Electronic Supplementary Information

Luminescent zinc(II) and copper(I) complexes for high-performance solution-processed monochromic and white organic light-emitting devices

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1. Device fabrication and characterization

Materials: PEDOT:PSS [poly(3,4-ethylenedioxythiophene):poly(styrene sulfonic acid)] (Clevios P AI 4083) was purchased from Heraeus, PVK (polyvinylcarbazole) from Sigma-Aldrich, FIrpic, OXD-7, PYD2, 3TPYMB, DPEPO, and TPBi from Luminescence Technology Corp. All of these materials were used as received. The synthetic procedures of **Zn-1–Zn-3** and **Cu-1**–**Cu-5** are described below (see pages S24–S27 and S39–S40). All Zn(II) complexes were purified by gradient sublimation before use.

Substrate cleaning: Glass slides with pre-patterned ITO electrodes used as substrates of OLEDs were cleaned in an ultrasonic bath of Decon 90 detergent and deionized water, rinsed with deionized water, and then cleaned in sequential ultrasonic baths of deionized water, acetone, and isopropanol, and subsequently dried in an oven for 1 h.

Fabrication and characterization of devices: PEDOT:PSS were spin-coated onto the cleaned ITO-coated glass substrate and baked at 120 ˚C for 20 min to remove the residual water solvent in a clean room. Blends of PVK: OXD-7:emitter(s) or PYD2:emitter(s) were spin-coated from chlorobenzene atop the PEDOT:PSS layer inside a N_2-filled glove box. For the **Cu-5** device, the mixture of Cu-5 and PYD2 was spin-coated from dimethylformamide as EML. The thickness for all EMLs was about 60 nm. Afterwards, all devices except for those with PYD2 as the host were annealed at 110 ˚C for 10 min inside the glove box and subsequently transferred into a Kurt J. Lesker SPECTROS vacuum deposition system without exposing to air. Finally, TmPyPb or 3TPYMB or DPEPO (5 nm), TPBi (40 nm), LiF (1.2 nm), and Al (150 nm) were deposited in sequence by thermal evaporation at a pressure of 10^{-8} mbar. EL spectra were recorded by an Ocean Optics Maya 2000 pro spectrometer or a Photo Research Inc PR-655. Luminance, CIE coordination, and CRI were measured by a Photo Research Inc PR-655. Voltage-current characteristics were measured by a Keithley 2400 source-meter measurement unit. All devices were characterized at room temperature without encapsulation. EQE and power efficiency were calculated by assuming a Lambertian distribution.

2. Experimental details for time-resolved emission and temperature dependent emission measurements

The instrumental set-up for the femtosecond time-resolved emission (fs-TRE) and nanosecond time-resolved emission (ns-TRE) and the related spectral calibrations have been described previously.[1,2] Briefly, all the measurements were performed based on a commercial Ti:Sapphire regenerative amplifier laser system (800 nm, 40 fs, 1 kHz, and 3.5 mJ/pulse). A 350 nm excitation wavelength was used for all the measurements. The 350 nm pump pulse was produced from an optical parametric amplifier (TOPAS) pumped by the 800 nm fundamental laser pulse. The fs-TRE was measured using a Kerr-gate technique.[3] A Kerr device composed of a 1 mm thick Kerr medium (benzene contained in a quartz cell) equipped within a crossed polarizer pair was driven by the 800 nm laser to function as an ultrafast optical shutter to sample transient emission spectra at various selected pump/probe delays. The delay between the probe and pump pulse was controlled by an optical delay line. The fs-TRE signals were collected by a monochromator and detected with a liquid nitrogen cooled CCD detector. The instrument response function (IRF) of the fs-TRE is wavelength-dependent, varying from ~0.5 ps to ~2 ps. For the ns-TRE measurement, an intensified CCD (ICCD) detector, which was synchronized to the fs laser system, was used to detect transient emission spectra with the controlled pump/probe time delay covering from ~2 ns and afterwards. To eliminate the effect of rotational diffusion, the polarization direction of the pump laser was set at the magic angle in relative to that of probe for all the measurements. The measurements were done at room temperature and atmospheric pressure with the samples (concentration of ~1 mM) of ~15 mL flowed in a cell with 0.5 mm path length. The samples were monitored by UV-vis absorption and revealed no degradation after the time-resolved measurement.

3. Experimental details for emission and lifetime measurements

Steady-state excitation and emission spectra were obtained on a SPEX Fluorolog-3 spectrophotometer. All solutions for photophysical measurements were degassed with no less than three freeze-pump-thaw cycles prior to the measurements. For measurement of emission spectrum at low-temperature (77 K), the solution or solid sample was loaded in a 5-mm-diameter quartz tube that was immersed in a liquid nitrogen Dewar flask equipped with quartz windows. The emission spectra were corrected for monochromator and photomultiplier efficiency and for Xenon-lamp stability. Emission lifetime measurements were performed with a Quanta Ray GCR 150-10 pulsed Nd:YAG laser system (pulse output 355 nm, 8 ns). Luminescence quantum yields were measured relative to that of a degassed benzene solution of 9,10-bis(phenylethynyl)anthracene (BPEA, Φ_r = 0.85) or acetonitrile solution of $Ru(bpy)_3(PF_6)_2$ (Φ_r = 0.062) as a standard reference. Errors for λ values (±1 nm), τ (±10%), and Φ (±10%) were estimated.

4. Experimental details for cyclic voltammetry and X-ray diffraction

Cyclic voltammetry was performed using PAR potentiostat 273A equipped with PowerSuite program at a scan rate of 100 mV s^{-1}. The electrolytic cell used was a conventional two compartment cell. Electrochemical measurements were performed at room temperature after purging with nitrogen using 0.1 M tetrabutylammonium hexafluorophosphate (TBAP)/dichloromethane as the supporting electrolyte. The working electrode was a glassy carbon electrode (geometric area 0.35 cm^2) and the counter electrode was platinum gauze. A non-aqueous $Ag/AgNO_3$ (0.1 M in acetonitrile) reference electrode was contained in a separate compartment connected to the test solution via fine sintered glass disks. The ferrocenium/ferrocene couple was used as the internal standard.

X-ray diffraction data were collected by a Bruker X8 diffractometer with MICROSTAR copper rotating anode (Cu K-alpha, 1.54178 angstrom) and Platinum 135 CCD detector. Proteum was used for data collection strategy, integration and scaling. Shelx-97 program suite was used for structure solution (XS) and refinement (XL).

5. Thermogravimetric properties of Zn-1–Zn-3

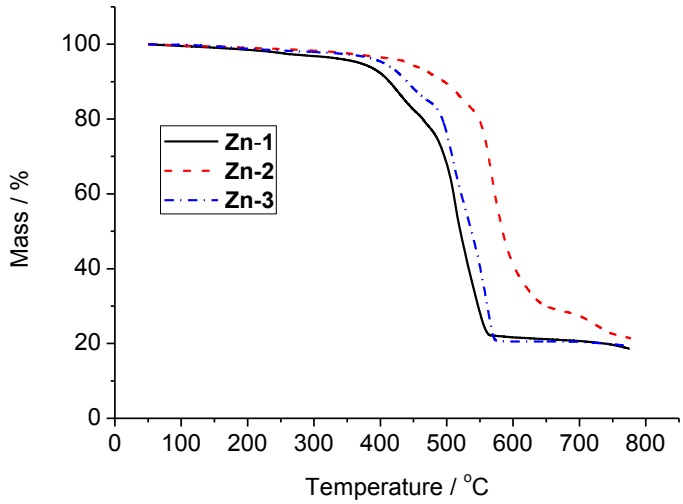


Fig. S1 Thermogravimetric curves of complexes **Zn-1**–**Zn-3** under a constant heating rate of 10 °C min^{-1}.

6. Photophysical properties of Zn-1–Zn-3

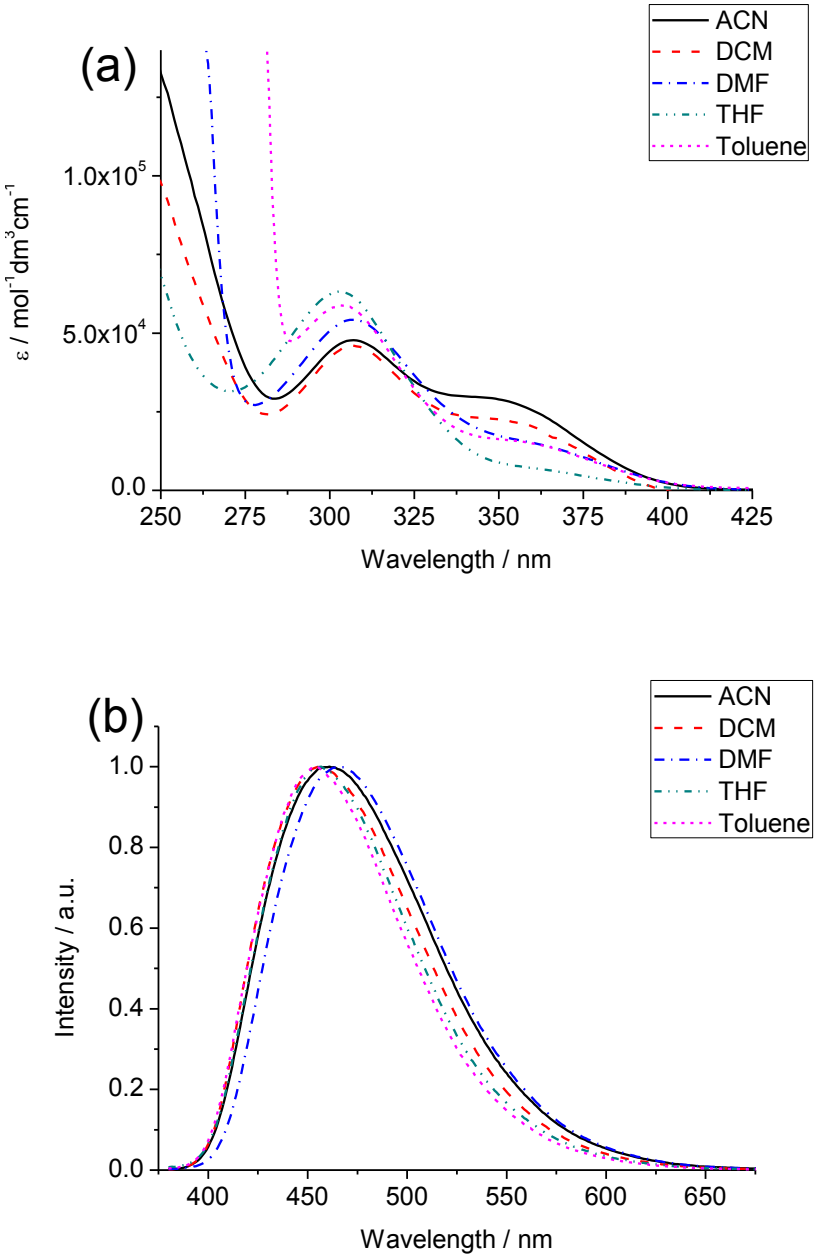


Fig. S2 (a) Absorption and (b) emission spectra of **Zn-1** in various solvents (ACN = MeCN; DCM = CH_2Cl_2).

