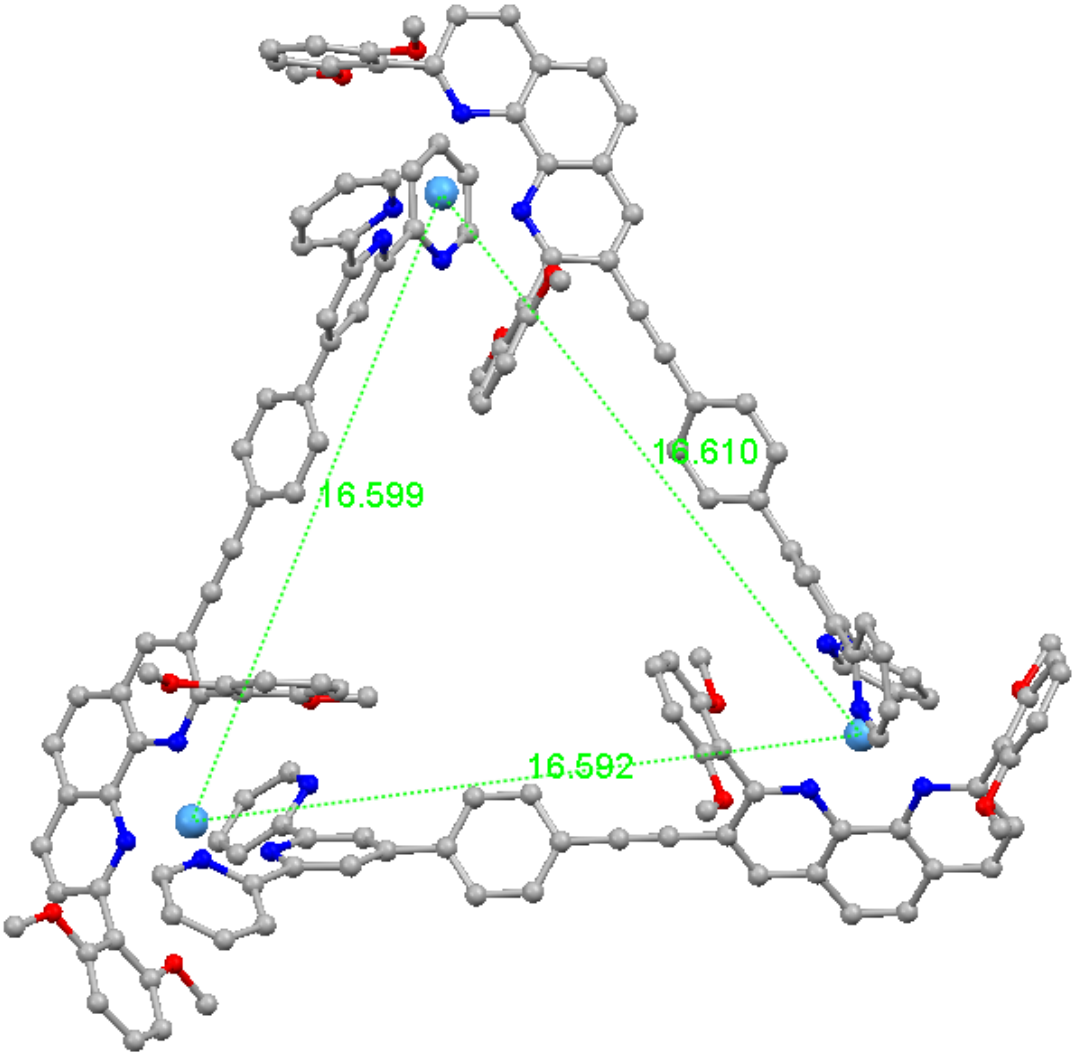


Figure S22. Energy minimised structure of equilateral triangle **T1**. Counter anions are not included. Hydrogens are omitted for clarity.

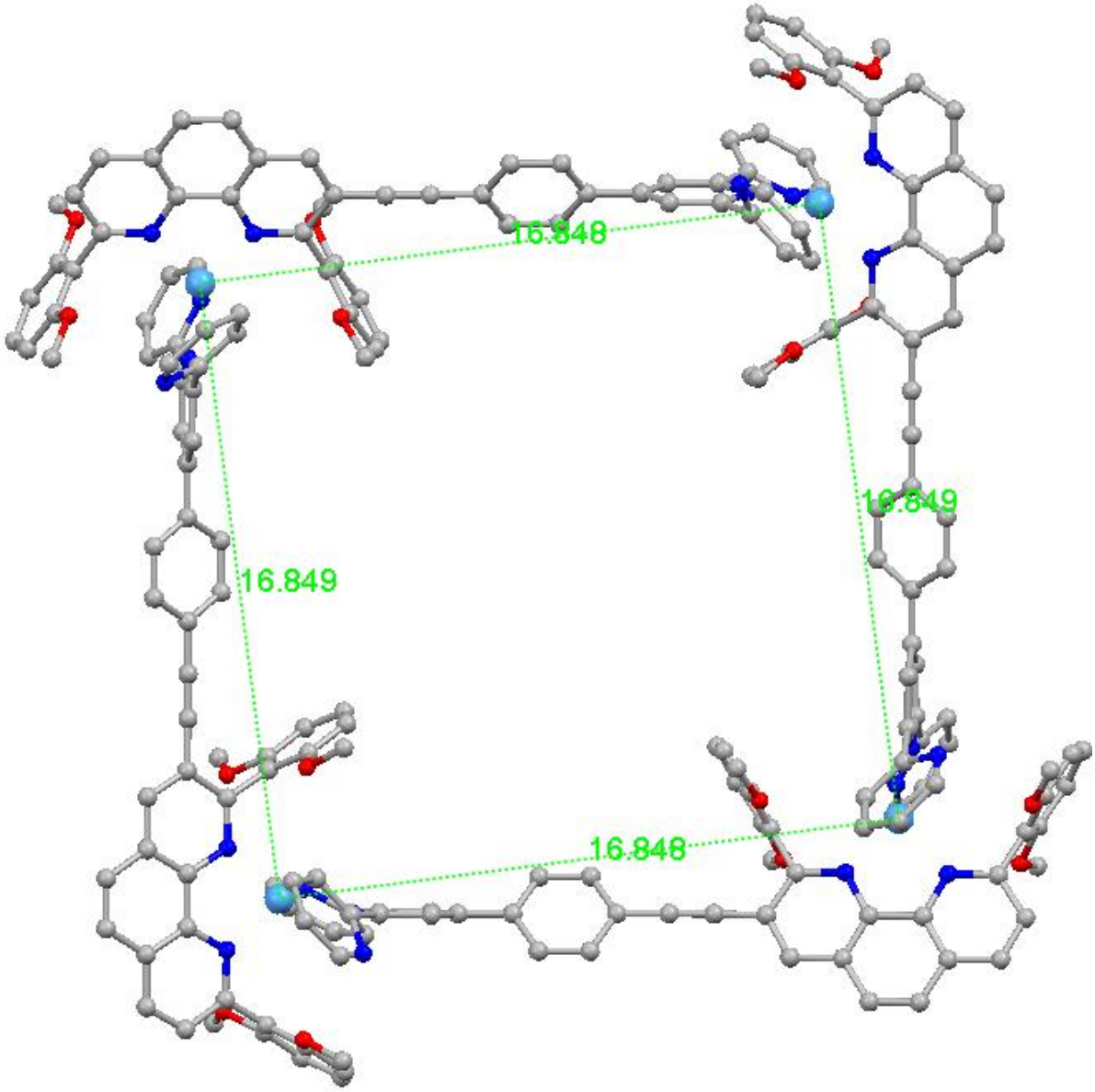


Figure S23. Energy minimised structure of the experimentally not formed square **S1**. Counter anions are not included. Hydrogens are omitted for clarity.

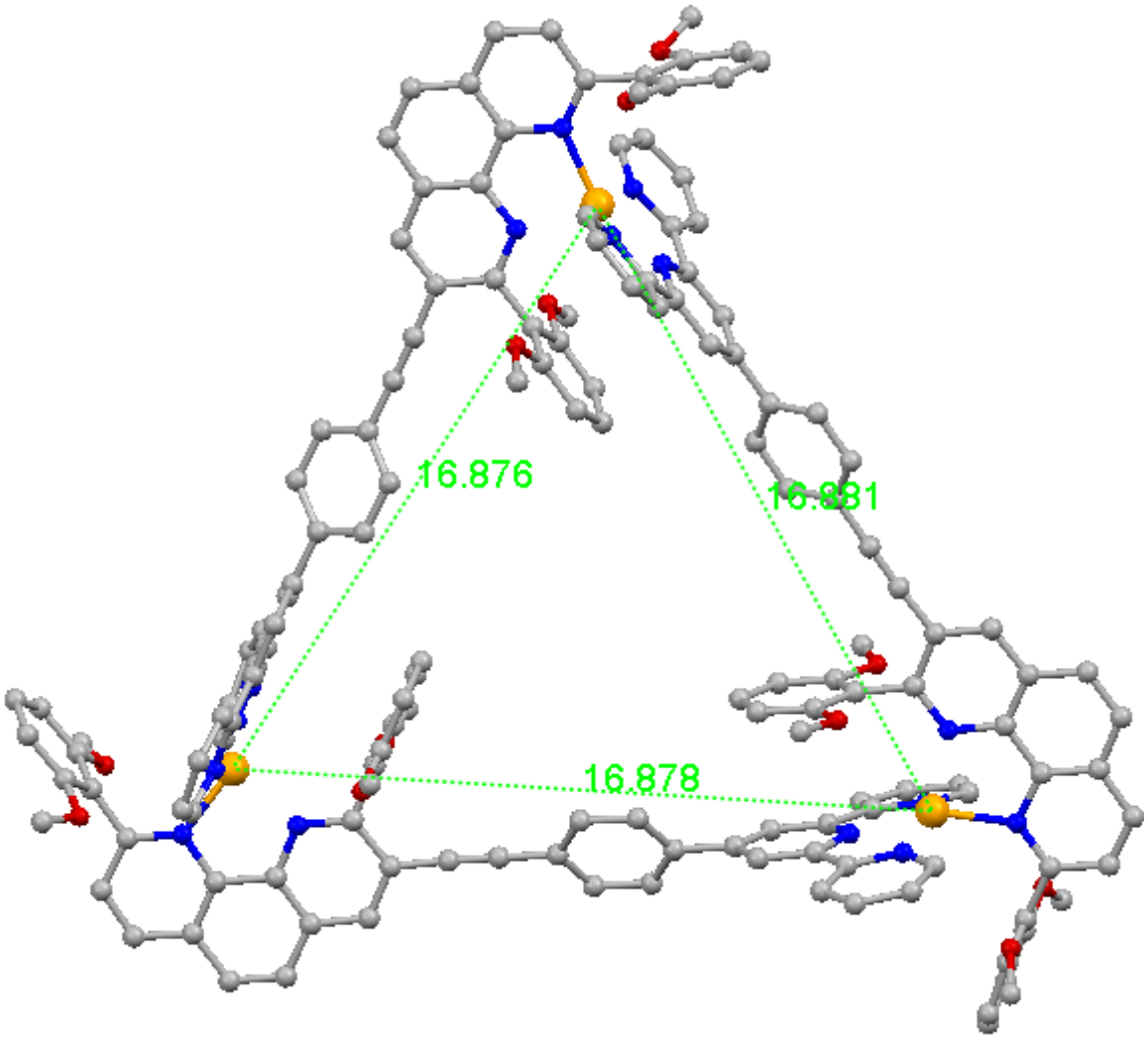


Figure S24. Energy minimised structure of equilateral triangle **T2**. Counter anions are not included. Hydrogens are omitted for clarity.