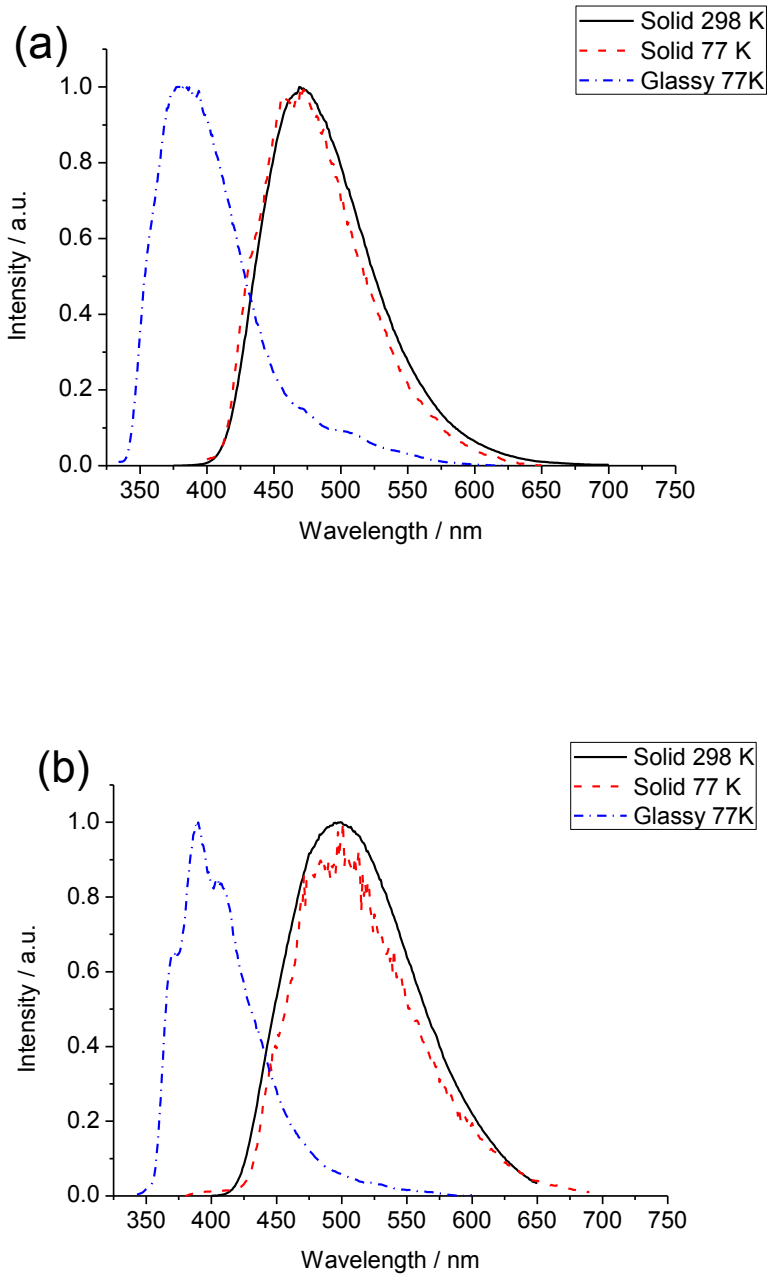


Fig. S3 Emission spectra of (a) **Zn-1** and (b) **Zn-2** in solid state at 298 and 77 K, and in 2-MeTHF glassy solution at 77 K.

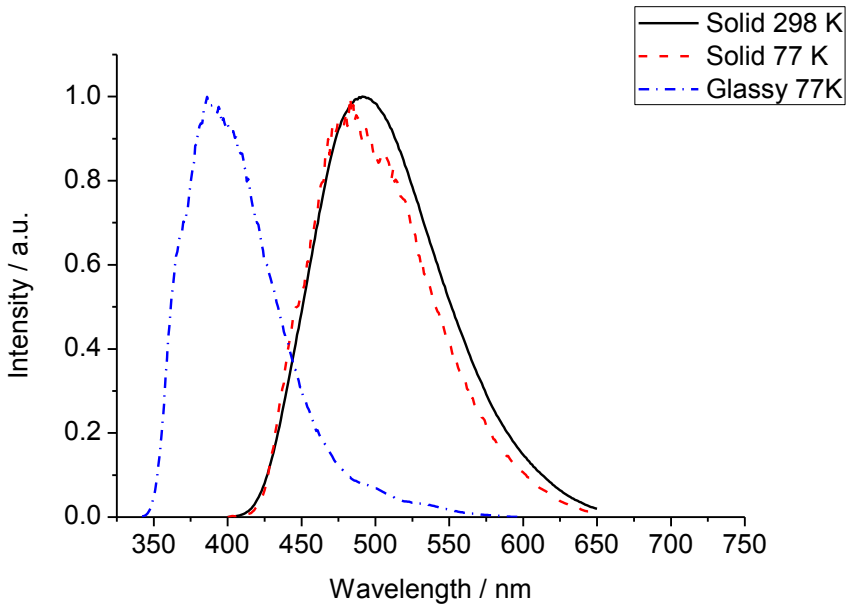


Fig. S4 Emission spectra of **Zn-3** in solid state at 298 and 77 K, and in 2-MeTHF glassy solution at 77 K.

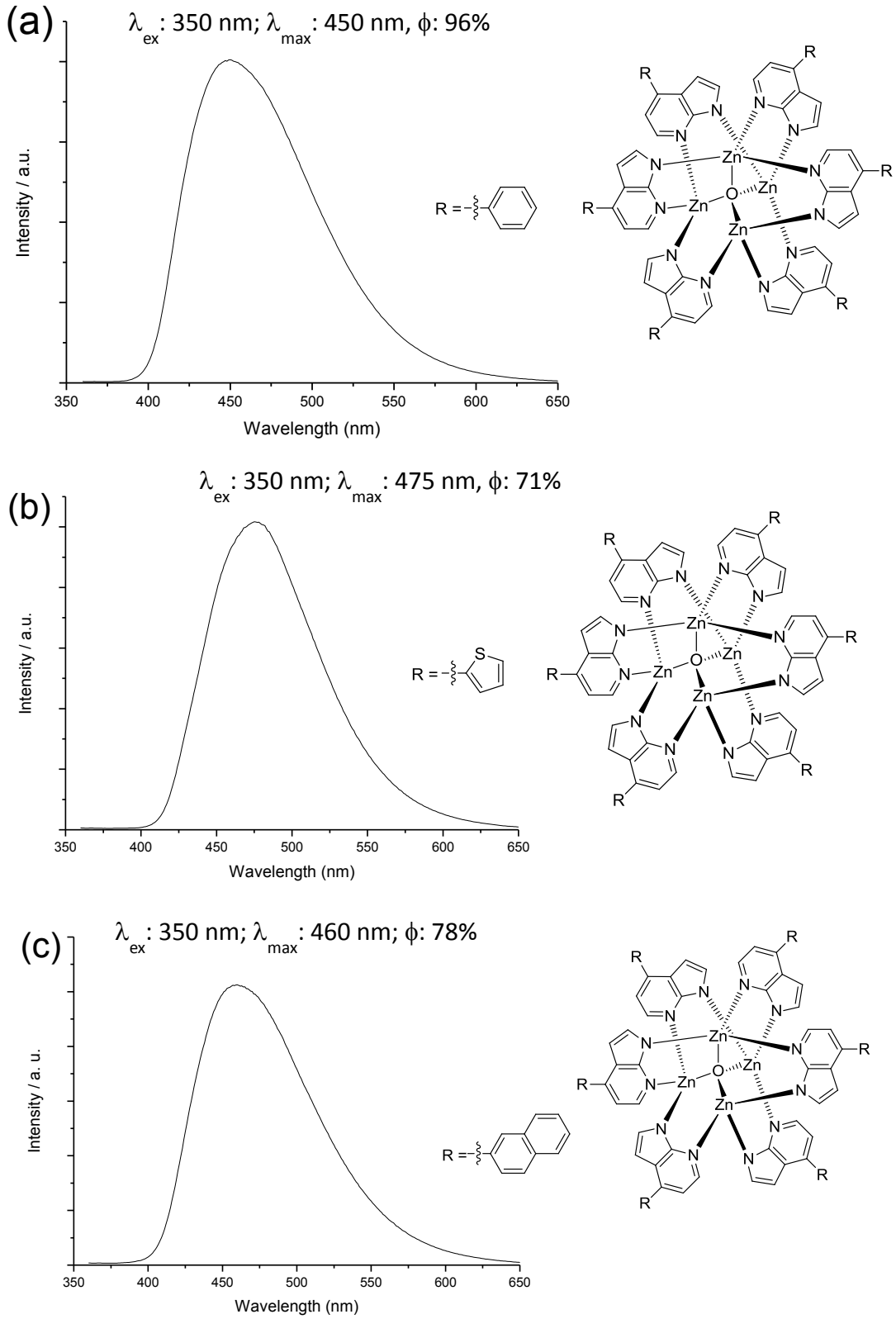


Fig. S5 PL spectra of (a) **Zn-1**, (b) **Zn-2**, and (c) **Zn-3** in PMMA thin film with concentration of 5 wt%.

7. Photophysical properties of Cu-1–Cu-5

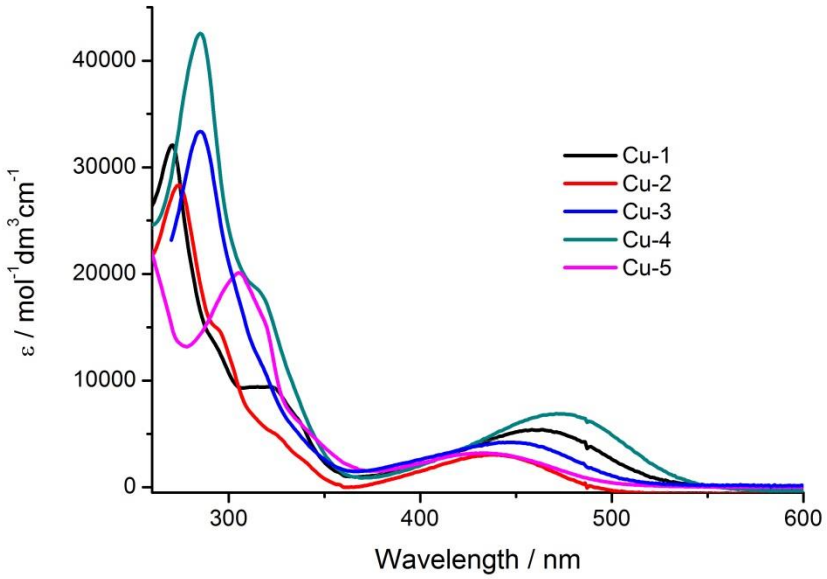


Fig. S6 Absorption spectra of complexes **Cu-1–Cu-5** in CH_2Cl_2 solution.

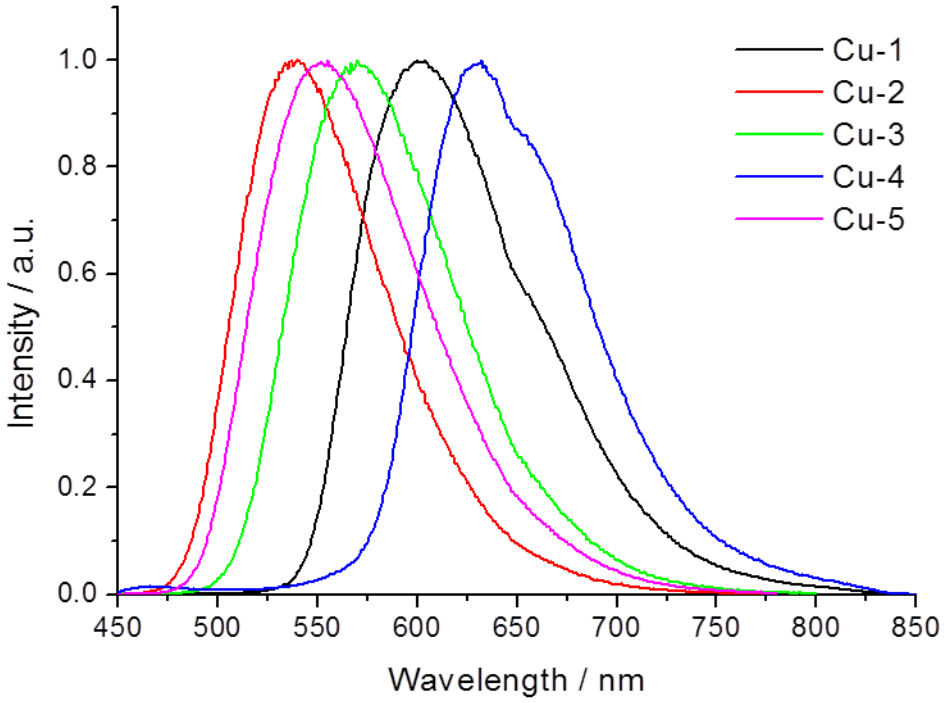


Fig. S7 Solid-state emission spectra of **Cu-1–Cu-5** at room temperature (λ_{ex} = 365 nm).

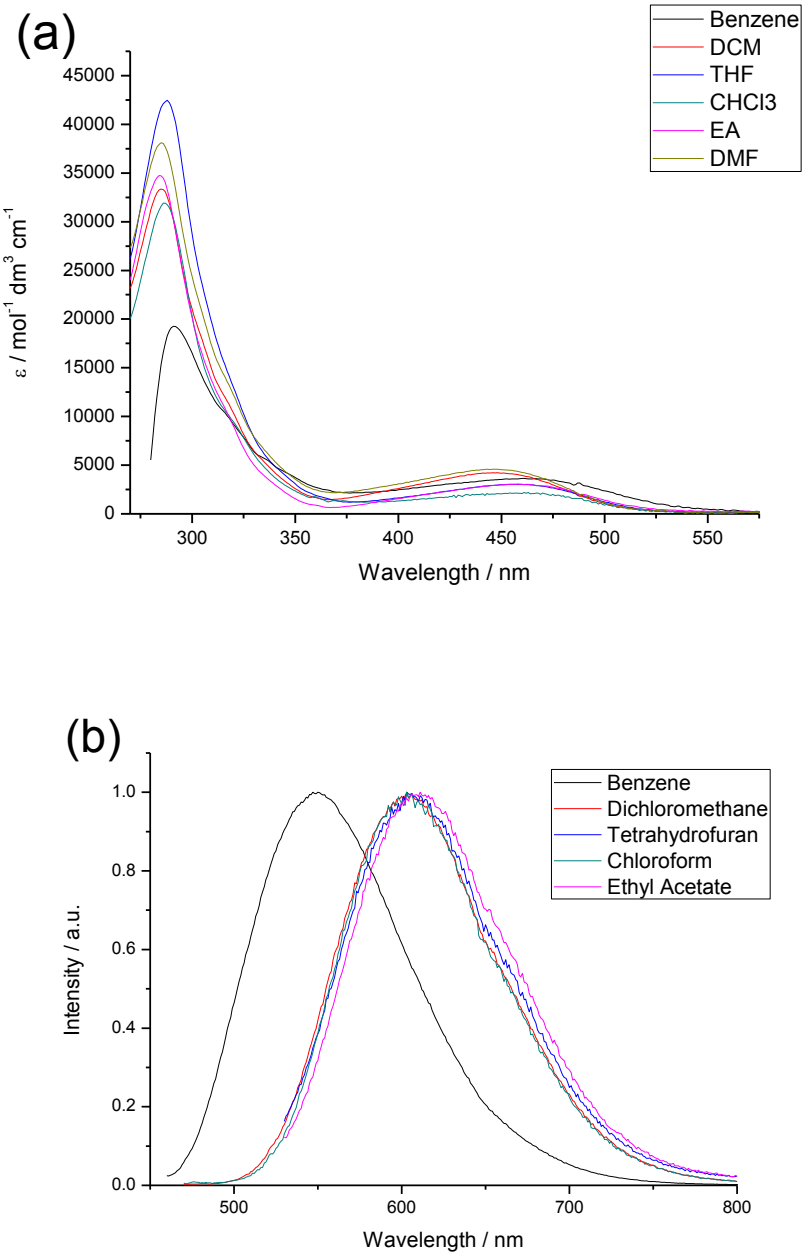


Fig. S8 (a) Absorption and (b) emission spectra of **Cu-3** in different solvents.

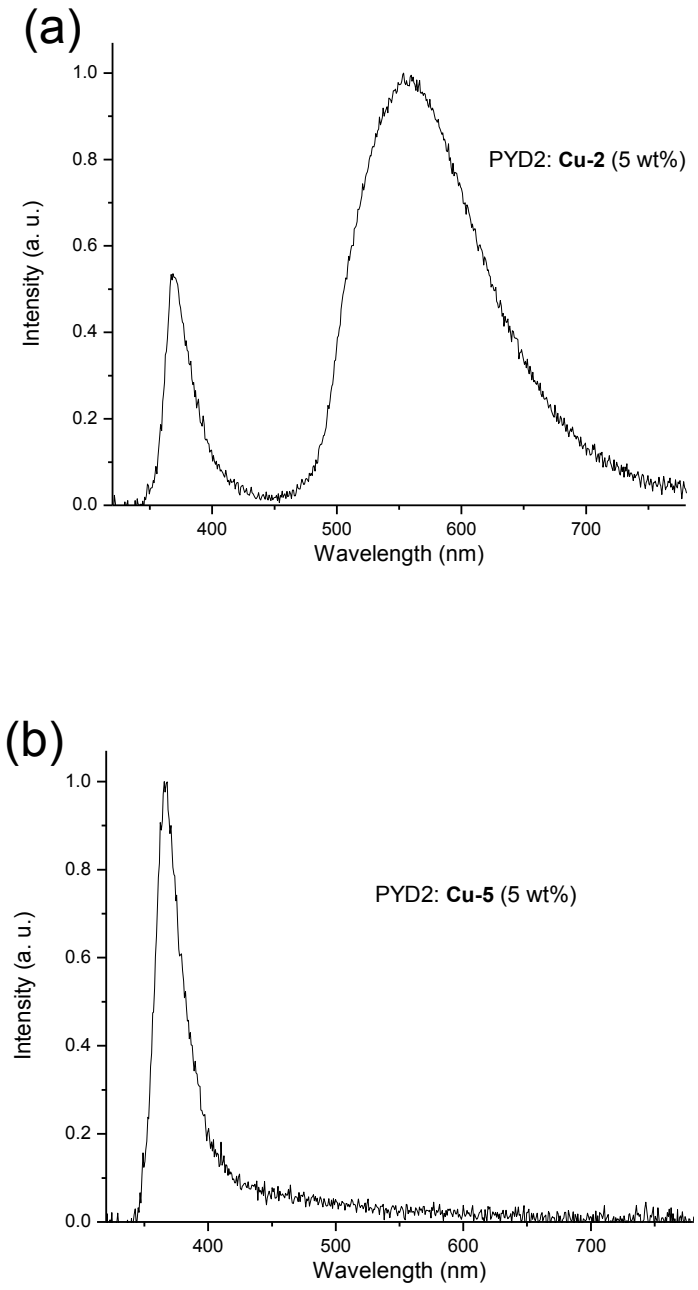


Fig. S9. PL emission of (a) **Cu-2** and (b) **Cu-5** in PYD2 thin film. λ_{ext} = 310 nm.

8. fs-Time-resolved fluorescence of Zn-1–Zn-3

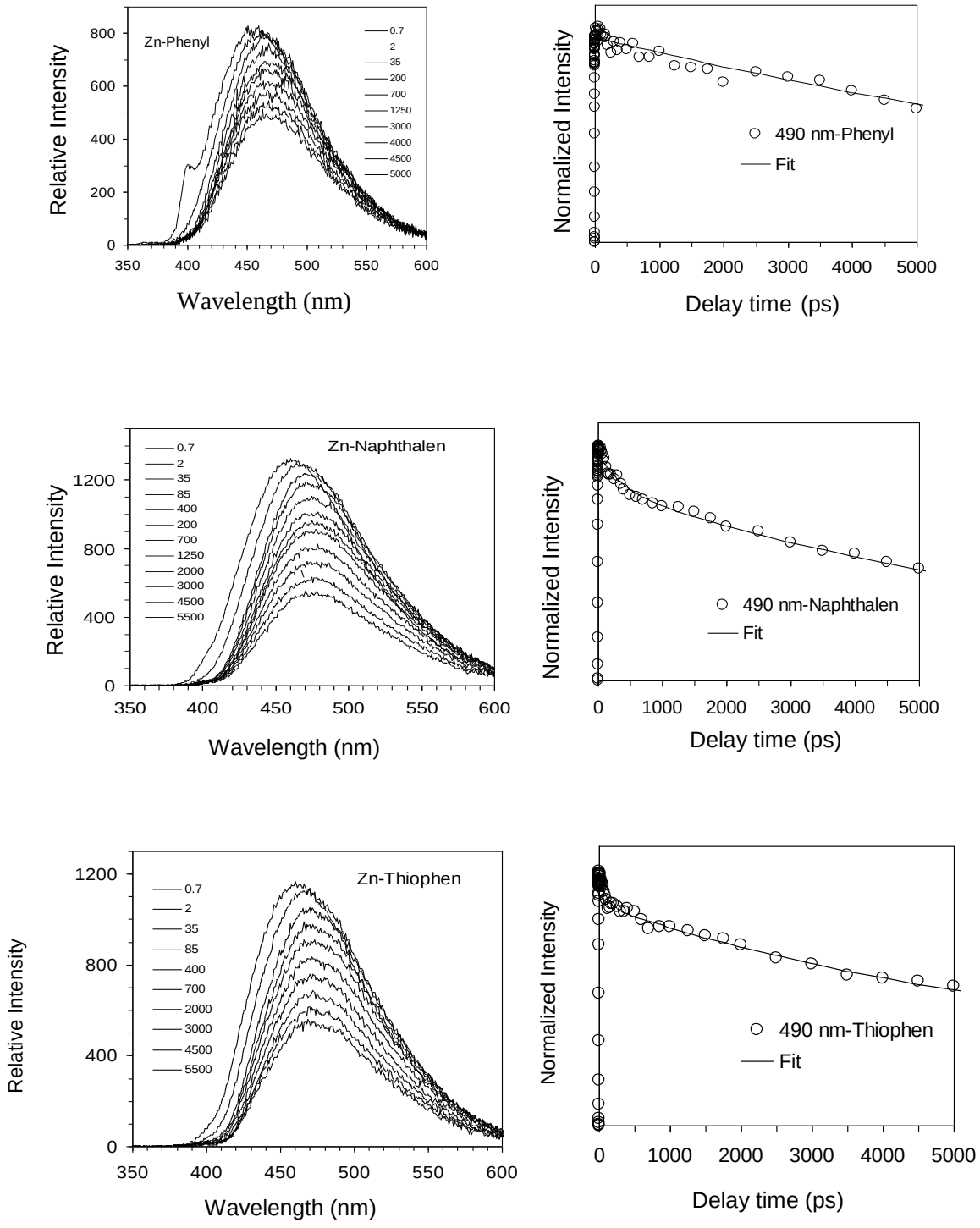


Fig. S10 Time-resolved fluorescence of **Zn-1** (Zn-Phenyl), **Zn-2** (Zn-Naphthalen), and **Zn-3** (Zn-Thiophen) in CH_2Cl_2 with excitation at 350 nm.

9. ns-Time-resolved fluorescence of Cu complexes

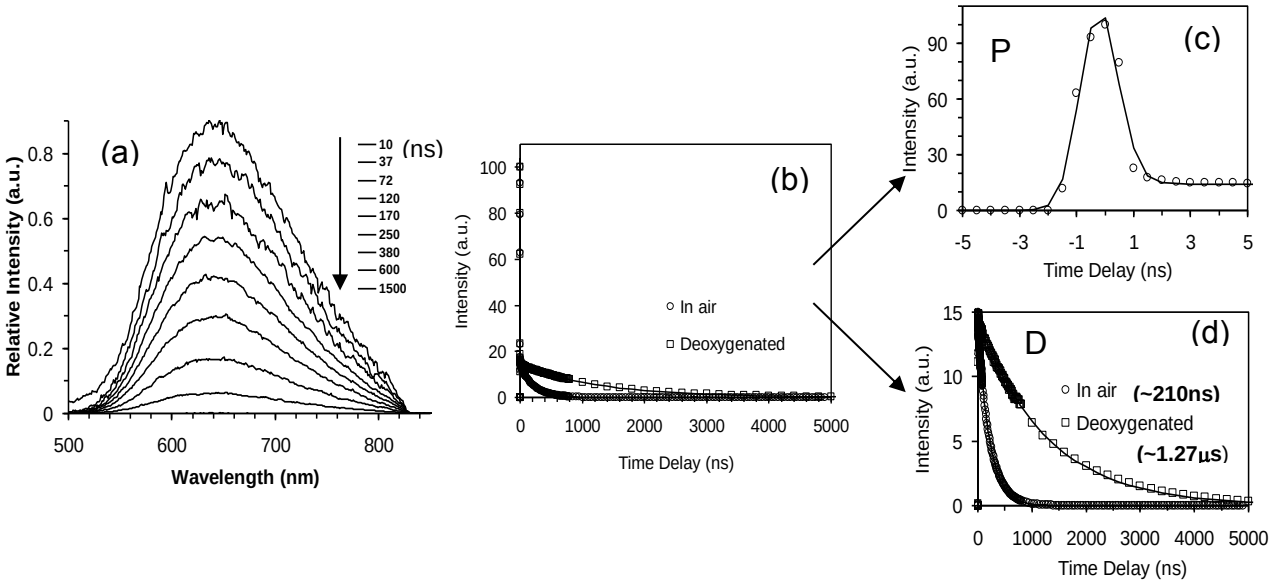


Fig. S11 (a) ns-TRE of **Cu-3** in CH_2Cl_2 (deoxygenated by purging the sample solution with nitrogen) recorded at indicated time intervals after excitation at 350 nm. (b)–(d) ns-TRE decay profile of **Cu-3** in CH_2Cl_2 recorded at 350 nm

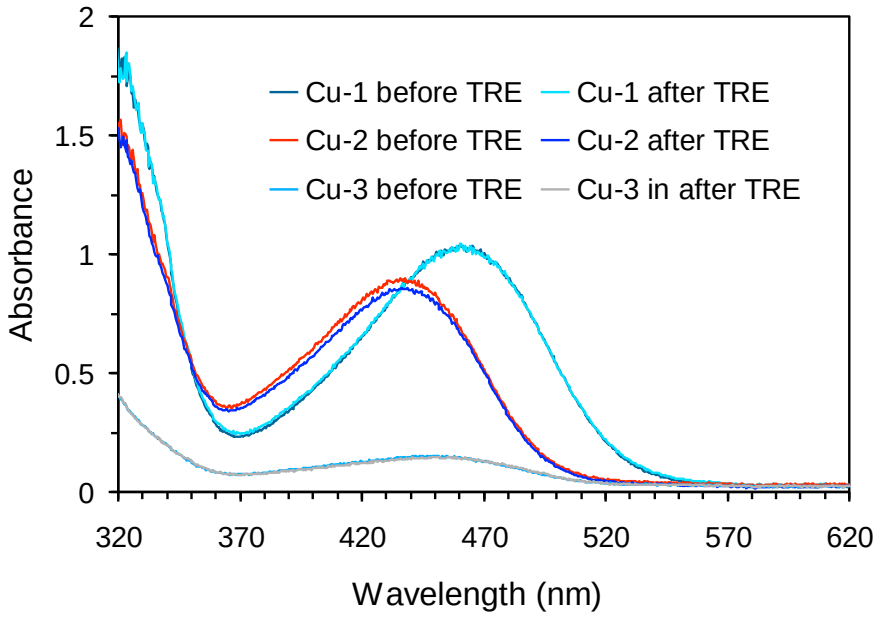
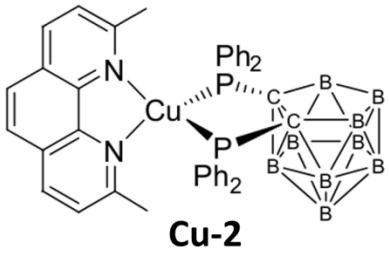


Fig. S12 UV-vis absorption spectra of **Cu-1**, **Cu-2**, and **Cu-3** in CH_2Cl_2 recorded before and after the nanosecond time-resolved emission measurement with excitation at 350 nm.