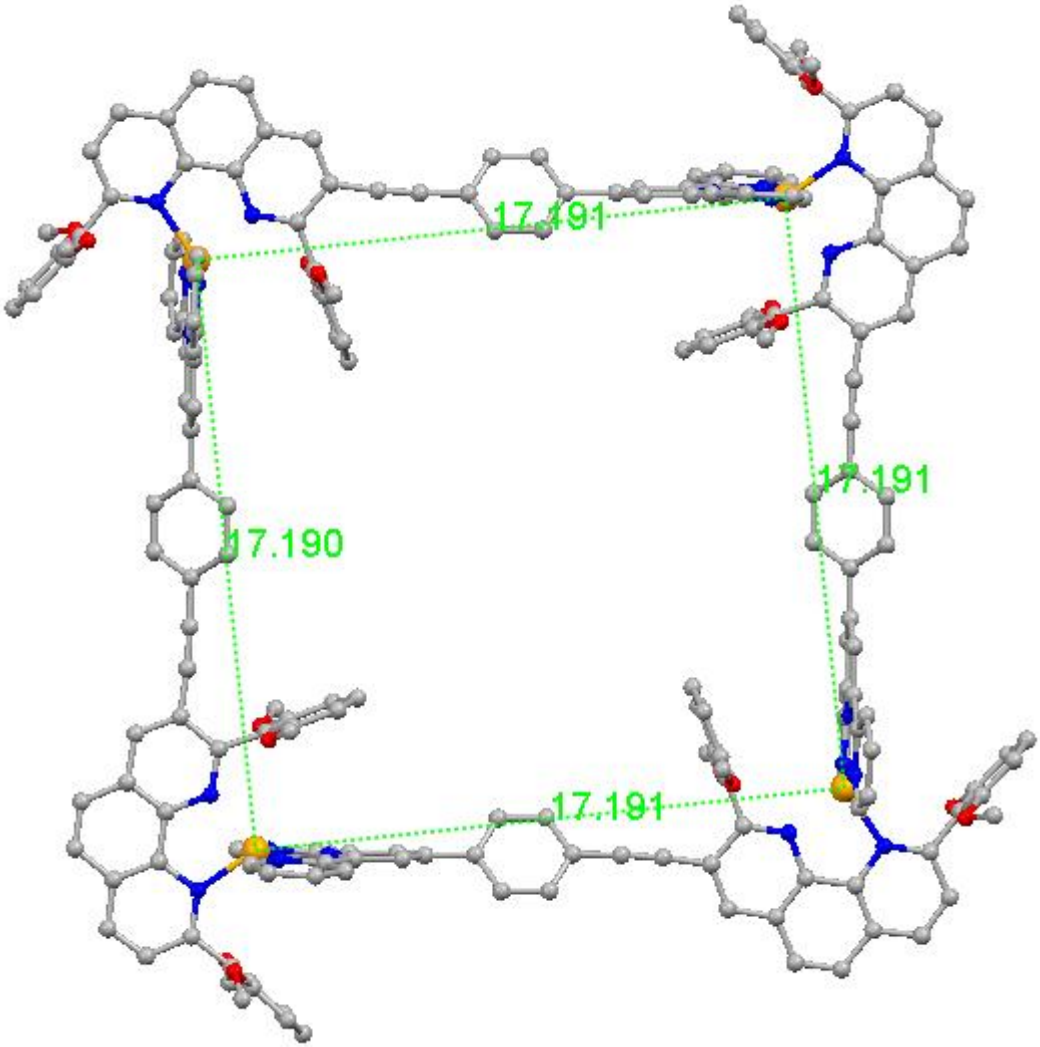


Figure S25. Energy minimised structure of square **S2**. Counter anions are not included. Hydrogens are omitted for clarity.

Table 3: PM6 Calculations of T1, S1, T2 and S2: Cartesian coordinates (x,y,z) for all structures calculated using Gaussian09.

S1				T1				S2				T2			
Charge = 4, Multiplicity = 1				Charge = 3, Multiplicity = 1				Charge = 8, Multiplicity = 1				Charge = 6, Multiplicity = 1			
E = 1.934529				E = 1.4137876				E = 3.1466125				E = 2.2412357			
C	10.613200	1.667300	-1.140500	C	-7.335200	3.600700	-0.736700	C	-8.142900	6.809200	0.719900	C	6.531100	-5.308700	-0.070300
C	8.852300	1.158600	0.463700	C	-8.312000	4.227000	-1.493200	C	-6.689300	5.389800	-0.616500	C	7.389700	-6.394200	-0.150400
C	10.259700	3.015500	-1.097400	C	-9.600000	3.639600	-1.608900	C	-7.168100	7.808000	0.717800	C	8.798000	-6.191000	-0.166900
H	11.436600	1.337600	-1.776200	C	-9.832900	2.412900	-0.945300	H	-9.091400	6.976500	1.237600	C	9.275700	-4.864100	-0.110600
C	8.507900	2.509700	0.508700	C	-7.644200	2.344000	-0.086700	C	-5.720800	6.395400	-0.623700	C	7.084200	-3.972900	-0.005100
H	8.308900	0.432500	1.068700	C	-10.657900	4.262800	-2.367600	H	-6.504300	4.449200	-1.136400	C	9.740400	-7.280500	-0.235300
C	9.204700	3.443900	-0.274800	C	-11.164100	1.809200	-1.011100	C	-5.951600	7.610500	0.043200	C	10.714000	-4.614900	-0.120600
H	10.810500	3.739500	-1.701000	C	-12.178600	2.461100	-1.748600	H	-7.366300	8.752000	1.230900	C	11.605000	-5.704500	-0.181700
H	7.690000	2.838700	1.149500	C	-11.891900	3.696800	-2.435800	H	-4.779800	6.231300	-1.148600	C	11.082200	-7.047400	-0.241300
C	8.411600	6.933700	0.951400	C	-13.473300	1.866200	-1.770800	C	-3.459200	10.189100	-1.174600	C	13.006800	-5.422700	-0.179500
C	8.760000	5.576100	0.971000	H	-14.275900	2.347400	-2.335800	C	-4.435600	9.183000	-1.189600	H	13.724400	-6.252900	-0.226300
C	8.158200	6.914800	-1.376300	C	-13.694200	0.704100	-1.073700	C	-3.450800	10.209200	1.200000	C	13.432100	-4.120200	-0.117700
C	8.827500	4.874100	-0.244000	C	-12.621700	0.098100	-0.338900	C	-4.925000	8.678500	0.030700	C	12.484800	-3.044900	-0.058500
H	8.982600	5.070900	1.910800	H	-10.437000	5.202200	-2.879000	H	-4.831500	8.802300	-2.134700	H	9.347500	-8.302600	-0.280100
C	8.530700	5.557200	-1.429500	H	-8.104100	5.173600	-1.999700	C	-4.430700	9.207000	1.238700	H	6.995100	-7.417100	-0.198600
H	8.597000	5.053100	-2.397300	H	-12.698800	4.165300	-3.004900	H	-4.811700	8.835400	2.193200	H	11.798900	-7.877500	-0.290900
N	8.094900	7.617900	-0.203600	H	-14.675700	0.224700	-1.058300	N	-2.966600	10.673500	0.007100	H	14.501300	-3.867700	-0.111800
C	7.831500	7.624600	-2.648100	N	-11.376200	0.620200	-0.314400	C	-2.851200	10.888000	2.386200	N	11.153300	-3.284100	-0.062800
C	6.603400	8.272900	-2.850300	N	-8.852100	1.756300	-0.204200	C	-3.284600	10.658800	3.693400	N	8.415500	-3.763200	-0.036000
C	8.557000	8.162200	-4.798700	C	-6.052100	4.181500	-0.612200	C	-1.277400	12.476800	3.119100	C	5.131300	-5.516300	-0.054800
C	6.374700	8.895100	-4.084900	C	-4.958500	4.693600	-0.528400	C	-2.684800	11.373300	4.745300	C	3.941700	-5.745200	-0.047700
H	5.835600	8.291100	-2.070400	C	-3.677000	5.294600	-0.452100	H	-4.086900	9.949100	3.906600	C	2.551400	-6.032400	-0.038200
C	7.356800	8.845100	-5.073800	C	-2.545600	4.595900	-0.915900	C	-1.675700	12.285600	4.459100	C	1.653500	-5.184500	0.640300
H	9.354700	8.088900	-5.550100	C	-3.530700	6.593600	0.070300	H	-0.486900	13.205300	2.873000	C	2.060300	-7.174700	-0.699800
H	5.433300	9.416400	-4.266500	C	-1.287800	5.195400	-0.866300	H	-3.019000	11.213800	5.777800	C	0.290000	-5.477100	0.654400
H	7.205900	9.323100	-6.041600	H	-2.660300	3.590000	-1.319200	H	-1.194200	12.862600	5.256900	H	2.031100	-4.304300	1.161200
C	8.344400	7.743900	2.198600	C	-2.268300	7.185500	0.125100	C	-2.873600	10.853800	-2.375600	C	0.692800	-7.458100	-0.691100
C	9.170400	7.505800	3.308100	H	-4.406900	7.137000	0.427600	C	-3.324400	10.611300	-3.674400	H	2.751900	-7.844900	-1.218100
C	9.016100	8.312100	4.441400	C	-1.142700	6.491900	-0.346200	C	-2.736300	11.312700	-4.741800	C	-0.200400	-6.611200	-0.016400
H	9.927300	6.722000	3.284700	H	-0.414700	4.656000	-1.231400	H	-4.133000	9.903200	-3.869100	H	-0.397100	-4.821300	1.188600
C	7.282100	9.529800	3.284300	H	-2.160900	8.195400	0.523000	C	-1.306600	12.431800	-3.146000	H	0.326500	-8.353100	-1.199800
C	8.058400	9.329100	4.437600	C	0.195600	7.121400	-0.304600	C	-1.721500	12.225400	-4.478800	C	-1.653600	-6.895700	-0.006800
H	9.642000	8.145000	5.321100	C	0.943300	7.282000	-1.477900	H	-3.084800	11.143100	-5.768000	C	-2.360200	-7.032100	-1.217200
H	6.521500	10.324200	3.233900	C	0.738800	7.571000	0.908800	H	-0.512200	13.162000	-2.918000	C	-2.343800	-7.014700	1.215000
H	7.913800	9.961700	5.313300	C	2.233200	7.844400	-1.412900	H	-1.248700	12.792200	-5.289000	C	-3.747600	-7.230100	-1.178200
N	8.799600	7.557300	-3.611100	H	0.531400	6.982100	-2.446800	N	-1.844200	11.795200	2.093900	H	-1.829300	-6.977300	-2.170100
N	7.408000	8.754800	2.169600	C	2.016200	8.150500	0.902300	N	-1.862200	11.763300	-2.106100	C	-3.730700	-7.215900	1.198300
C	9.907200	0.728000	-0.363500	H	0.180800	7.457600	1.837800	C	-7.912800	5.589800	0.051200	H	-1.795900	-6.962600	2.158800
C	10.259700	-0.643400	-0.423300	N	2.791600	8.263100	-0.231000	C	-8.926300	4.594200	0.041700	N	-4.413600	-7.283100	0.015200
C	10.569900	-1.811900	-0.489800	C	3.017400	8.044100	-2.666500	C	-9.824300	3.780400	0.034900	Zn	9.534100	-2.024400	-0.017500
C	10.954300	-3.168100	-0.592600	C	3.842500	9.164000	-2.860000	C	-10.946800	2.917100	0.032900	C	-4.643800	-7.435600	-2.354000
C	12.151900	-3.508300	-1.202500	C	3.502100	7.236800	-4.803700	C	-12.218200	3.471800	0.056700	C	-4.167700	-7.559200	-3.659500
C	10.107100	-4.220800	-0.074500	C	4.518700	9.297000	-4.079700	C	-10.807300	1.477100	0.009700	C	-6.859400	-7.808600	-3.058100
C	12.532000	-4.872600	-1.302000	H	3.958400	9.925000	-2.079000	C	-13.367500	2.633500	0.060500	C	-5.082300	-7.813100	-4.697800
H	12.813100	-2.734700	-1.603000	C	4.352400	8.327500	-5.068000	H	-12.352000	4.561100	0.071800	H	-3.101300	-7.483600	-3.881600
C	11.650200	-5.847400	-0.778600	H	3.335400	6.453800	-5.554300	C	-13.166100	1.236800	0.042400	C	-6.432700	-7.941300	-4.397100