10. Emission lifetime measurements at various temperatures for Cu-2 and Cu-5



Cu-2

$$\tau(T) = \frac{3 + \exp\left[-\frac{\Delta E(S_1 - T_1)}{k_B T}\right]}{\frac{3}{\tau(T_1)} + \frac{1}{\tau(S_1)}\exp\left[-\frac{\Delta E(S_1 - T_1)}{k_B T}\right]} \quad (1)$$

$\Delta E(S_1 - T_1)$: 1195 cm^{-1}

$\tau(T_1)$: 564 µs

$\tau(S_1)$: 0.01 µs

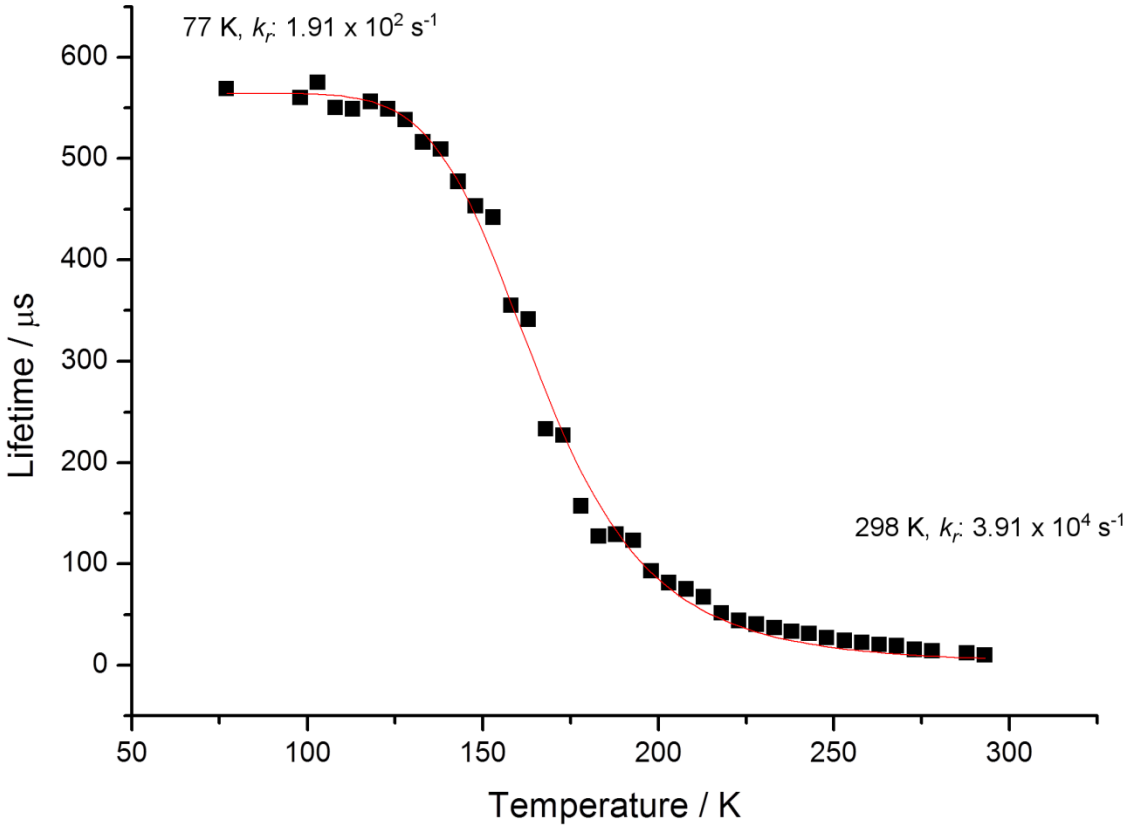


Fig. S13 Emission decay time of **Cu-2** powder versus temperature.

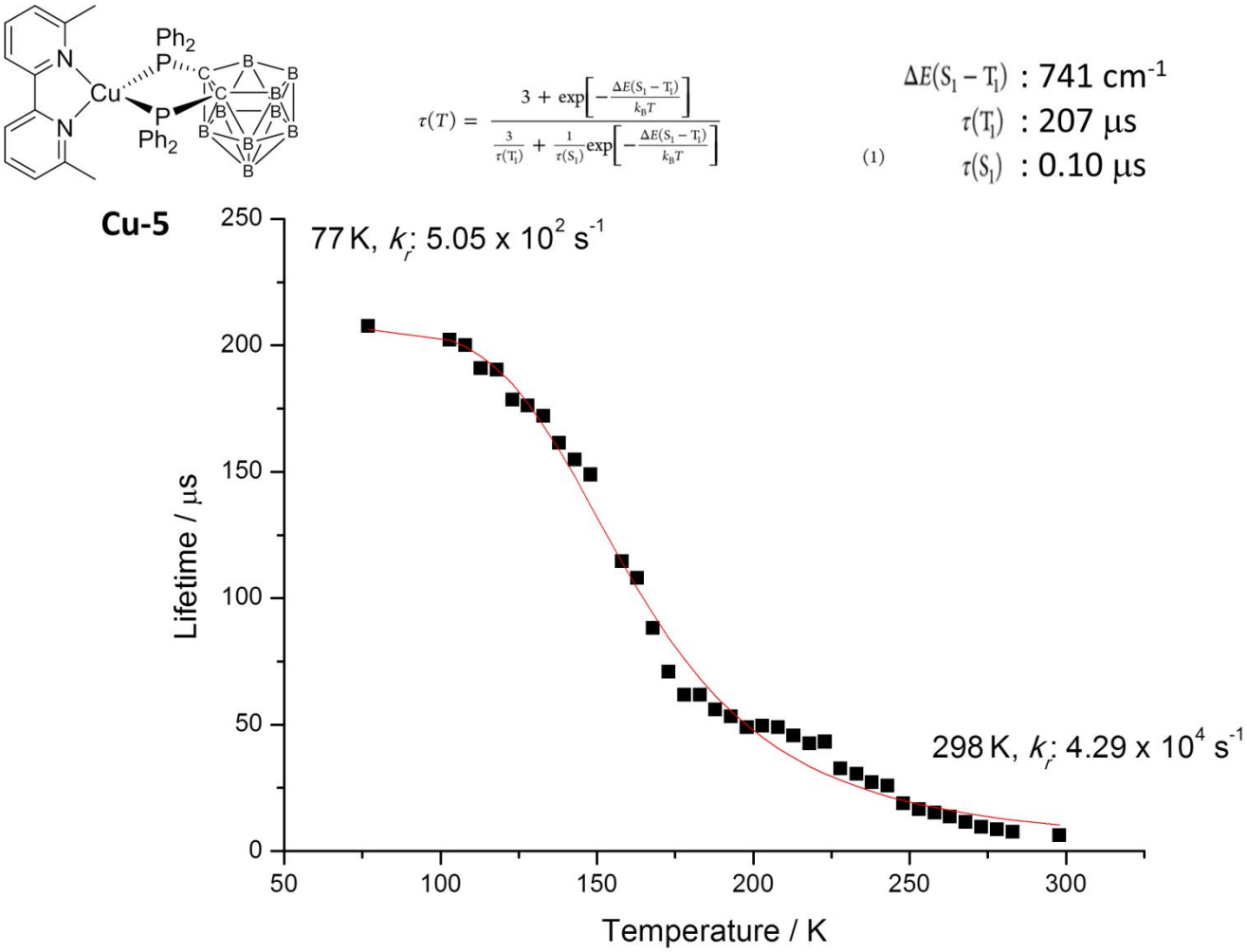


Fig. S14 Emission decay time of **Cu-5** powder versus temperature.

11. Electrochemical properties of Zn-1–Zn-3

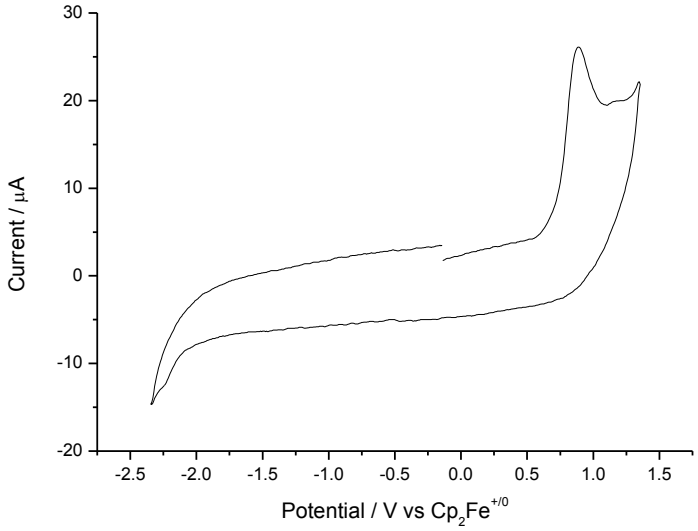


Fig. S15 Cyclic voltammogram of **Zn-1** in CH_2Cl_2 containing $[^nBu_4N]PF_6$ (0.1 mol dm^{-3}) as supporting electrolyte. Scan rate: 100 mV s^{-1}.

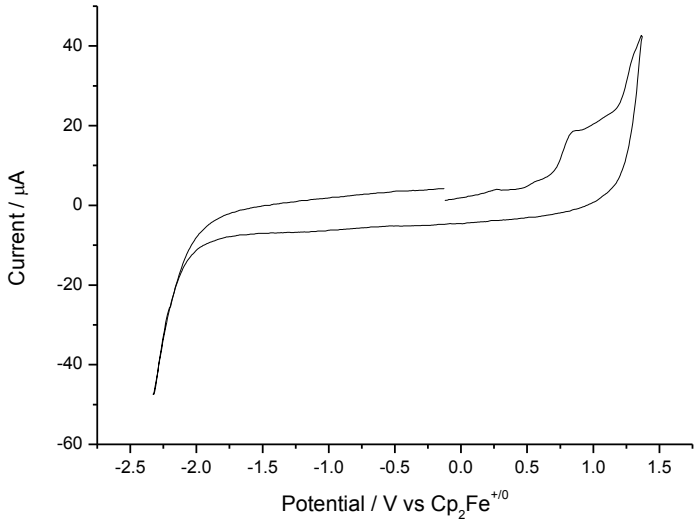


Fig. S16 Cyclic voltammogram of **Zn-2** in CH_2Cl_2 containing $[^nBu_4N]PF_6$ (0.1 mol dm^{-3}) as supporting electrolyte. Scan rate: 100 mV s^{-1}.

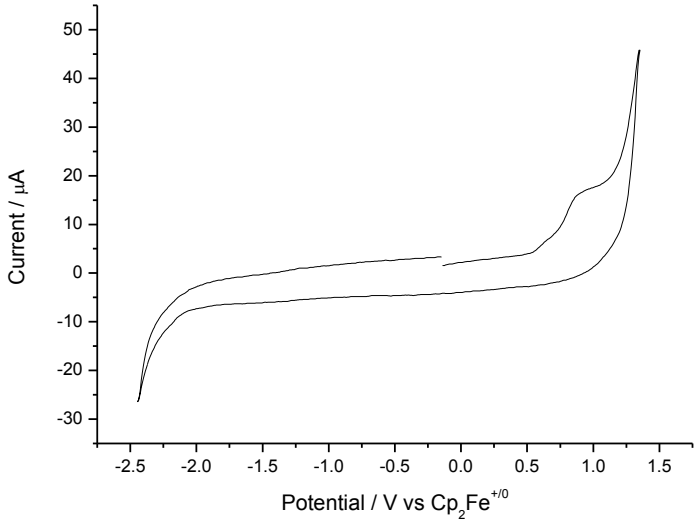


Fig. S17 Cyclic voltammogram of **Zn-3** in CH_2Cl_2 containing $[^nBu_4N]PF_6$ (0.1 mol dm^{-3}) as supporting electrolyte. Scan rate: 100 mV s^{-1}.

12. Electrochemical properties of Cu-1–Cu-5

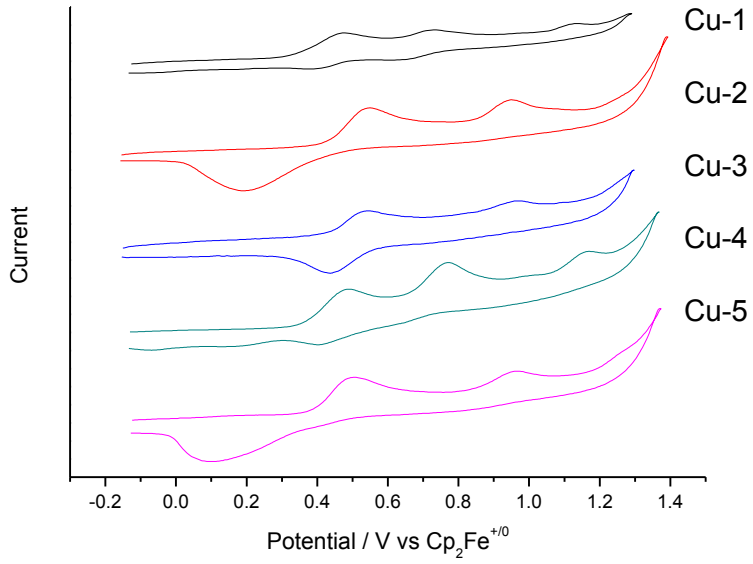


Fig. S18 Cyclic voltammogram of **Cu-1–Cu-5** in CH_2Cl_2 containing $[^nBu_4N]PF_6$ (0.1 mol dm^{-3}) as supporting electrolyte (oxidation). Scan rate: 100 mV s^{-1}.

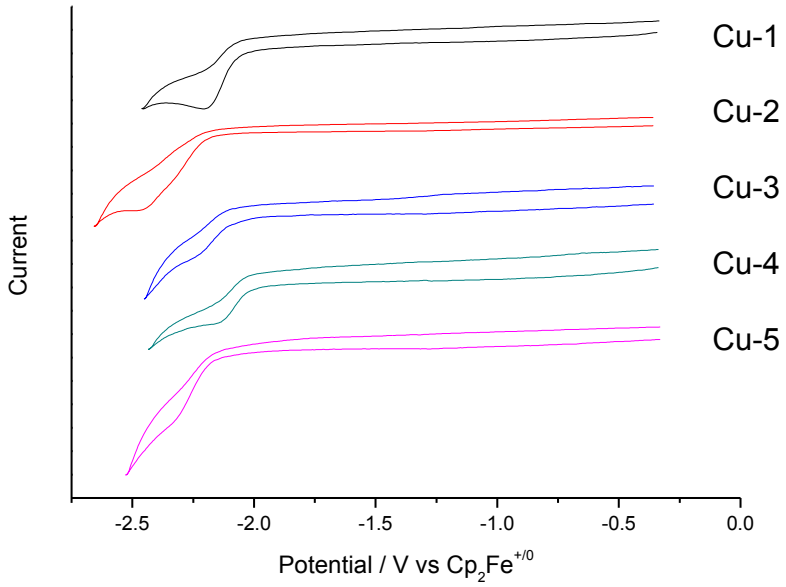


Fig. S19 Cyclic voltammogram of **Cu-1–Cu-5** in CH_2Cl_2 containing $[^nBu_4N]PF_6$ (0.1 mol dm^{-3}) as supporting electrolyte (reduction). Scan rate: 100 mV s^{-1}.

13. EL properties of Zn-1

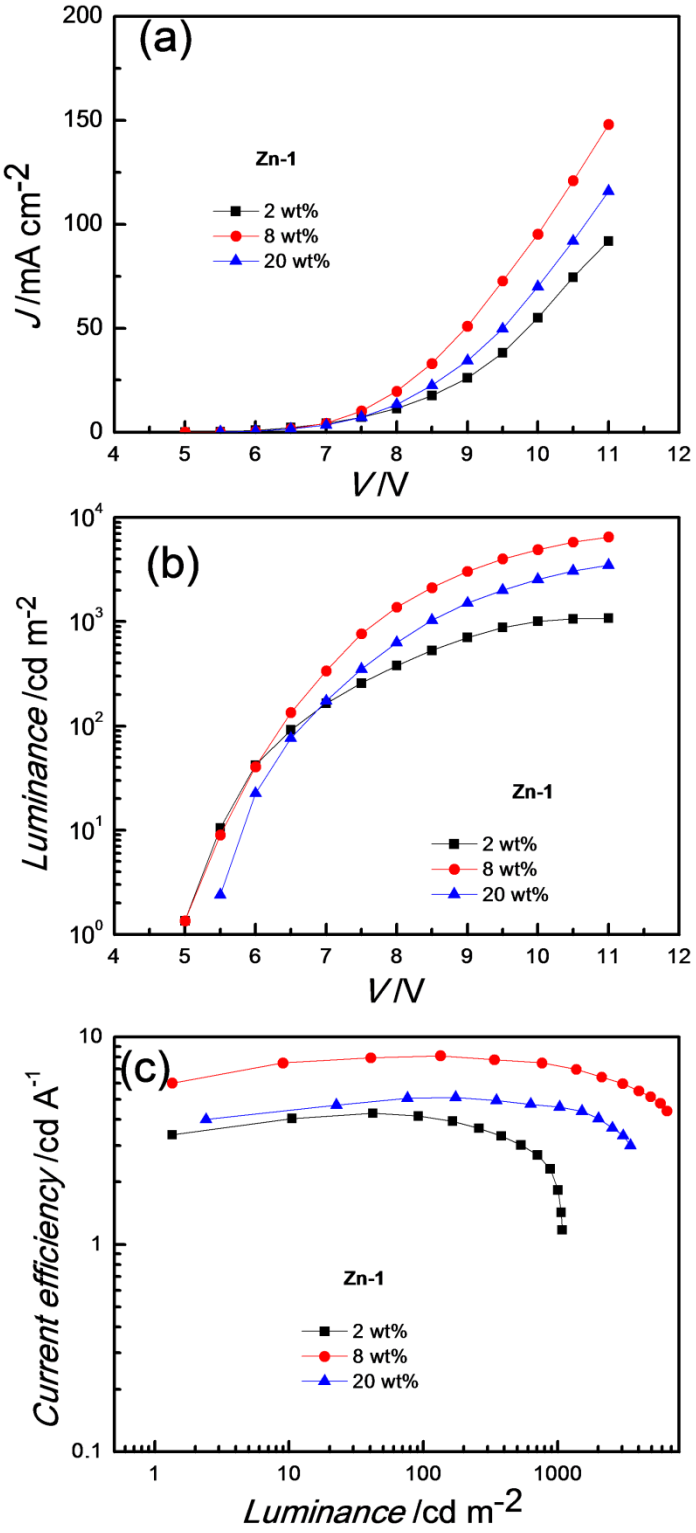


Fig. S20 (a) Current density-voltage, (b) luminance-voltage, and (c) current efficiency-luminance characteristics of PLEDs based on **Zn-1** at different doping concentrations.

14. EL properties of Zn-2

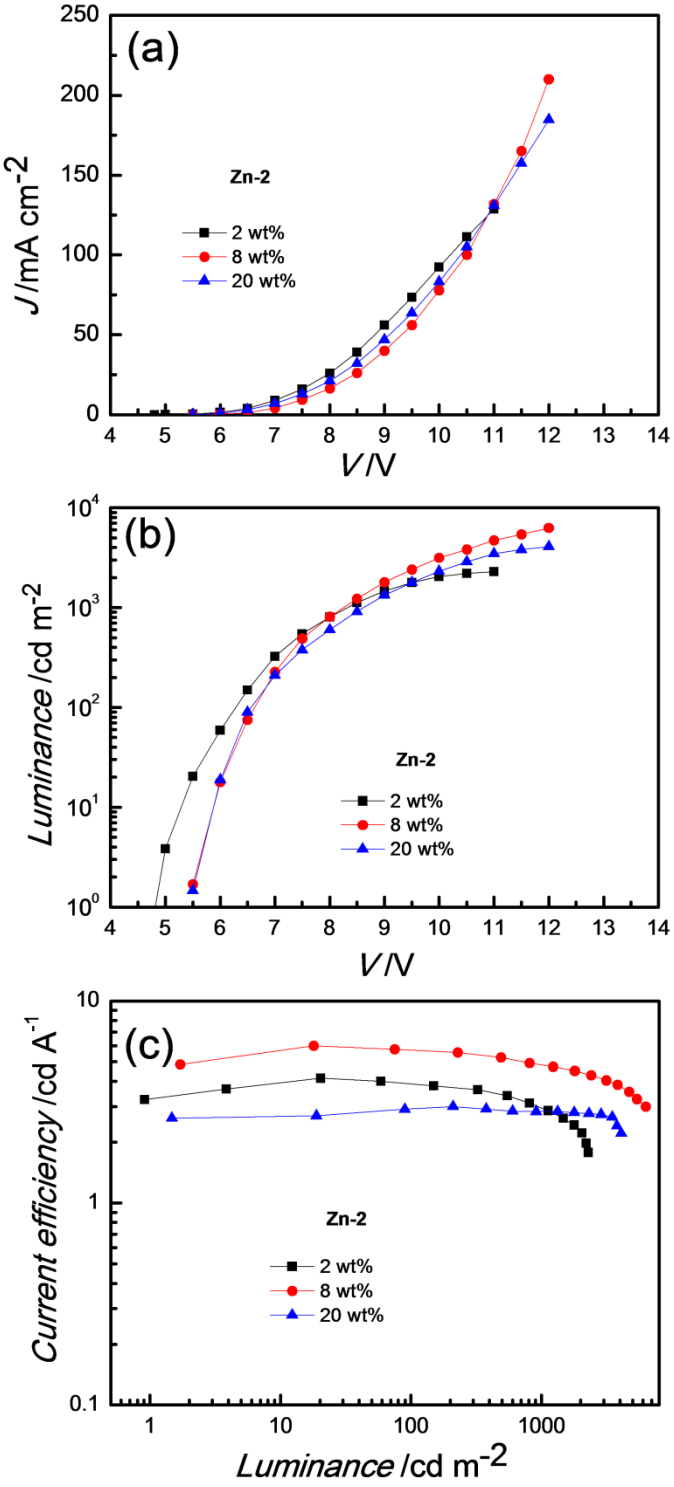


Fig. S21 (a) Current density-voltage, (b) luminance-voltage, and (c) current efficiency-luminance characteristics of PLEDs based on **Zn-2** at different doping concentrations.