C	13.778300	-5.278900	-1.905800	H	5.170700	10.156100	-4.249900	C	-14.711200	3.156200	0.082600	H	-7.925200	-7.943900	-2.797100
C	12.032500	-7.257600	-0.836000	H	4.863600	8.407900	-6.026900	C	-14.321200	0.343900	0.048200	H	-4.725300	-7.920500	-5.729400
C	14.130700	-6.591000	-1.961100	C	2.626900	8.714200	2.137600	C	-15.787900	2.322100	0.086900	H	-7.167900	-8.149900	-5.182400
H	14.429900	-4.501300	-2.310200	C	1.859600	9.269900	3.173300	H	-14.843800	4.244100	0.095300	C	-4.607900	-7.410000	2.389800
C	13.270600	-7.613300	-1.416400	C	4.624400	9.221100	3.254100	C	-15.619500	0.889900	0.069900	C	-4.109400	-7.532600	3.687300
H	15.075400	-6.904600	-2.413500	C	2.520500	9.793000	4.290600	H	-16.811000	2.720900	0.103200	C	-6.813400	-7.755100	3.134600
C	13.628600	-8.993400	-1.426200	H	0.772800	9.308400	3.106800	C	-16.726400	-0.016000	0.073700	C	-5.008100	-7.769100	4.743000
C	11.537800	-9.486100	-0.289800	C	3.915800	9.768000	4.337300	C	-15.149700	-1.875300	0.034200	H	-3.038200	-7.470300	3.889800
C	12.779000	-9.915600	-0.866600	H	5.725900	9.217900	3.237000	C	-16.491500	-1.366800	0.056000	C	-6.365400	-7.882500	4.466900
H	14.578100	-9.298700	-1.873900	H	1.946900	10.223400	5.115200	H	-17.750200	0.382500	0.090600	H	-7.884200	-7.877100	2.894100
H	13.022800	-10.980700	-0.847000	H	4.450900	10.168200	5.198200	H	-17.318400	-2.090500	0.058000	H	-4.634600	-7.873300	5.769100
N	10.432500	-5.524100	-0.183700	N	2.842500	7.088200	-3.630700	N	-11.887200	0.668500	0.017600	H	-7.089100	-8.074500	5.266900
N	11.155600	-8.189800	-0.284400	N	4.003100	8.679700	2.169500	N	-14.086800	-1.039200	0.031000	N	-5.993900	-7.546800	-2.049000
C	8.852300	-3.851500	0.607600	C	-6.606700	1.697200	0.737500	C	-9.479100	0.847400	-0.023400	N	-5.963100	-7.510400	2.108100
C	7.663200	-3.591900	-0.111600	C	-6.507400	1.945300	2.127100	C	-8.772900	0.559200	1.169600	C	6.195500	-2.806000	0.107700
C	8.807800	-3.672000	2.011200	C	-5.621700	0.860100	0.159500	C	-8.838900	0.546900	-1.250200	C	5.793800	-2.315300	1.374000
C	6.485400	-3.170400	0.523900	C	-5.495000	1.367300	2.911800	C	-7.487600	-0.004800	1.145300	C	5.663200	-2.170100	-1.039400
C	7.638600	-3.249300	2.666200	C	-4.601500	0.274800	0.928000	C	-7.554600	-0.017800	-1.290300	C	4.904200	-1.235000	1.494200
C	6.492000	-3.006400	1.910900	C	-4.555900	0.538900	2.297700	C	-6.895500	-0.280400	-0.088200	C	4.772900	-1.089000	-0.934500
H	5.581100	-2.974400	-0.040000	H	-5.433100	1.559800	3.977200	H	-6.950400	-0.213600	2.064600	C	4.401700	-0.642800	0.335300
H	7.616300	-3.116400	3.742700	H	-3.855200	-0.363300	0.470600	H	-7.069100	-0.240000	-2.235100	H	4.596600	-0.869400	2.468600
H	5.579000	-2.680300	2.414700	H	-3.765000	0.089800	2.902800	H	-5.891900	-0.713200	-0.113900	H	4.361600	-0.617300	-1.819800
C	10.662900	-10.501300	0.323800	C	-12.922900	-1.130800	0.420200	C	-14.930200	-3.326100	0.014100	H	3.702700	0.193300	0.425400
C	10.773200	-10.841900	1.692600	C	-12.936100	-2.403200	-0.198600	C	-14.920200	-4.050700	-1.204000	C	12.966600	-1.661000	0.010000
C	9.736200	-11.240200	-0.451500	C	-13.323600	-1.075400	1.776400	C	-14.879700	-4.079800	1.213200	C	13.267300	-0.924800	-1.162700
C	9.978600	-11.839800	2.275600	C	-13.310900	-3.563200	0.495200	C	-14.844300	-5.448000	-1.230700	C	13.290400	-1.056300	1.250000
C	8.924400	-12.235800	0.117500	C	-13.709300	-2.222100	2.485500	C	-14.803300	-5.477400	1.203300	C	13.831100	0.354500	-1.106700
C	9.063400	-12.526600	1.474100	C	-13.699500	-3.455700	1.831500	C	-14.800400	-6.148400	-0.022300	C	13.854800	0.221000	1.324200
H	10.079100	-12.099600	3.323700	H	-13.317000	-4.534400	0.009600	H	-14.856900	-5.997000	-2.170200	C	14.127300	0.912300	0.139900
H	8.214300	-12.791800	-0.485900	H	-14.027100	-2.163900	3.521700	H	-14.783600	-6.049100	2.129100	H	14.067000	0.910300	-2.012700
H	8.447600	-13.312800	1.919600	H	-14.005100	-4.354200	2.375400	H	-14.767500	-7.243900	-0.036000	H	14.109600	0.674100	2.280800
O	7.789700	-3.798400	-1.462800	O	-7.473400	2.791400	2.597900	O	-9.474600	0.869800	2.299600	H	14.585600	1.907200	0.190100
O	9.995600	-3.942600	2.636500	O	-13.279600	0.187900	2.312200	O	-9.599200	0.850700	-2.343800	O	6.365400	-2.984100	2.416300
O	9.742900	-10.894300	-1.772000	O	-5.778900	0.700800	-1.186600	O	-14.899500	-3.308000	2.346600	O	12.983900	-1.837200	2.339100
O	11.713100	-10.102200	2.362500	O	-12.559400	-2.374100	-1.518200	O	-14.976700	-3.251400	-2.317100	O	6.120500	-2.703700	-2.209500
C	8.861900	-11.611400	-2.680300	C	-12.698900	-3.594300	-2.296900	C	-15.268200	-3.956500	3.599300	O	12.943900	-1.584400	-2.323600
H	9.065100	-12.685000	-2.647100	H	-12.400500	-3.255300	-3.298200	H	-16.217800	-4.495600	3.488100	C	13.578500	-1.126800	-3.554500
H	7.819100	-11.368800	-2.452400	H	-12.019000	-4.363000	-1.919000	H	-14.463300	-4.616800	3.929800	H	13.328900	-1.934400	-4.254500
H	9.153800	-11.181600	-3.648700	H	-13.741400	-3.929800	-2.293900	H	-15.395400	-3.096700	4.270300	H	13.147700	-0.170500	-3.861700
C	6.677400	-3.432500	-2.321900	C	-13.960200	0.416700	3.575600	C	-8.796200	0.789200	3.583400	H	14.666400	-1.059300	-3.425100
H	7.083500	-3.660600	-3.317700	H	-13.450400	-0.114100	4.383000	H	-9.568900	1.177900	4.264100	C	13.660900	-1.532300	3.594500
H	5.806500	-4.055000	-2.099300	H	-13.863100	1.506200	3.684800	H	-8.547600	-0.249100	3.815400	H	13.247800	-0.617200	4.026100

H	6.459500	-2.364800	-2.224800	H	-15.014600	0.129300	3.499400	H	-7.915200	1.438600	3.591800
C	12.063000	-10.501100	3.714900	C	-4.814300	-0.106000	-1.912900	C	-15.390200	-3.868200	-3.571700
H	12.895300	-9.818800	3.937600	H	-4.731700	-1.104900	-1.476700	H	-15.540300	-2.991800	-4.216100
H	11.217100	-10.333700	4.386200	H	-5.291000	-0.159200	-2.907400	H	-14.598000	-4.519800	-3.947100
H	12.403100	-11.542100	3.731600	H	-3.855300	0.414300	-1.950500	H	-16.335700	-4.409900	-3.440800
C	10.120300	-3.619600	4.047600	C	-7.427400	3.184500	3.995700	C	-8.995400	0.743400	-3.662400
H	9.449500	-4.246500	4.641000	H	-8.285200	3.869500	4.057500	H	-8.773000	-0.301300	-3.892500
H	11.174700	-3.868000	4.237000	H	-7.570900	2.313000	4.640000	H	-9.800200	1.133300	-4.304200
H	9.940400	-2.552800	4.212400	H	-6.492300	3.709400	4.212100	H	-8.108300	1.380600	-3.730800
N	8.187800	11.151900	-0.286600	C	-7.959000	-1.963000	-1.395300	Zn	-12.079000	-1.392100	0.006500