15. EL properties of Zn-3

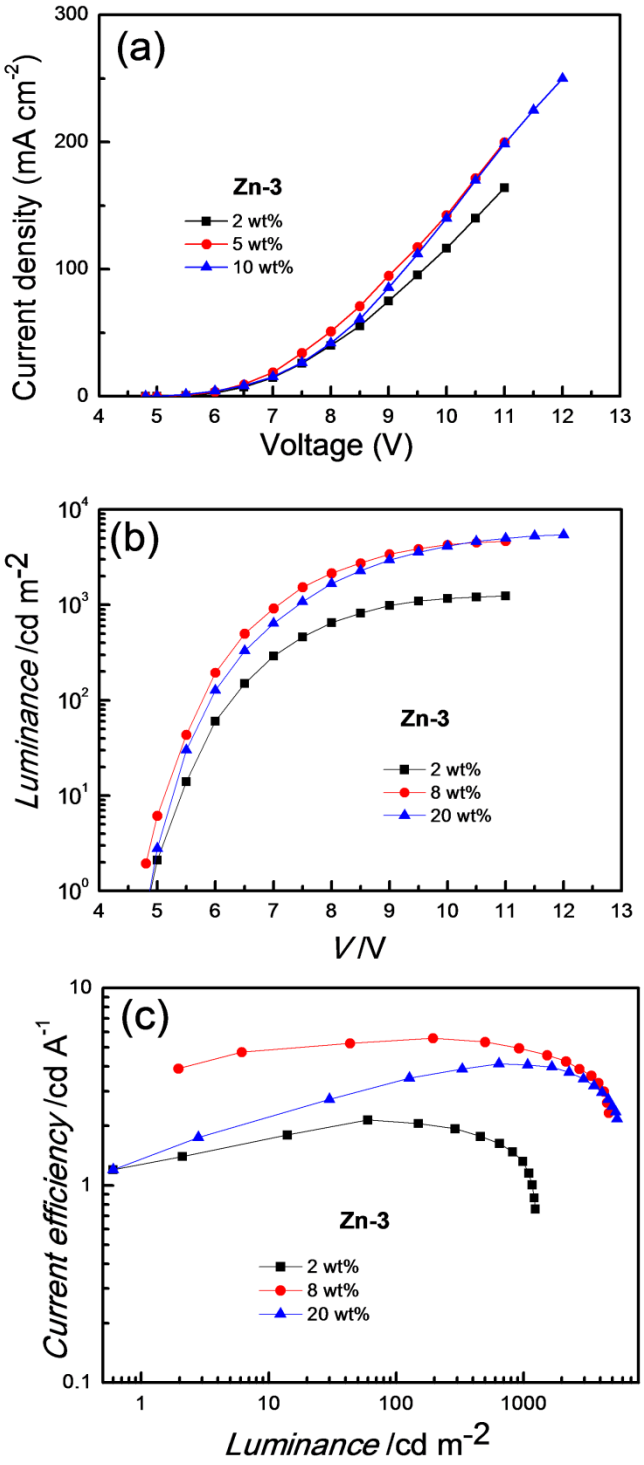


Fig. S22 (a) Current density-voltage, (b) luminance-voltage, and (c) current efficiency-luminance characteristics of PLEDs based on **Zn-3** at different doping concentrations.

16. EL properties of Cu(I) complexes

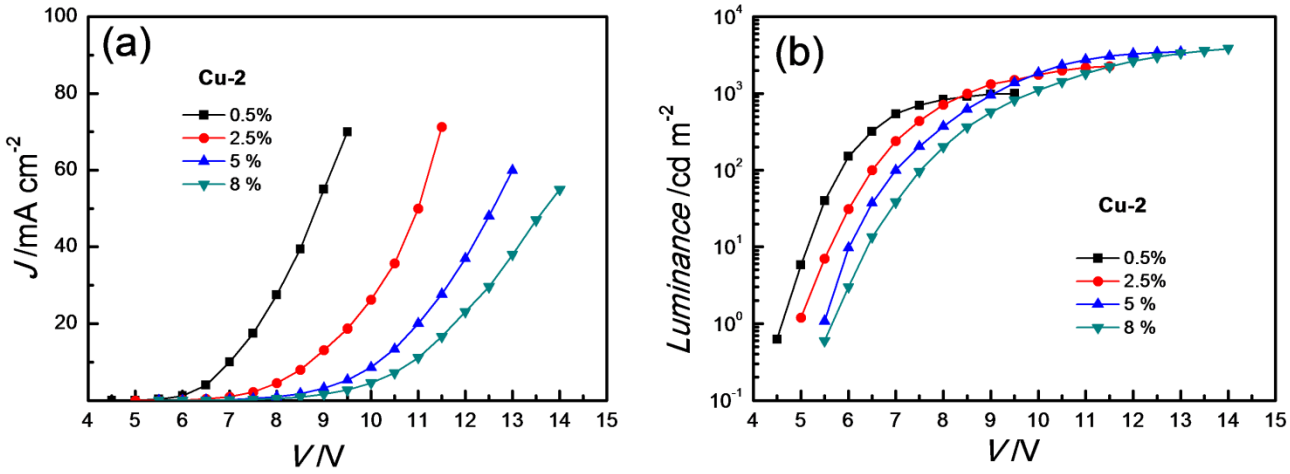


Fig. S23 Current density-luminance-voltage characteristics of PYD2/DPEOP devices based on **Cu-2** at different doping concentrations.

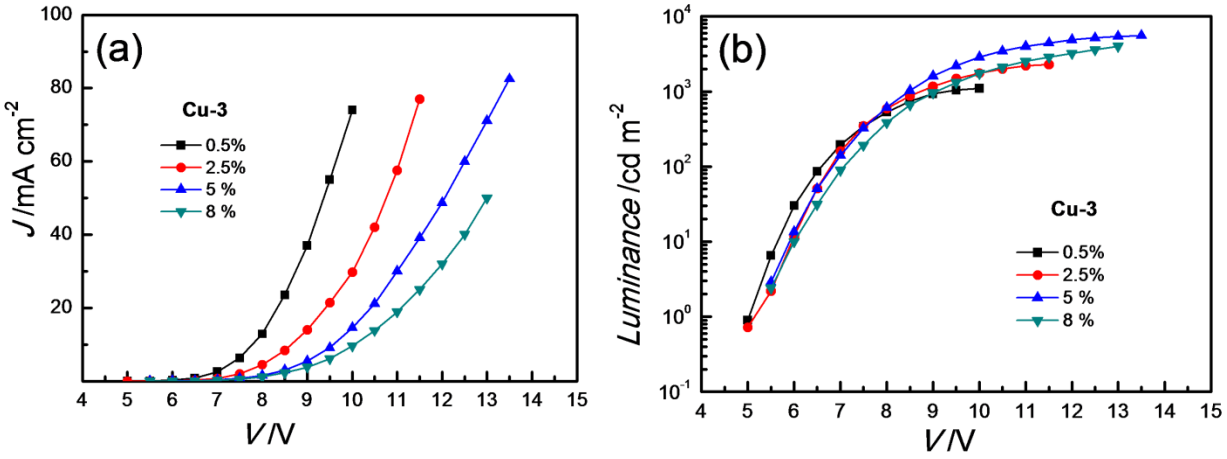


Fig. S24 Current density-luminance-voltage characteristics of PYD2/DPEOP devices based on **Cu-3** at different doping concentrations.

Table S1 Key performance parameters of PVK/3TPYMB devices with **Cu-3**

Doping concentration of **Cu-3**	L[a] (cd m^{-2})	Max. CE[b] (cd A^{-1})	Max. PE[c] (lm W^{-1})	Max. EQE[d] (%)	CIE coordinates (x, y) at 1000 cd m^{-2}
2 wt%	1200	23.33	12.22	10.77	(0.54, 0.45)
5 wt%	1350	22.58	11.88	10.59	(0.54, 0.45)
10 wt%	2520	22.88	13.20	11.43	(0.55, 0.44)

[a] Luminance at 17 V. [b] Current efficiency. [c] Power efficiency. [d] External quantum efficiency.

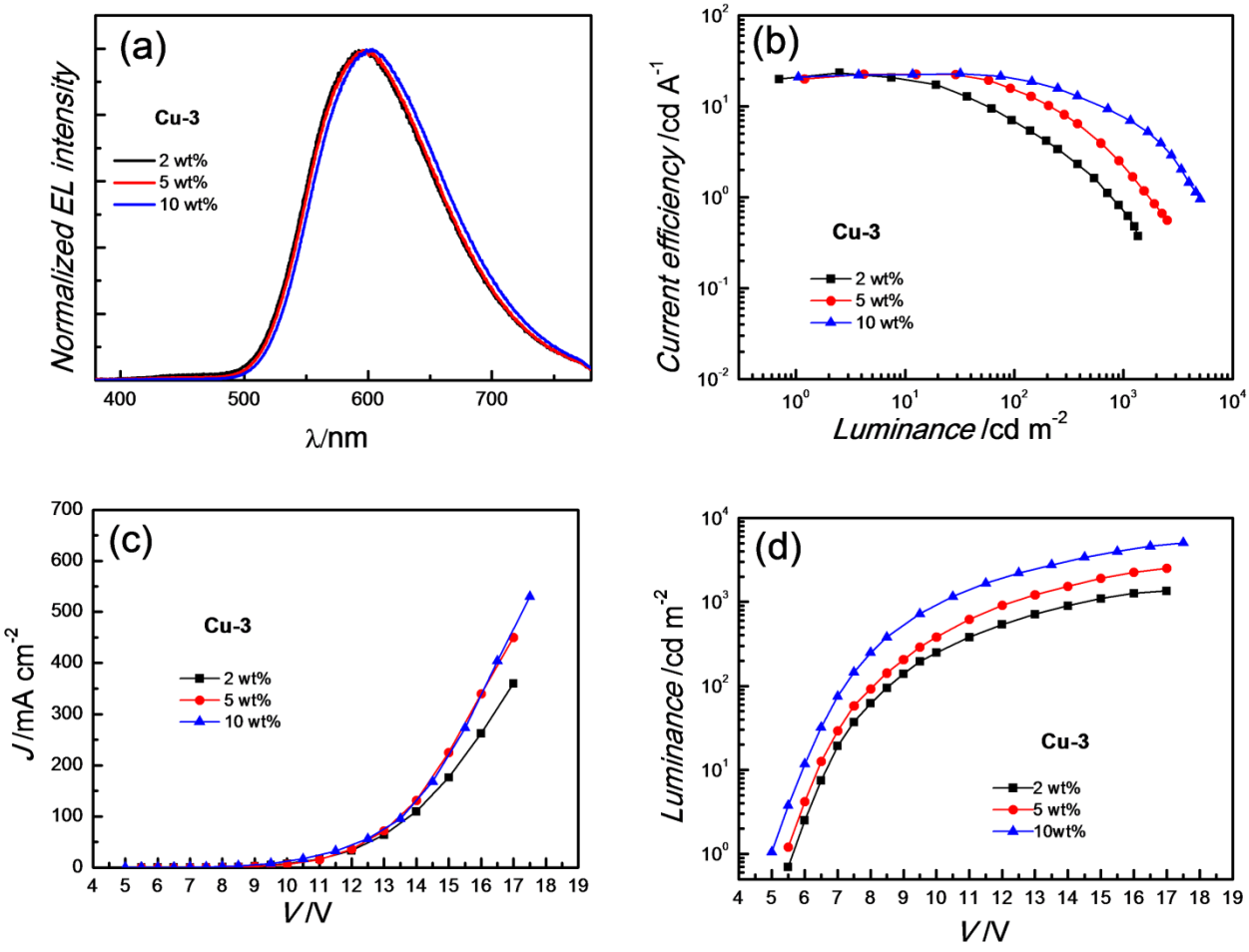


Fig. S25 (a) Normalized EL spectra, (b) current efficiency-luminance, (c) current density-voltage, and (d) luminance-voltage characteristics of PVK/3TPYMB devices based on **Cu-3** at different doping concentrations.

17. EL properties of Cu(pop)(pz_2Bph_2)

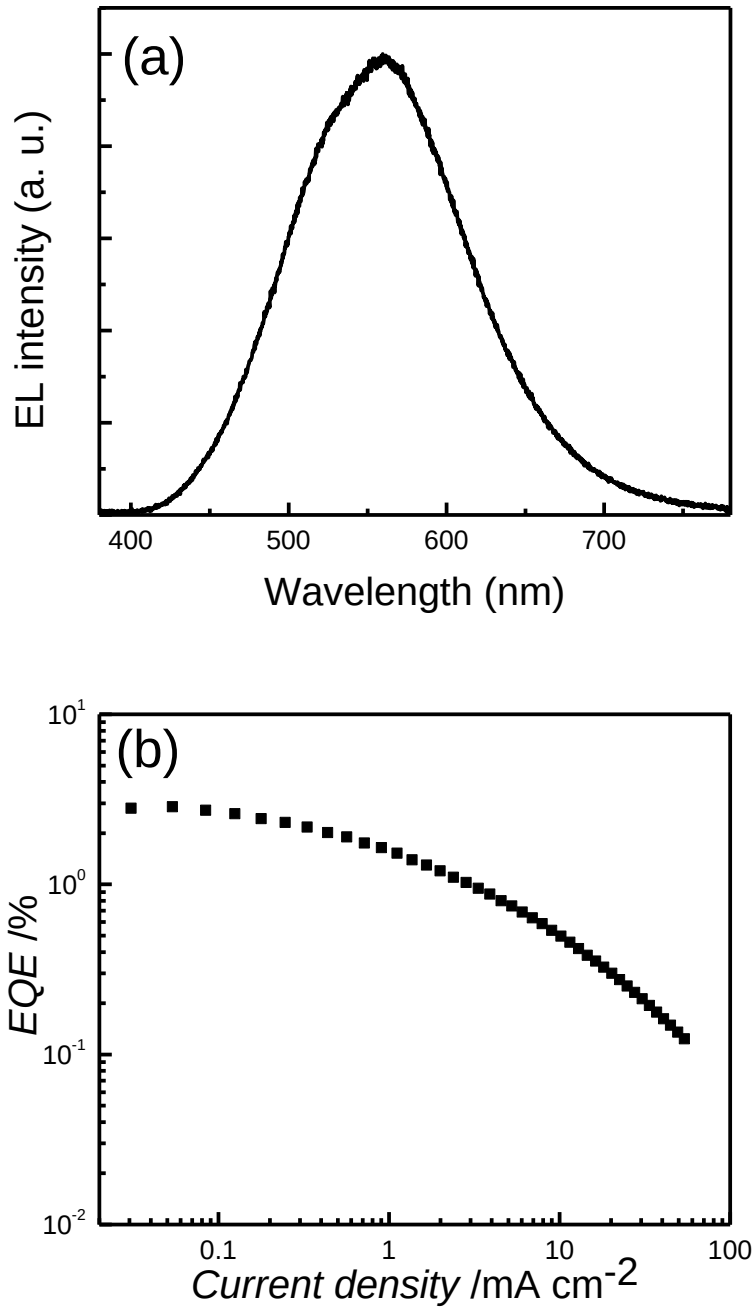


Fig. S26 (a) EL spectrum and (b) current efficiency-luminance characteristics of PYD2/DPEOP devices based on 10 wt% Cu(pop)(pz_2Bph_2).