N	5.521800	10.430000	-0.185100	C	-8.099700	-2.364600	0.910500	N	-1.038900	14.080800	-0.024600
C	7.255900	12.029100	-0.838200	C	-6.824000	-2.792100	-1.489300	N	0.668600	11.881100	-0.012000
C	9.484200	11.533600	-0.292300	C	-6.950500	-3.168100	0.890900	C	0.344300	14.315300	-0.023100
C	5.845400	11.647400	-0.780500	C	-6.295900	-3.379700	-0.332800	C	-1.874900	15.143800	-0.033000
C	4.218300	10.105200	-0.075500	H	-6.357900	-2.958800	-2.465100	C	1.237200	13.160100	-0.014400
C	7.611900	13.266800	-1.418900	H	-6.571000	-3.623400	1.805400	C	1.477100	10.801000	-0.006200
C	9.914100	12.774500	-0.869400	N	-8.595900	-1.724000	-0.203800	C	0.890500	15.613700	-0.029500
C	4.870900	12.529400	-1.303900	C	-5.071900	-4.207100	-0.402400	C	-1.366200	16.485600	-0.040800
C	3.165900	10.952600	-0.593800	C	-3.971600	-3.907500	0.417500	C	2.633900	13.361500	-0.009800
C	8.992100	13.624300	-1.429100	C	-5.004100	-5.289900	-1.294100	C	2.917200	10.940700	0.004200
C	6.589800	14.127200	-1.963800	C	-2.810000	-4.676100	0.342800	C	-0.015200	16.720600	-0.039000
H	10.979300	13.017900	-0.850100	H	-4.023900	-3.069200	1.112500	C	2.322900	15.782000	-0.026200
C	5.277600	13.775400	-1.908100	C	-3.847600	-6.065100	-1.368900	H	-2.089800	17.312600	-0.048000
C	3.506500	12.149800	-1.204100	H	-5.860400	-5.532200	-1.925900	C	3.156900	14.705200	-0.016400
H	9.297700	14.573600	-1.877100	C	-2.740300	-5.760200	-0.553100	C	3.472100	12.212100	0.001500
H	6.903800	15.071700	-2.416500	H	-1.954400	-4.444500	0.977700	H	0.383400	17.744400	-0.044700
H	4.500200	14.427100	-2.312600	H	-3.798000	-6.909300	-2.058600	H	2.721800	16.805200	-0.031800
H	2.733000	12.811200	-1.604600	C	-1.564300	-6.545300	-0.641700	H	4.244800	14.837800	-0.013800
C	1.809500	10.568800	-0.490600	C	-0.567200	-7.225900	-0.732500	H	4.561500	12.346000	0.006700
C	0.640900	10.259000	-0.423900	C	0.579900	-8.040700	-0.865600	C	3.780300	9.818200	0.019100
C	10.499200	10.658500	0.321400	C	0.550200	-9.148400	-1.697300	C	4.594000	8.920100	0.034200
C	10.839900	10.768900	1.690100	C	1.797200	-7.734100	-0.143000	C	-3.325800	14.924200	-0.033500
C	11.237700	9.731500	-0.453800	C	1.700800	-9.971800	-1.818000	C	-4.063700	14.886600	-1.242900
C	11.837600	9.974000	2.273200	H	-0.353900	-9.401100	-2.257700	C	-4.066200	14.901400	1.174800
C	12.233100	8.919400	0.115100	C	2.854400	-9.613500	-1.083000	C	-5.461400	14.810200	-1.252200
C	12.524100	9.058500	1.471800	C	1.710900	-11.150700	-2.650600	C	-5.463800	14.825300	1.182300
H	12.097500	10.074500	3.321200	C	4.040100	-10.467600	-1.159400	C	-6.148300	14.794300	-0.035500
H	12.788900	8.209100	-0.488200	C	2.814100	-11.941300	-2.724200	H	-6.020800	14.800400	-2.185600
C	3.848600	8.850700	0.607000	H	0.805400	-11.389000	-3.212700	H	-6.025000	14.827900	2.114600
C	3.669300	8.806700	2.010600	C	4.003300	-11.624000	-1.971600	C	0.847100	9.472600	-0.012100
C	3.588500	7.661400	-0.111800	H	2.827000	-12.838700	-3.347700	C	0.545800	8.808600	-1.226000
C	3.246100	7.637900	2.666100	C	5.162100	-12.452800	-2.004400	C	0.559600	8.789800	1.194600
C	3.166500	6.484100	0.524200	C	6.228000	-10.924300	-0.445900	C	-0.018600	7.523700	-1.241100
C	3.002600	6.491200	1.911200	C	6.257900	-12.111300	-1.250800	C	-0.004800	7.504400	1.195300
C	-3.446800	9.205600	-0.274500	H	5.160900	-13.353600	-2.623600	C	-0.280800	6.888200	-0.025900
C	-2.512700	8.508500	0.508800	H	7.160500	-12.726400	-1.243100	C	7.611200	5.946400	0.050000
C	-3.018100	10.260400	-1.097100	N	2.909000	-8.487400	-0.263200	C	6.396100	5.712300	-0.615800
C	-1.161400	8.852300	0.463600	N	5.154100	-10.106300	-0.403000	C	7.807500	7.164800	0.721200
H	-2.841800	7.690700	1.149700	C	-8.893000	-2.156400	2.152900	C	5.389900	6.680200	-0.612300
C	-1.669800	10.613400	-1.140600	C	-9.001500	-3.135600	3.152600	H	6.232500	4.769300	-1.137400
H	-3.742000	10.811500	-1.700700	C	-10.323900	-0.711000	3.317900	C	6.808100	8.139200	0.719700
C	-0.730600	9.907000	-0.363800	C	-9.788800	-2.861000	4.276600	H	8.751000	7.365100	1.234300
H	-0.435400	8.308700	1.068400	H	-8.497500	-4.096700	3.052000	C	5.589400	7.906400	0.050700
H	-1.339900	11.436700	-1.776400	C	-10.456500	-1.637700	4.365400	H	4.449500	6.492800	-1.131500
C	-4.877100	8.829000	-0.243300	H	-10.861200	0.250200	3.335900	H	6.974500	9.089400	1.234600
C	-5.578800	8.761600	0.971800	H	-9.884000	-3.602500	5.073700	C	8.680700	4.921300	0.037800
C	-5.560600	8.532700	-1.428700	H	-11.075000	-1.403200	5.231600	C	9.183700	4.431900	-1.183000
C	-6.936500	8.413800	0.952500	C	-8.531600	-1.349500	-2.628800	C	9.211900	4.428500	1.245200
H	-5.073200	8.983900	1.911600	C	-9.917400	-1.241000	-2.829200	C	10.191200	3.456900	-1.169200
C	-6.918300	8.160700	-1.375200	C	-8.087900	-0.409100	-4.719100	H	8.800900	4.826700	-2.127700
H	-5.056800	8.598900	-2.396700	C	-10.379900	-0.686600	-4.029500	C	10.215200	3.449700	1.205300
C	-7.746500	8.346900	2.199900	H	-10.626700	-1.581300	-2.065200	H	8.841500	4.809800	2.200200
C	-7.507800	9.172900	3.309300	C	-9.461900	-0.262500	-4.989800	C	10.854300	2.871700	-2.371300
C	-8.313900	9.019000	4.442800	H	-7.329500	-0.093400	-5.446900	C	10.610400	3.323400	-3.669600
H	-6.723800	9.929500	3.285600	H	-11.452800	-0.589800	-4.207100	C	11.310100	2.735500	-4.738100
C	-9.532500	7.285300	3.286100	H	-9.794100	0.170300	-5.933000	H	9.902200	4.132100	-3.863100
C	-9.331300	8.061600	4.439300	N	-7.620700	-0.943600	-3.566000	C	12.430600	1.304600	-3.144300
H	-8.146500	9.644800	5.322400	N	-9.541400	-0.943600	2.227100	C	12.222900	1.720100	-4.476600
H	-10.327300	6.525000	3.235900	C	1.807300	-6.568800	0.760600	H	11.139100	3.084100	-5.764000
H	-9.963700	7.917200	5.315200	C	1.480900	-6.697000	2.131800	H	13.160500	0.509600	-2.917600
C	-7.628700	7.834600	-2.646800	C	2.064400	-5.262800	0.278000	H	12.788000	1.247100	-5.287900
C	-8.277200	6.606700	-2.849300	C	1.431400	-5.583700	2.987800	C	10.896900	2.851200	2.390400
C	-8.166800	8.561000	-4.797000	C	2.013300	-4.138000	1.117500	C	10.668500	3.283600	3.698100
C	-8.899800	6.378600	-4.083800	C	1.701700	-4.318700	2.466000	C	12.490700	1.280800	3.120700
H	-8.295300	5.838600	-2.069700	H	1.188900	-5.695600	4.038900	C	11.386100	2.685200	4.748800
C	-8.850000	7.361000	-5.072400	H	2.213600	-3.144700	0.734400	H	9.957500	4.084400	3.912600
H	-8.093600	9.358900	-5.548100	H	1.666700	-3.449800	3.127600	C	12.300300	1.678400	4.461100
H	-9.421300	5.437300	-4.265600	C	7.423700	-10.616400	0.361700	H	13.220900	0.492200	2.873200
H	-9.328400	7.210600	-6.040100	C	8.543300	-9.952600	-0.193300	H	11.227700	3.019200	5.781600
N	-8.757700	7.410900	2.171300	C	7.546600	-11.071700	1.695900	H	12.880100	1.198400	5.257800
N	-7.621200	8.097500	-0.202300	C	9.718000	-9.735300	0.541900	N	11.763700	1.859900	-2.103300
N	-7.561500	8.803000	-3.609500	C	8.715300	-10.871800	2.445100	N	10.678100	2.965500	0.011800
H	2.970000	5.579700	-0.039300	C	9.790400	-10.205300	1.854200	N	11.806200	1.846400	2.096700
H	2.676200	5.578500	2.415300	H	10.570900	-9.224800	0.105200	H	-0.215100	6.985400	2.125100
H	3.113400	7.616100	3.742600	H	8.801800	-11.238200	3.463100	H	-0.713400	5.884200	-0.031200
H	13.310100	8.442600	1.917200	H	10.708100	-10.051400	2.429200	H	-0.239400	7.019600	-2.176100
O	3.794900	7.787400	-1.463100	O	1.217100	-7.984700	2.508600	H	-7.243900	14.761300	-0.036500
O	3.940700	9.994600	2.635600	O	6.421300	-11.699800	2.168100	O	0.871200	9.512700	2.310800
O	10.891700	9.738100	-1.774300	O	2.361900	-5.235200	-1.054000	O	0.848500	9.548100	-2.334200
O	10.100600	11.709100	2.360000	O	8.358800	-9.564900	-1.497000	O	-3.281700	14.946200	2.298800
C	10.499600	12.059000	3.712300	C	9.498700	-9.021200	-2.217900	O	-3.277000	14.918000	-2.365800
H	9.817700	12.891600	3.934900	H	9.079300	-8.877600	-3.222800	C	-3.908700	15.300900	-3.622800
H	10.332000	11.213300	4.383700	H	9.805300	-8.069200	-1.775900	H	-3.039900	15.435900	-4.280700
H	11.540800	12.398800	3.728900	H	10.317500	-9.748200	-2.237900	H	-4.564200	14.499700	-3.971400
C	11.608400	8.856700	-2.682600	C	6.532600	-12.467300	3.397100	H	-4.449600	16.249100	-3.508200
H	11.178500	9.148400	-3.650900	H	6.711500	-11.802200	4.245100	C	-3.915200	15.345800	3.549600
H	12.682100	9.059700	-2.649600	H	5.540100	-12.936100	3.455200	H	-3.047500	15.488300	4.207300
H	11.365600	7.814000	-2.454300	H	7.314100	-13.229100	3.302700	H	-4.454900	16.292900	3.421900
C	3.428200	6.675100	-2.321800	C	2.539900	-3.952600	-1.707900	H	-4.572100	14.549700	3.907200
H	2.360500	6.457800	-2.224400	H	3.311900	-3.352500	-1.207700	C	0.789600	8.858900	3.607500
H	3.656500	7.080600	-3.317600	H	2.887900	-4.274900	-2.705800	H	1.438300	7.977700	3.632800
H	4.050200	5.803800	-2.098900	H	1.580400	-3.433500	-1.762400	H	1.178600	9.644000	4.273400
C	3.617500	10.120000	4.046500	C	0.789500	-8.232600	3.874800	H	-0.249000	8.615300	3.843500

H	13.427600	-2.416700	4.201400
H	14.744800	-1.454400	3.439800
C	5.541000	-2.244200	-3.461100
H	5.809600	-1.200600	-3.640000
H	6.031800	-2.912700	-4.186000
H	4.458600	-2.403800	-3.464600
C	5.939400	-2.666400	3.770100
H	6.496300	-3.416000	4.354400
H	6.245400	-1.650800	4.032700
H	4.861700	-2.819200	3.880100
Zn	-6.520300	-7.240900	0.025300
C	-4.397900	6.850400	-1.203200
C	-4.383600	6.850600	1.173300
C	-4.921700	5.550600	-1.227800
C	-4.908500	5.551100	1.204400
C	-5.155600	4.882400	-0.010200
H	-5.160200	5.060100	-2.174400
H	-5.119700	5.055800	2.154600
N	-4.103600	7.463800	-0.016700
C	-5.639100	3.482900	-0.007700
C	-6.800500	3.125900	0.695700
C	-4.923400	2.498200	-0.711100
C	-7.238800	1.800000	0.703400
H	-7.378100	3.885500	1.228100
C	-5.351500	1.171100	-0.698200
H	-4.028400	2.770700	-1.270000
C	-6.514000	0.810100	0.011700
H	-8.150400	1.531000	1.244500
H	-4.794100	0.409600	-1.244200
C	-6.958400	-0.538100	0.023700
C	-7.352900	-1.683500	0.034700
C	-7.870600	-3.000400	0.056000
C	-9.239600	-3.203200	0.137300
C	-6.988300	-4.146100	-0.003500
C	-9.765500	-4.525300	0.161000
H	-9.929700	-2.351000	0.180800
C	-8.853300	-5.601100	0.110700
C	-11.179700	-4.798800	0.231300
C	-9.354100	-6.972100	0.129000
C	-11.646400	-6.078200	0.245000
H	-11.870000	-3.948500	0.271100
C	-10.742800	-7.201200	0.191900
H	-12.723300	-6.285500	0.296000
C	-11.197200	-8.556900	0.198200
C	-8.875500	-9.290100	0.080800
C	-10.279900	-9.575000	0.142300
H	-12.274500	-8.764900	0.246500
H	-10.593900	-10.627900	0.143000
N	-8.419300	-8.016600	0.077100
N	-7.470200	-5.404500	0.034300
C	-4.133200	7.717300	-2.388700
C	-4.496700	7.358900	-3.687200
C	-3.331100	9.805700	-3.120000
C	-4.257500	8.264500	-4.736500
H	-4.981400	6.402700	-3.895200
C	-3.674000	9.493400	-4.453100
H	-2.899900	10.792300	-2.873300
H	-4.541600	8.002600	-5.763100
H	-3.482800	10.223200	-5.247800
C	-4.104000	7.718300	2.355100
C	-4.440300	7.356200	3.659800
C	-3.312900	9.816500	3.072400
C	-4.194900	8.265700	4.704500
H	-4.906900	6.393200	3.876700
C	-3.632100	9.501700	4.410900
H	-2.898000	10.808500	2.817300
H	-4.458600	8.001100	5.735800
H	-3.438800	10.235300	5.201500
N	-3.539000	8.938100	-2.100000
N	-3.526400	8.945100	2.057000
C	-5.533700	-3.958400	-0.118000
C	-4.716300	-3.808100	1.027800
C	-4.908600	-3.862700	-1.385200
C	-3.335200	-3.577600	0.920700
C	-3.528500	-3.632500	-1.507600
C	-2.763800	-3.486300	-0.349900
H	-2.720500	-3.451600	1.805000
H	-3.058700	-3.554300	-2.482700
H	-1.690400	-3.299100	-0.441500
C	-7.916000	-10.397900	0.018600
C	-7.553800	-10.987700	-1.217900
C	-7.426900	-11.018300	1.194900
C	-6.727900	-12.114200	-1.285500
C	-6.599000	-12.145000	1.145600
C	-6.263700	-12.687600	-0.098000
H	-6.462600	-12.566800	-2.239500
H	-6.234200	-12.621000	2.054300
H	-5.629700	-13.581100	-0.143000
O	-7.836900	-10.401900	2.352300
O	-5.406400	-3.930800	2.199000
O	-8.078600	-10.339700	-2.310700
O	-5.774200	-4.029700	-2.426100
C	-5.286900	-3.827700	-3.781500
H	-4.560500	-4.602100	-4.039900
H	-6.214900	-3.938700	-4.364600
H	-4.880500	-2.818700	-3.897800
C	-8.152200	-11.086200	-3.561600
H	-8.802800	-10.446800	-4.172200
H	-7.153100	-11.186700	-3.993000
H	-8.624700	-12.063700	-3.400800
C	-7.756200	-11.172600	3.587900
H	-6.712300	-11.274200	3.895300
H	-8.331400	-10.549200	4.284300

H	3.866300	11.174300	4.235500	H	0.631200	-9.320700	3.859000	C	0.741300	8.919500	-3.640900	H	-8.240200	-12.149900	3.464700
H	2.550500	9.940700	4.211200	H	1.582100	-7.959100	4.576400	H	1.130000	9.712600	-4.297900	C	-4.718000	-3.651400	3.448600
H	4.243900	9.449200	4.640400	H	-0.146400	-7.705400	4.081500	H	1.379400	8.032100	-3.692800	H	-5.541700	-3.738100	4.174500
H	-8.982600	-5.070900	1.910800	C	5.706800	-5.863000	-1.305400	H	-0.303300	8.692100	-3.866500	H	-3.948300	-4.404800	3.631300