18. Performances of the white OLEDs with 10 wt% Zn-1 and 1 wt% Cu-3

Table S2 Key performance parameters of the white PLEDs with 10 wt% **Zn-1** and 1 wt% **Cu-3** at different voltages

Voltage (V)	Luminance (cd m^{-2})	CE (cd A^{-1})	EQE (%)	CIE coordinates (x, y)	CRI
7	22	14.67	6.88	(0.44, 0.44)	80
9	300	9.38	4.27	(0.42, 0.44)	81
12	1540	3.67	1.62	(0.38, 0.44)	79
15	3150	1.66	0.73	(0.35, 0.44)	76

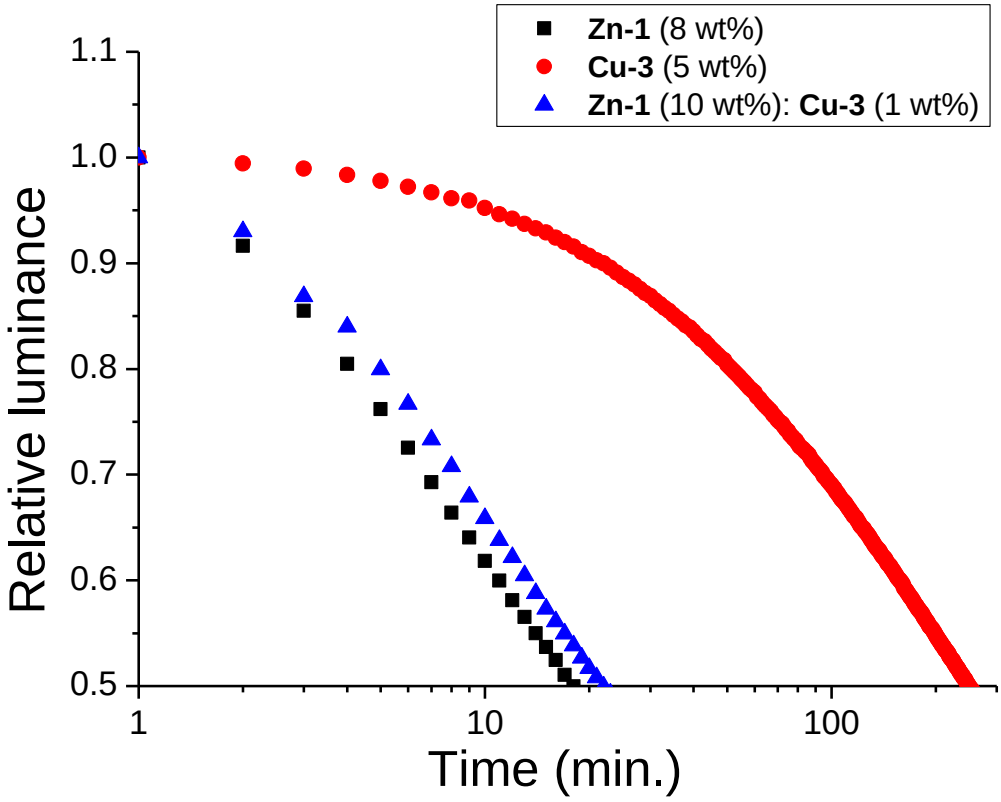
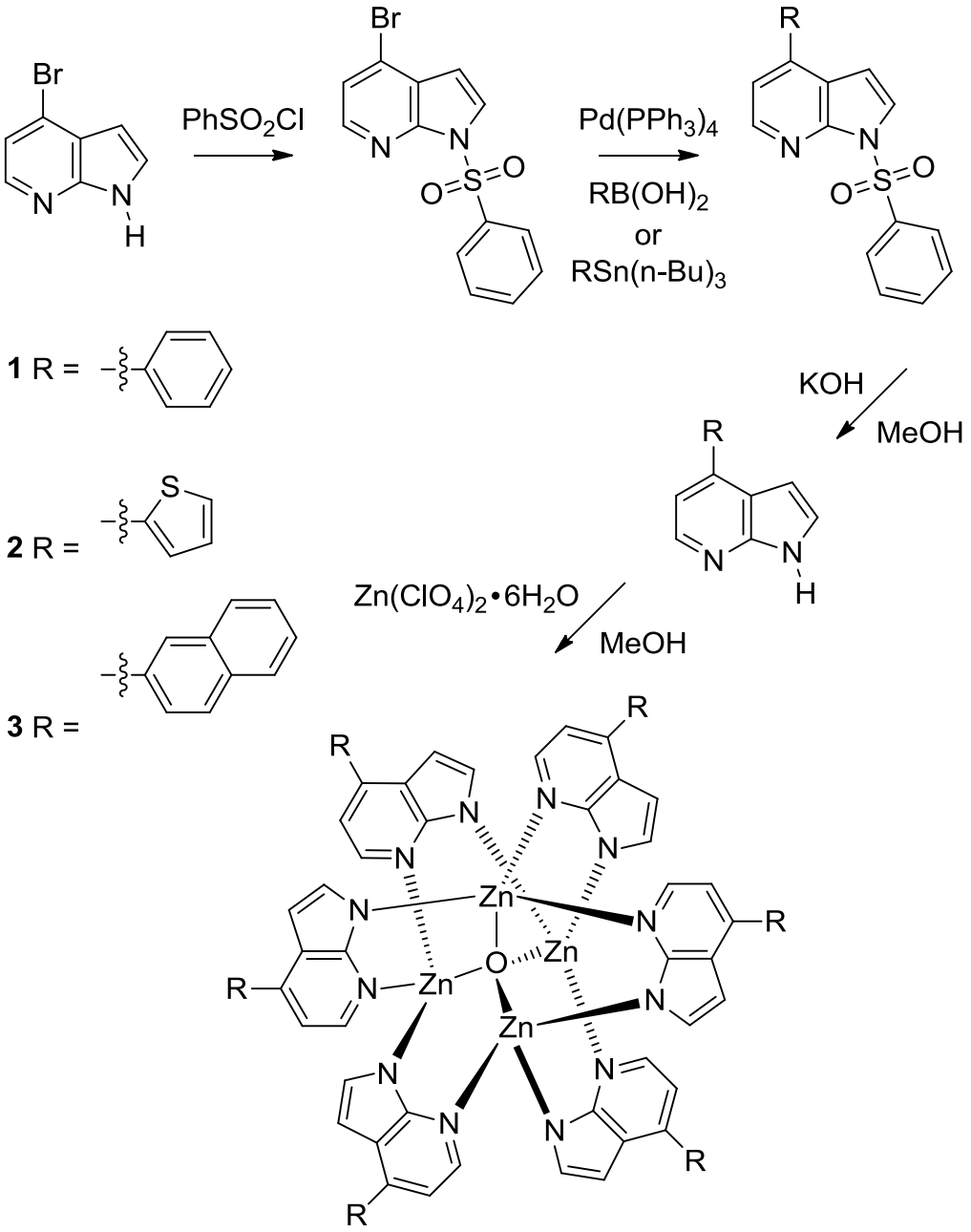


Fig. S27 Device lifetime of solution-processed OLEDs with **Zn-1** (8 wt%), **Cu-3** (5 wt%), as well as that of the white device with both **Zn-1** (10 wt%) and **Cu-3** (1 wt%).

19. Synthesis of Zn(II) complexes

Synethic procedures



4-Bromo-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine. Sodium hydroxide (4.3 g, 107.5 mmol) and benzenesulfonyl chloride (5.5 mL, 43.1 mmol) were added to a solution of 4-bromo-1*H*-pyrrolo[2,3-*b*]pyridine (6.9 g, 35.0 mmol) and benzyltriethylammonium chloride (0.21 g, 0.9 mmol) in dichloromethane (150 mL) under ice-cooling. The reaction mixture was stirred at room temperature for 3 h. The resultant mixture was filtered through Celite and the filtrate was concentrated under reduced pressure. The crude product was purified by column chromatography over silica gel using *n*-hexane/dichloromethane mixture (1:1) as eluent to afford a white solid. The solid was further purified by recrystallization in *n*-hexane/ethyl acetate mixture to give a white solid. Yield: 8.62 g (73%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (d, *J* = 5.2 Hz, 1H), 8.21–8.12 (m, 2H), 7.79 (d, *J* = 4.0 Hz, 1H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.36 (d, *J* = 5.2 Hz, 1H), 6.65 (d, *J* = 4.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 146.83, 145.16, 138.11, 134.38, 129.19, 128.15, 127.00, 125.83, 124.44, 122.23, 105.13. EI-MS (+ve): *m*/*z* 338 $[M + H]^+$.

4-Phenyl-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine. Suzuki coupling was employed to synthesize the compound. A mixture of 4-bromo-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine (3.60 g, 10.68 mmol), phenylboronic acid (1.43 g, 11.73 mmol), tetrakis(triphenylphosphine)palladium(0) (0.62 g, 0.54 mmol) and potassium carbonate solution (2 M, 50 mL) in toluene (250 mL) was refluxed under nitrogen atmosphere for 24 h. After cooling, the toluene layer was washed with water (3 × 250 mL), brine solution (100 mL) and dried over anhydrous magnesium sulphate. The solvent was removed under reduced pressure and the crude product was purified by column chromatography over silica gel using *n*-hexane/dichloromethane mixture (1:1) as eluent to afford a yellow solid. Yield: 2.96 g (83%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.48 (d, *J* = 5.0 Hz, 1H), 8.27–8.20 (m, 2H), 7.78 (d, *J* = 4.1 Hz, 1H), 7.62–7.54 (m, 3H), 7.54–7.41 (m, 5H), 7.24 (d, *J* = 5.0 Hz, 1H), 6.78 (d, *J* = 4.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 147.94, 145.31, 143.34, 138.51, 137.68, 134.15, 129.13, 129.10, 128.95, 128.57, 128.18, 126.57, 120.99, 118.20, 104.90. EI-MS (+ve): *m*/*z* 334 $[M]^+$.

1-(Phenylsulfonyl)-4-(thiophen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine. Stille coupling was employed to synthesize the compound. A mixture of 4-bromo-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine (3.60 g, 10.68 mmol), tributyl(thiophen-2-yl)stannane (3.73 mL, 11.74 mmol) and tetrakis(triphenylphosphine)palladium(0) (0.62 g, 0.54 mmol) in anhydrous *N*,*N*-dimethylformamide (40 mL) was refluxed under nitrogen atmosphere for 24 h. After cooling, the resultant mixture was filtered through Celite and the filtrate was concentrated under reduced pressure. The crude product was purified by column chromatography over silica gel using *n*-hexane/dichloromethane mixture (1:1) as eluent to afford a yellow solid. Yield: 3.49 g (96%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.37 (d, *J* = 5.1 Hz, 1H), 8.25–8.16 (m, 2H), 7.82 (d, *J* = 4.1 Hz, 1H), 7.65–7.44 (m, 5H), 7.36 (d, *J* = 5.2 Hz, 1H), 7.19 (dd, *J* = 5.1, 3.7 Hz, 1H), 7.02 (d, *J* = 4.2 Hz, 1H). ^{13}C NMR (101 MHz, CD_2Cl_2): δ 148.47, 145.22, 140.04, 138.58, 135.84, 134.55, 129.40, 128.61, 128.45, 128.06, 127.60, 127.04, 119.63, 116.96, 105.30. EI-MS (+ve): *m*/*z* 340 $[M]^+$.