C	-8.760000	-5.576100	0.971000	C	6.155600	-5.878700	0.996300	Zn	-1.392100	12.073000	-0.011100	H	-4.314900	-2.634300	3.445900
C	-8.411600	-6.933700	0.951400	C	5.879900	-4.466200	-1.348900	H	4.812400	-8.835800	-2.192800	Zn	-3.011300	9.265700	-0.021100
C	-8.827500	-4.874100	-0.244000	C	6.313600	-4.485100	1.026000	C	4.431400	-9.207500	-1.238300	C	8.127700	0.382200	-1.195300
C	-8.530700	-5.557200	-1.429500	C	6.160600	-3.766100	-0.168800	C	3.451400	-10.209600	-1.199700	C	8.134300	0.371400	1.181300
C	-8.158200	-6.914800	-1.376300	H	5.794200	-3.939500	-2.304200	C	4.925700	-8.679100	-0.030300	C	7.260600	1.483000	-1.215500
H	-8.597000	-5.053100	-2.397300	H	6.534600	-3.966100	1.958300	C	4.436200	-9.183500	1.190000	C	7.269500	1.474200	1.216800
C	-9.204700	-3.443900	-0.274800	N	5.818700	-6.579700	-0.140700	C	3.459800	-10.189600	1.174900	C	6.805100	2.019500	0.004500
C	-8.507900	-2.509700	0.508700	C	6.281100	-2.291700	-0.190900	H	4.832100	-8.803000	2.135100	H	6.947200	1.933000	-2.160500
C	-10.259700	-3.015500	-1.097400	C	7.477600	-1.665900	0.189300	C	5.952300	-7.611100	-0.042800	H	6.951200	1.905500	2.168500
C	-8.852300	-1.158600	0.463700	C	5.187000	-1.517100	-0.609900	C	5.721300	-6.395800	0.623700	N	8.519900	-0.177500	-0.010600
H	-7.690000	-2.838700	1.149500	C	7.587200	-0.275700	0.135300	C	7.169000	-7.808900	-0.716800	C	5.831100	3.134900	0.008500
C	-10.613200	-1.667300	-1.140500	H	8.329100	-2.264900	0.514200	C	6.689700	-5.390200	0.616500	C	4.607200	2.989300	-0.667900
H	-10.810500	-3.739500	-1.701000	C	5.287500	-0.127900	-0.657600	H	4.780100	-6.231500	1.148300	C	6.113300	4.333900	0.681500
H	-8.308900	-0.432500	1.068700	H	4.255000	-2.013000	-0.900200	C	8.143900	-6.810100	-0.718900	C	3.671700	4.023300	-0.662400
H	-11.436600	-1.337600	-1.776200	C	6.494300	0.501400	-0.293400	H	7.367300	-8.753000	-1.229500	H	4.386200	2.064200	-1.199900
N	-8.094900	-7.617900	-0.203600	H	8.521200	0.211400	0.420300	H	6.504500	-4.449400	1.136000	C	5.183700	5.376300	0.681300
C	-8.344400	-7.743900	2.198600	H	4.440600	0.476200	-0.982100	H	9.092600	-6.977500	-1.236200	H	7.068500	4.466100	1.195600
C	-9.170400	-7.505800	3.308100	C	6.613600	1.911100	-0.378200	N	2.967200	-10.673900	-0.006800	C	3.953300	5.227900	0.012400
C	-9.016100	-8.312100	4.441400	C	6.725000	3.112900	-0.471100	C	2.851600	-10.888200	-2.385900	H	2.723400	3.907800	-1.187700
H	-9.927300	-6.722000	3.284700	C	6.876700	4.512300	-0.603700	C	3.285400	-10.659300	-3.693100	H	5.414900	6.312200	1.197700
C	-7.282100	-9.529800	3.284300	C	7.992000	5.034900	-1.238000	C	2.685300	-11.373500	-4.745000	C	3.010000	6.289100	0.006300
C	-8.058400	-9.329100	4.437600	C	5.869200	5.417400	-0.092600	H	4.088200	-9.950100	-3.906200	C	2.216700	7.204600	-0.005600
H	-9.642000	-8.145000	5.321100	C	8.139500	6.442000	-1.362300	C	1.276900	-12.476000	-3.119000	C	1.336300	8.312400	-0.022900
H	-6.521500	-10.324200	3.233900	H	8.764000	4.374800	-1.642900	C	1.675600	-12.285100	-4.458900	C	1.847000	9.600600	-0.060300
H	-7.913800	-9.961700	5.313300	C	7.126000	7.266900	-0.821500	H	3.019800	-11.214300	-5.777500	C	-0.098100	8.120600	-0.003100
C	-7.831500	-7.624600	-2.648100	C	9.283200	7.035800	-2.012300	H	0.485800	-13.203900	-2.872900	C	0.965800	10.717900	-0.077000
C	-6.603400	-8.272900	-2.850300	C	7.278400	8.720500	-0.888700	H	1.193800	-12.861900	-5.256800	H	2.930800	9.772400	-0.077500
C	-8.557000	-8.162200	-4.798700	C	9.413900	8.386400	-2.093700	C	2.874000	-10.854200	2.375900	C	-0.422700	10.465700	-0.057500
C	-6.374700	-8.895100	-4.084900	H	10.037700	6.367800	-2.433400	C	3.324900	-10.612100	3.674700	C	1.437700	12.080100	-0.110800
H	-5.835600	-8.291100	-2.070400	C	8.420100	9.262300	-1.522000	C	1.306500	-12.431800	3.146200	C	-1.358800	11.585800	-0.066600
C	-7.356800	-8.845100	-5.073800	H	10.276700	8.842900	-2.585100	C	2.736800	-11.313400	4.742000	C	0.563800	13.124700	-0.119500
H	-9.354700	-8.088900	-5.550100	C	8.554600	10.680600	-1.554200	H	4.133900	-9.904400	3.869400	H	2.519800	12.252800	-0.128700
H	-5.433300	-9.416400	-4.266500	C	6.473800	10.847300	-0.311400	C	1.721500	-12.225700	4.479000	C	-0.861300	12.903600	-0.095500
H	-7.205900	-9.323100	-6.041600	C	7.598200	11.462700	-0.955100	H	0.511800	-13.161700	2.918200	H	0.923900	14.161500	-0.144500
N	-7.408000	-8.754800	2.169600	H	9.422000	11.127000	-2.047500	H	3.085400	-11.144100	5.768200	C	-1.807600	13.975500	-0.098200
N	-8.799600	-7.557300	-3.611100	H	7.673000	12.552500	-0.948900	H	1.248600	-12.792500	5.289200	C	-3.605700	12.330900	-0.042700
C	-9.907200	-0.728000	-0.363500	N	6.294500	9.508500	-0.292000	N	1.844000	-11.794700	-2.093800	C	-3.148800	13.690200	-0.071400
C	-10.259700	0.643400	-0.423300	N	5.985100	6.756200	-0.206400	N	1.862200	-11.763400	2.106400	H	-1.447900	15.013100	-0.120900
C	-10.569900	1.811900	-0.489800	C	5.436500	-6.613600	-2.565900	C	7.913500	-5.590400	-0.050700	H	-3.903300	14.488900	-0.071200
C	-10.954300	3.168100	-0.592600	C	6.027500	-7.860700	-2.826400	C	8.927000	-4.594800	-0.041200	N	-0.945900	9.168500	-0.024000
C	-12.151900	3.508300	-1.202500	C	4.369200	-6.609600	-4.641900	C	9.824900	-3.780800	-0.034500	N	-2.731400	11.298600	-0.042200
C	-10.107100	4.220800	-0.074500	C	5.758900	-8.487200	-4.050000	C	10.947200	-2.917500	-0.032400	C	8.753100	-0.304300	2.359700
C	-12.532000	4.872600	-1.302000	H	6.685300	-8.337000	-2.089600	C	12.218700	-3.471900	-0.056100	C	8.615300	0.168300	3.665100
H	-12.813100	2.734700	-1.603000	C	4.920700	-7.862100	-4.972900	C	10.807500	-1.477400	-0.009500	C	10.178000	-2.039200	3.069500
C	-11.650200	5.847400	-0.778600	H	3.708100	-6.078900	-5.338700	C	13.367900	-2.633400	-0.059900	C	9.286000	-0.498900	4.706200
C	-13.778300	5.278900	-1.905800	H	6.206100	-9.457200	-4.275500	H	12.352700	-4.561200	-0.071000	H	8.016500	1.054400	3.885000
C	-12.032500	7.257600	-0.836000	H	4.697400	-8.325500	-5.933300	C	13.166300	-1.236800	-0.042000	C	10.072600	-1.604900	4.408500
C	-14.130700	6.591000	-1.961100	C	6.355100	-6.719400	2.208400	C	14.711700	-3.155900	-0.081700	H	10.828500	-2.894900	2.811000
H	-14.429900	4.501300	-2.310200	C	7.277100	-6.389500	3.213900	C	14.321200	-0.343600	-0.048000	H	9.195200	-0.137400	5.737800
C	-13.270600	7.613300	-1.416400	C	5.755800	-8.698200	3.312800	C	15.788200	-2.321600	-0.086000	H	10.615900	-2.138900	5.196100
H	-15.075400	6.904600	-2.413500	C	7.410700	-7.250300	4.309200	H	14.844400	-4.243800	-0.094100	C	8.740800	-0.279200	-2.384200
C	-13.628600	8.993400	-1.426200	H	7.887800	-5.490100	3.140100	C	15.619600	-0.889400	-0.069400	C	8.606200	0.216200	-3.681700
C	-11.537800	9.486100	-0.289800	C	6.643300	-8.415800	4.364400	H	16.811400	-2.720200	-0.102200	C	10.144600	-2.017300	-3.123400
C	-12.779000	9.915600	-0.866600	H	5.157300	-9.622200	3.305600	C	16.726400	0.016700	-0.073500	C	9.265900	-0.443100	-4.734500
H	-14.578100	9.298700	-1.873900	H	8.115000	-7.013100	5.110500	C	15.149400	1.875700	-0.034600	H	8.019100	1.113900	-3.886300
H	-13.022800	10.980700	-0.847000	H	6.731000	-9.100100	5.208300	C	16.491200	1.367500	-0.056200	C	10.039600	-1.563300	-4.455500
N	-11.155600	8.189800	-0.284400	N	4.618000	-5.986400	-3.465500	H	17.750200	-0.381600	-0.090200	H	10.783100	-2.884900	-2.880400
N	-10.432500	5.524100	-0.183700	N	5.588000	-7.862600	2.249600	H	17.318000	2.091300	-0.058400	H	9.176100	-0.065700	-5.760600
C	-10.662900	10.501300	0.323800	C	4.673900	4.861800	0.567200	N	14.086500	1.039400	-0.031100	H	10.571800	-2.093500	-5.253300
C	-10.773200	10.841900	1.692600	C	4.599600	4.702200	1.970600	N	11.887300	-0.668700	-0.017400	N	9.502200	-1.404100	-2.099700
C	-9.736200	11.240200	-0.451500	C	3.566700	4.413900	-0.194100	C	14.929600	3.326400	-0.014900	N	9.524800	-1.418400	2.057600
C	-9.978600	11.839800	2.275600	C	3.458500	4.168700	2.594200	C	14.879700	4.079800	-1.214200	C	-0.664700	6.764000	0.049100
C	-8.924400	12.235800	0.117500	C	2.415900	3.884200	0.412100	C	14.918600	4.051400	1.203000	C	-0.890200	6.114300	1.286900
C	-9.063400	12.526600	1.474100	C	2.380000	3.773100	1.803200	C	14.803100	5.477500	-1.204800	C	-0.948000	6.037500	-1.132400
H	-10.079100	12.099600	3.323700	H	3.408600	4.059400	3.671800	C	14.842500	5.448700	1.229300	C	-1.380300	4.799300	1.347300
H	-8.214300	12.791800	-0.485900	H	1.569600	3.559900	-0.180600	C	14.799200	6.148800	0.020700	C	-1.438200	4.722500	-1.087500
H	-8.447600	13.312800	1.919600	H	1.488400	3.362600	2.283200	H	14.783900	6.048900	-2.130800	C	-1.639300	4.120800	0.156600
C	-8.852300	3.851500	0.607600	C	5.509400	11.733200	0.368700	H	14.854300	5.997900	2.168600	H	-1.541900	4.305900	2.300400
C	-7.663200	3.591900	-0.111600	C	4.454700	12.369900	-0.326300	H	14.766200	7.244300	0.034100	H	-1.642600	4.171400	-1.998500
C	-8.807800	3.672000	2.011200	C	5.675000	12.076300	1.732100	C	9.479200	-0.848000	0.023400	H	-2.011800	3.093700	0.199900
C	-6.485400	3.170400	0.523900	C	3.596400	13.284600	0.302200	C	8.838800	-0.547600	1.250100	C	-5.045800	12.053500	-0.012100
C	-7.638600	3.249300	2.666200	C	4.832500	12.992800	2.376900	C	8.773100	-0.559900	-1.169700	C	-5.806400	11.971700	-1.204900
C	-6.492000	3.006400	1.910900	C	3.800500	13.588500	1.648900	C	7.554300	0.016800	1.290000	C	-5.759700	12.002700	1.210900
H	-5.581100	2.974400	-0.040000	H	2.789700	13.766800	-0.241900	C	7.487800	0.003800	-1.145600	C	-7.196600	11.817600	-1.184900
H	-7.616300	3.116400	3.742700	H	4.977300	13.254600	3.420200	C	6.895300	0.279400	0.087800	C	-7.149300	11.849300	1.249100
H	-5.579000	2.680300	2.414700	H	3.142200	14.309400	2.142300	H	7.068700	0.239000	2.234800	C	-7.856400	11.765800	0.046100
O	-7.789700	3.798400	-1.462800	O	6.715900	11.419500	2.342100	H	6.950600	0.212600	-2.065000	H	-7.774700	11.764200	-2.106000
O	-9.995600	3.942600	2.636500	O	5.730600	5.106500	2.624900	H	5.891600	0.712000	0.113300	H	-7.691100	11.820800	2.193000
O	-9.742900	10.894300	-1.772000	O	4.371400	12.009000	-1.648000	O	9.598900	-0.851200	2.343900	H	-8.947900	11.662800	0.068700
O	-11.713100	10.102200	2.362500	O	3.759500	4.539000	-1.539500	O	9.475000	-0.870400	-2.299600	O	-0.602400	6.897600	2.366100
C	-8.861900	11.611400	-2.680300	C	2.680800	4.163800	-2.436700	O	14.974400	3.252400	2.316300	O	-4.956100	12.105800	2.321300
H	-7.819100	11.368800	-2.452400	H	1.816100	4.815200	-2.274800	O	14.900400	3.307700	-2.347400	O	-0.709400	6.751400	-2.271100
H	-9.153800	11.181600	-3.648700	H	3.133200	4.382200	-3.416600	C	15.387100	3.869600	3.571100	O	-5.046600	12.047400	-2.347300
H	-9.065100	12.685000	-2.647100	H	2.445800	3.103900	-2.328700	H	14.594600	4.521300	3.945700	C	-5.730500	12.403100	-3.585500
C	-12.063000	10.501100	3.714900	C	3.440900	12.735800	-2.497400	H	15.537000	2.993400	4.215700	H	-4.889800	12.610500	-4.259900
H	-12.895300	9.818800	3.937600	H	3.644200	12.292800	-3.481600	H	16.332600	4.411400	3.440500	H	-6.335300	11.560900	-3.931000
H	-11.217100	10.333700	4.386200	H	2.411800	12.543700	-2.181000	C	15.269700	3.955900	-3.600100	H	-6.336300	13.307500	-3.445300
H	-12.403100	11.542100	3.731600	H	3.679400	13.804600	-2.494500	H	15.397500	3.095900	-4.270700	C	-5.589900	12.505300	3.572600
C	-10.120300	3.619600	4.047600	C	7.183300	11.925300	3.621800	H	14.464800	4.615900	-3.931300	H	-6.182800	11.677300	3.969300
H	-9.449500	4.246500	4.641000	H	6.426100	11.764000	4.392600	H	16.219100	4.495300	-3.488500	H	-4.723000	12.732200	4.206400
H	-11.174700	3.868000	4.237000	H	8.073600	11.304100	3.793700	C	8.796800	-0.789900	-3.583500	H	-6.198700	13.406800	3.426500
H	-9.940400	2.552800	4.212400	H	7.461000	12.981600	3.536900	H	8.548000	0.248400	-3.815400	C	-0.834400	6.082800	-3.555800
C	-6.677400	3.432500	-2.321900	C	5.802400	4.915800	4.063100	H	9.569700	-1.178300	-4.264200	H	-1.877800	5.818000	-3.742500
H	-5.806500	4.055000	-2.099300	C	6.813000	5.289000	4.282200	H	7.916100	-1.439600	-3.592100	H	-0.493000	6.871300	-4.245100
H	-6.459500	2.364800	-2.224800	H	5.040800	5.518900	4.564200	C	8.994800	-0.744200	3.662300	H	-0.168300	5.216600	-3.605500
H	-7.083500	3.660600	-3.317700	H	5.717500	3.853400	4.310400	H	8.772100	0.300500	3.892400	C	-0.654700	6.305500	3.693600
N	-5.521800	-10.430000	-0.185100	Cu	4.776200	8.303700	0.358200	H	8.107900	-1.381700	3.730500	H	-0.289900	7.137100	4.316800
N	-8.187800	-11.151900	-0.286600	Cu	-9.594800	-0.024500	0.455100	H	9.799600	-1.133900	4.304200	H	-1.683800	6.040700	3.947700
C	-5.845400	-11.647400	-0.780500	Cu	4.800600	-8.288000	0.467000	Zn	12.078700	1.392000	-0.006700	H	0.024800	5.450400	3.759600

C	-4.218300	-10.105200	-0.075500
C	-7.255900	-12.029100	-0.838200
C	-9.484200	-11.533600	-0.292300
C	-4.870900	-12.529400	-1.303900
C	-3.165900	-10.952600	-0.593800
C	-7.611900	-13.266800	-1.418900
C	-9.914100	-12.774500	-0.869400
C	-5.277600	-13.775400	-1.908100
C	-3.506500	-12.149800	-1.204100
C	-1.809500	-10.568800	-0.490600
C	-8.992100	-13.624300	-1.429100
C	-6.589800	-14.127200	-1.963800
H	-10.979300	-13.017900	-0.850100
H	-4.500200	-14.427100	-2.312600
H	-2.733000	-12.811200	-1.604600
H	-9.297700	-14.573600	-1.877100
H	-6.903800	-15.071700	-2.416500
C	-0.640900	-10.259000	-0.423900
C	3.446800	-9.205600	-0.274500
C	2.512700	-8.508500	0.508800
C	3.018100	-10.260400	-1.097100
C	1.161400	-8.852300	0.463600
H	2.841800	-7.690700	1.149700
C	1.669800	-10.613400	-1.140600
H	3.742000	-10.811500	-1.700700
C	0.730600	-9.907000	-0.363800
H	0.435400	-8.308700	1.068400
H	1.339900	-11.436700	-1.776400
C	-10.499200	-10.658500	0.321400
C	-10.839900	-10.768900	1.690100
C	-11.237700	-9.731500	-0.453800
C	-11.837600	-9.974000	2.273200
C	-12.233100	-8.919400	0.115100
C	-12.524100	-9.058500	1.471800
H	-12.097500	-10.074500	3.321200
H	-12.788900	-8.209100	-0.488200
C	-3.848600	-8.850700	0.607000
C	-3.669300	-8.806700	2.010600
C	-3.588500	-7.661400	-0.111800
C	-3.246100	-7.637900	2.666100
C	-3.166500	-6.484100	0.524200
C	-3.002600	-6.491200	1.911200
C	4.877100	-8.829000	-0.243300
C	5.578800	-8.761600	0.971800
C	5.560600	-8.532700	-1.428700
C	6.936500	-8.413800	0.952500
H	5.073200	-8.983900	1.911600
C	6.918300	-8.160700	-1.375200
H	5.056800	-8.598900	-2.396700
C	7.628700	-7.834600	-2.646800
C	8.277200	-6.606700	-2.849300
C	8.166800	-8.561000	-4.797000
C	8.899800	-6.378600	-4.083800
H	8.295300	-5.838600	-2.069700
C	8.850000	-7.361000	-5.072400
H	8.093600	-9.358900	-5.548100
H	9.421300	-5.437300	-4.265600
H	9.328400	-7.210600	-6.040100
C	7.746500	-8.346900	2.199900
C	7.507800	-9.172900	3.309300
C	8.313900	-9.019000	4.442800
H	6.723800	-9.929500	3.285600
C	9.532500	-7.285300	3.286100
C	9.331300	-8.061600	4.439300
H	8.146500	-9.644800	5.322400
H	10.327300	-6.525000	3.235900
H	9.963700	-7.917200	5.315200
N	7.621200	-8.097500	-0.202300
N	7.561500	-8.803000	-3.609500
N	8.757700	-7.410900	2.171300
H	-13.310100	-8.442600	1.917200
H	-3.113400	-7.616100	3.742600
H	-2.676200	-5.578500	2.415300
H	-2.970000	-5.579700	-0.039300
O	-10.100600	-11.709100	2.360000
O	-10.891700	-9.738100	-1.774300
O	-3.794900	-7.787400	-1.463100
O	-3.940700	-9.994600	2.635600
C	-3.428200	-6.675100	-2.321800
H	-3.656500	-7.080600	-3.317600
H	-4.050200	-5.803800	-2.098900
H	-2.360500	-6.457800	-2.224400
C	-3.617500	-10.120000	4.046500
H	-3.866300	-11.174300	4.235500
H	-2.550500	-9.940700	4.211200
H	-4.243900	-9.449200	4.640400
C	-10.499600	-12.059000	3.712300
H	-9.817700	-12.891600	3.934900
H	-10.332000	-11.213300	4.383700
H	-11.540800	-12.398800	3.728900
C	-11.608400	-8.856700	-2.682600
H	-11.365600	-7.814000	-2.454300
H	-11.178500	-9.148400	-3.650900
H	-12.682100	-9.059700	-2.649600
Cu	-7.268300	-9.436900	0.282800
Cu	9.440200	-7.271100	0.284500
Cu	7.268300	9.436900	0.282800
Cu	-9.440200	7.271100	0.284500
N	-0.668600	-11.880900	0.011700
N	1.039000	-14.080500	0.024100
C	-1.237100	-13.160000	0.013400
C	-1.477200	-10.800900	0.006100
C	-0.344200	-14.315100	0.021900
C	1.875100	-15.143500	0.032400
C	-2.633800	-13.361500	0.008200
C	-2.917400	-10.940700	-0.004800
C	-0.890300	-15.613500	0.027600
C	1.366500	-16.485300	0.039500
C	-3.156700	-14.705300	0.014000
C	-3.472200	-12.212200	-0.002800
C	-3.780500	-9.818200	-0.019500
C	0.015600	-16.720400	0.037100
C	-2.322600	-15.782000	0.023700
H	2.090200	-17.312300	0.046700
H	-4.244600	-14.838000	0.011100
H	-4.561500	-12.346100	-0.008500
H	-0.383000	-17.744200	0.042300
H	-2.721500	-16.805200	0.028700
C	-4.594200	-8.920200	-0.034500
C	-7.611000	-5.946200	-0.050200
C	-6.395900	-5.712200	0.615700
C	-7.807500	-7.164600	-0.721400
C	-5.389800	-6.680100	0.612000
H	-6.232300	-4.769200	1.137200
C	-6.808200	-8.139000	-0.719800
H	-8.751100	-7.364800	-1.234400
C	-5.589400	-7.906400	-0.050900
H	-4.449300	-6.492800	1.131200
H	-6.974700	-9.089300	-1.234700
C	3.326000	-14.923800	0.033600
C	4.067000	-14.900500	-1.174300
C	4.063400	-14.886500	1.243400
C	5.464600	-14.824300	-1.181100
C	5.461000	-14.810100	1.253400
C	6.148500	-14.793700	0.037000
H	6.026200	-14.826600	-2.113200
H	6.020000	-14.800500	2.187000
C	-0.847400	-9.472400	0.012700
C	-0.559500	-8.789100	-1.193500
C	-0.546500	-8.808900	1.227000
C	0.004700	-7.503600	-1.193500
C	0.017700	-7.524000	1.242900
C	0.280300	-6.887900	0.028000
C	-8.680500	-4.921000	-0.037900
C	-9.212000	-4.428600	-1.245300
C	-9.183200	-4.431300	1.182900
C	-10.215300	-3.449800	-1.205400
H	-8.841900	-4.810100	-2.200200
C	-10.190700	-3.456300	1.169100
H	-8.800200	-4.825900	2.127600
C	-10.853700	-2.871000	2.371200
C	-10.609200	-3.322100	3.669600
C	-12.430600	-1.304500	3.144200
C	-11.308900	-2.734300	4.738100
H	-9.900500	-4.130400	3.863100
C	-12.222300	-1.719500	4.476500
H	-13.161100	-0.510000	2.917400
H	-11.137500	-3.082500	5.764100
H	-12.787600	-1.246600	5.287700
C	-10.897500	-2.851800	-2.390500
C	-10.669200	-3.284300	-3.698100
C	-11.387300	-2.686500	-4.748800
H	-9.957900	-4.084800	-3.912600
C	-12.492100	-1.282300	-3.120800
C	-12.301900	-1.680000	-4.461100
H	-11.228900	-3.020600	-5.781500
H	-13.222700	-0.494000	-2.873200
H	-12.882000	-1.200500	-5.257800
N	-10.677900	-2.965200	-0.012000
N	-11.763700	-1.859800	2.103100
N	-11.807200	-1.847300	-2.096800
H	7.244100	-14.760600	0.038600
H	0.215300	-6.984300	-2.123000
H	0.712800	-5.883900	0.033900
H	0.238300	-7.020300	2.178200
O	3.282900	-14.945000	-2.298700
O	3.276200	-14.918300	2.365900
O	-0.849400	-9.549000	2.334800
O	-0.870700	-9.511600	-2.310200
C	-0.742800	-8.920900	3.641900
H	-1.131900	-9.714200	4.298400
H	0.301700	-8.693700	3.868000
H	-1.380800	-8.033400	3.693800
C	-0.788900	-8.857100	-3.606500
H	-1.178100	-9.641900	-4.272900
H	-1.437500	-7.975900	-3.631500
H	0.249700	-8.613600	-3.842400
C	3.917100	-15.344100	-3.549300
H	3.049800	-15.486400	-4.207500
H	4.574100	-14.547800	-3.906400
H	4.456800	-16.291200	-3.421700
C	3.907200	-15.301600	3.623100
H	4.562600	-14.500600	3.972200
H	3.038200	-15.436800	4.280500
H	4.448100	-16.249800	3.508400
Zn	1.392000	-12.072700	0.011600

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