4-(Naphthalen-2-yl)-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine. Suzuki coupling was employed to synthesize the compound. A mixture of 4-bromo-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine (3.60 g, 10.68 mmol), naphthalen-2-ylboronic acid (2.02 g, 11.74 mmol), tetrakis(triphenylphosphine)palladium(0) (0.62 g, 0.54 mmol) and potassium carbonate solution (2 M, 50 mL) in toluene (250 mL) was refluxed under nitrogen atmosphere for 24 h. After cooling, the toluene layer was washed with water (3 × 250 mL), brine solution (100 mL) and dried over anhydrous magnesium sulphate. The solvent was removed under reduced pressure and the crude product was purified by column chromatography over silica gel using *n*-hexane/dichloromethane mixture (1:1) as eluent to afford a beige solid. Yield: 3.61 g (88%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.49 (d, *J* = 5.0 Hz, 1H), 8.29–8.20 (m, 2H), 8.08 (s, 1H), 7.98 (d, *J* = 8.5 Hz, 1H), 7.96–7.88 (m, 2H), 7.83 (d, *J* = 4.1 Hz, 1H), 7.71 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.64–7.47 (m, 5H), 7.37 (d, *J* = 5.0 Hz, 1H), 6.87 (d, *J* = 4.1 Hz, 1H). ^{13}C NMR (101 MHz, CD_2Cl_2): δ 148.24, 145.37, 143.45, 138.70, 135.32, 134.51, 133.76, 133.62, 129.41, 129.08, 128.69, 128.45, 128.28, 128.07, 127.23, 127.07, 126.99, 126.36, 121.37, 118.71, 105.15. EI-MS (+ve): *m*/*z* 384 $[M]^+$.

4-Phenyl-1*H*-pyrrolo[2,3-*b*]pyridine. A mixture of 4-phenyl-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine (1.10 g, 3.29 mmol) and 10 % potassium hydroxide (20 mL) in methanol (200 mL) was stirred at room temperature for 24 h. The methanol in the reaction mixture was removed under reduced pressure. The resultant mixture was diluted with water (30 mL) and extracted with dichloromethane (3 × 50 mL). The combined organic layer was dried over anhydrous magnesium sulphate. The solvent was removed under reduced pressure and the crude product was purified by column chromatography over silica gel using dichloromethane/methanol mixture (9:1) as eluent to afford a pink solid. Yield: 0.59 g (92%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 10.76 (s, 1H), 8.40 (d, *J* = 5.0 Hz, 1H), 7.86–7.76 (m, 2H), 7.62–7.51 (m, 2H), 7.51–7.43 (m, 2H), 7.22 (d, *J* = 4.9 Hz, 1H), 6.74 (d, *J* = 3.4 Hz, 1H). ^{13}C NMR (101 MHz, [D_6]DMSO): δ 149.15, 142.93, 140.26, 138.49, 128.96, 128.33, 128.20, 126.60, 117.23, 114.18, 98.95. EI-MS (+ve): *m*/*z* 194 $[M]^+$.

4-(Thiophen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine. A mixture of 1-(phenylsulfonyl)-4-(thiophen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine (1.12 g, 3.29 mmol) and 10% potassium hydroxide (20 mL) in methanol (200 mL) was stirred at room temperature for 24 h. The methanol in the reaction mixture was removed under reduced pressure.

The resultant mixture was diluted with water (30 mL) and extracted with dichloromethane (3 × 50 mL). The combined organic layer was dried over anhydrous magnesium sulphate. The solvent was removed under reduced pressure and the crude product was purified by column chromatography over silica gel using dichloromethane/methanol mixture (9:1) as eluent to afford a yellow solid. Yield: 0.55 g (83%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 10.82 (s, 1H), 8.34 (t, *J* = 4.7 Hz, 1H), 7.70 (td, *J* = 4.1, 1.1 Hz, 1H), 7.60–7.44 (m, 2H), 7.34 (t, *J* = 4.7 Hz, 1H), 7.27–7.18 (m, 1H), 6.93 (t, *J* = 3.7 Hz, 1H). ^{13}C NMR (101 MHz, [D_6]DMSO): δ 149.50, 142.81, 140.75, 132.75, 128.40, 127.55, 126.91, 126.77, 115.58, 112.60, 99.43. EI-MS (+ve): *m*/*z* 200 $[M]^+$.

4-(Naphthalen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine. A mixture of 4-(naphthalen-2-yl)-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine (1.26 g, 3.28 mmol) and 10% potassium hydroxide (20 mL) in methanol (200 mL) was stirred at room temperature for 24 h. The methanol in the reaction mixture was removed under reduced pressure. The resultant mixture was diluted with water (30 mL) and extracted with dichloromethane (3 × 50 mL). The combined organic layer was dried over anhydrous magnesium sulphate. The solvent was removed under reduced pressure and the crude product was purified by column chromatography over silica gel using dichloromethane/methanol mixture (9:1) as eluent to afford a beige solid. Yield: 0.60 g (75%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 9.78 (s, 1H), 8.41 (d, *J* = 5.0 Hz, 1H), 8.26 (s, 1H), 8.02 (d, *J* = 8.5 Hz, 1H), 8.00–7.88 (m, 3H), 7.60–7.53 (m, 2H), 7.47 (t, *J* = 2.9 Hz, 1H), 7.33 (d, *J* = 5.0 Hz, 1H), 6.81 (dd, *J* = 3.5, 1.9 Hz, 1H). ^{13}C NMR (101 MHz, [D_6]DMSO): δ 149.23, 142.97, 140.13, 135.97, 133.15, 132.66, 128.47, 128.40, 127.56, 127.28, 126.74, 126.59, 126.53, 126.13, 117.42, 114.51, 99.13. EI-MS (+ve): *m*/*z* 244 $[M]^+$.

[Zn_4O(AID-4-Phenyl)$_6$] (Zn-1). A solution of zinc perchlorate hexahydrate (0.37 g, 1 mmol) in methanol (30 mL) was added dropwise to a hot solution of 4-phenyl-1*H*-pyrrolo[2,3-*b*]pyridine (0.29 g, 1.5 mmol) and triethylamine (1 mL) in methanol (20 mL). The reaction mixture was stirred at 60 °C for 3 h. After cooling, the resultant mixture was filtered and the residue was washed with hot methanol (3 × 10 mL). The solid collected was dissolved in dichloromethane (20 mL) and filtered through Celite. The filtrate was concentrated under reduced pressure and added dropwise to methanol (10 mL). The white solid precipitated was collected by centrifugation and dried under vacuum at 40 °C for 24 h. Yield: 0.25 g (71%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.06–7.80 (m, 6H), 7.80–7.54 (m, 18H), 7.54–7.27 (m, 18H), 7.10–6.99 (m, 6H), 6.85–6.67 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 156.30–155.37 (m), 144.76–143.33 (m), 139.80–137.56 (m), 129.85–127.79 (m), 124.36–123.23 (m), 113.24–112.11 (m), 101.29–100.27 (m). FAB-MS (+ve): *m*/*z* 1436 $[M]^+$. Elemental analyses calcd. for $C_{78}H_{54}N_{12}OZn_4 \cdot CH_2Cl_2$: C 62.35, H 3.71, N 11.04; found: C 62.34, H 3.91, N 10.78.

[Zn_4O(AID-4-Thiophen-2-yl)$_6$] (Zn-2). A solution of zinc perchlorate hexahydrate (0.37 g, 1 mmol) in methanol (30 mL) was added dropwise to a hot solution of 4-(thiophen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine (0.30 g, 1.5 mmol) and triethylamine (1 mL) in methanol (20 mL). The reaction mixture was stirred at 60 °C for 3 h. After cooling, the resultant mixture was filtered and the residue was washed with hot methanol (3 × 10 mL). The solid collected was dissolved in dichloromethane (20 mL) and filtered through Celite. The filtrate was concentrated under reduced pressure and added dropwise to methanol (10 mL). The yellow solid precipitated was collected by centrifugation and dried under vacuum at 40 °C for 24 h. Yield: 0.31 g (84%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.00–7.34 (m, 24H), 7.23–7.06 (m, 12H), 7.06–6.89 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 156.58–155.79 (m), 142.07–141.15 (m), 139.95–137.28 (m), 136.91–135.60 (m), 128.78–126.39 (m), 122.70–121.39 (m), 111.86–110.88 (m), 101.87–100.71 (m). FAB-MS (+ve): *m*/*z* 1473 $[M + H]^+$. Elemental analyses calcd. for $C_{66}H_{42}N_{12}OS_6Zn_4$: C 53.81, H 2.87, N 11.41; found: C 53.82, H 3.09, N 11.34.

[Zn_4O(AID-4-Naphthalen-2-yl)$_6$] (Zn-3). A solution of zinc perchlorate hexahydrate (0.37 g, 1 mmol) in methanol (30 mL) was added dropwise to a hot solution of 4-(naphthalen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine (0.37 g, 1.5 mmol) and triethylamine (1 mL) in methanol (20 mL). The reaction mixture was stirred at 60 °C for 3 h. After cooling, the resultant mixture was filtered and the residue was washed with hot methanol (3 × 10 mL). The solid collected was dissolved in dichloromethane (20 mL) and filtered through Celite. The filtrate was concentrated under reduced pressure and added dropwise to methanol (10 mL). The yellow solid precipitated was collected by

centrifugation and dried under vacuum at 40 °C for 24 h. Yield: 0.26 g (60%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.37–8.18 (m, 6H), 8.17–7.60 (m, 36H), 7.59–7.43 (m, 12H), 7.24–7.12 (m, 6H), 7.04–6.81 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 156.29–155.57 (m), 144.54–143.56 (m), 139.78–137.63 (m), 137.17–136.29 (m), 134.03–132.58 (m), 129.63–125.40 (m), 124.54–123.44 (m), 113.56–112.57 (m), 101.42–100.39 (m). FAB-MS (+ve): *m*/*z* 1737 $[M]^+$. Elemental analyses calcd. for $C_{102}H_{66}N_{12}OZn_4$: C 70.52, H 3.83, N 9.67; found: C 70.57, H 4.13, N 9.33.

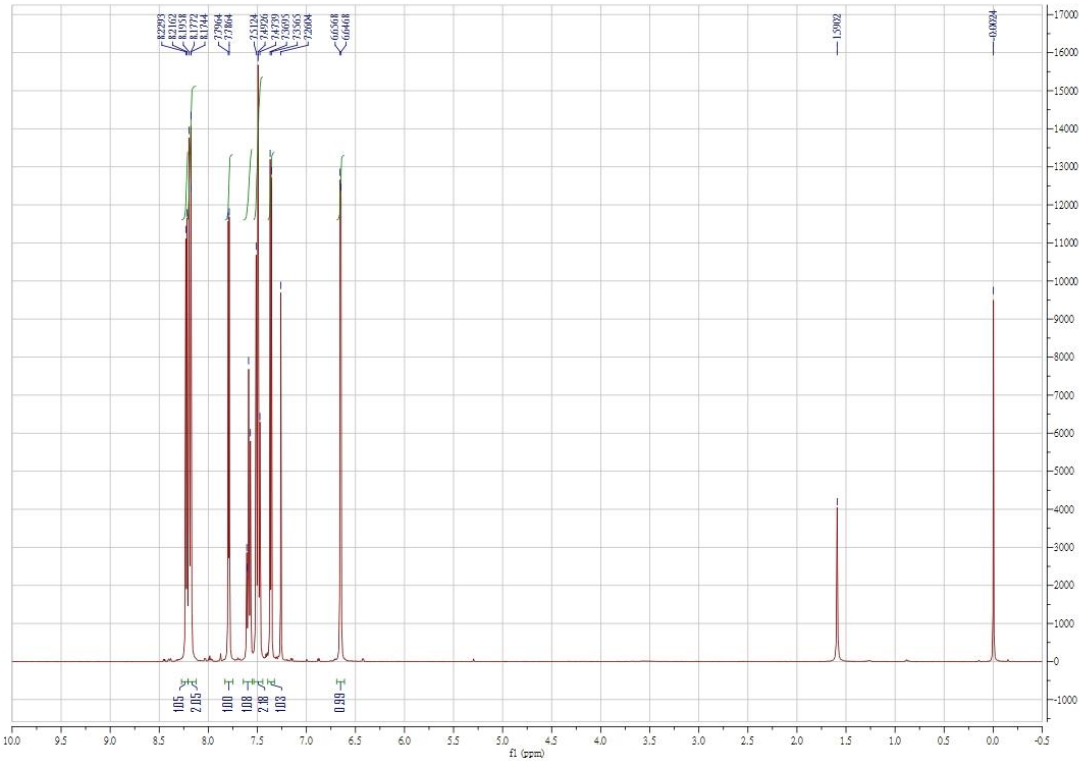


Fig. S28 ^{1}H NMR spectrum of 4-bromo-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine in $CDCl_3$.

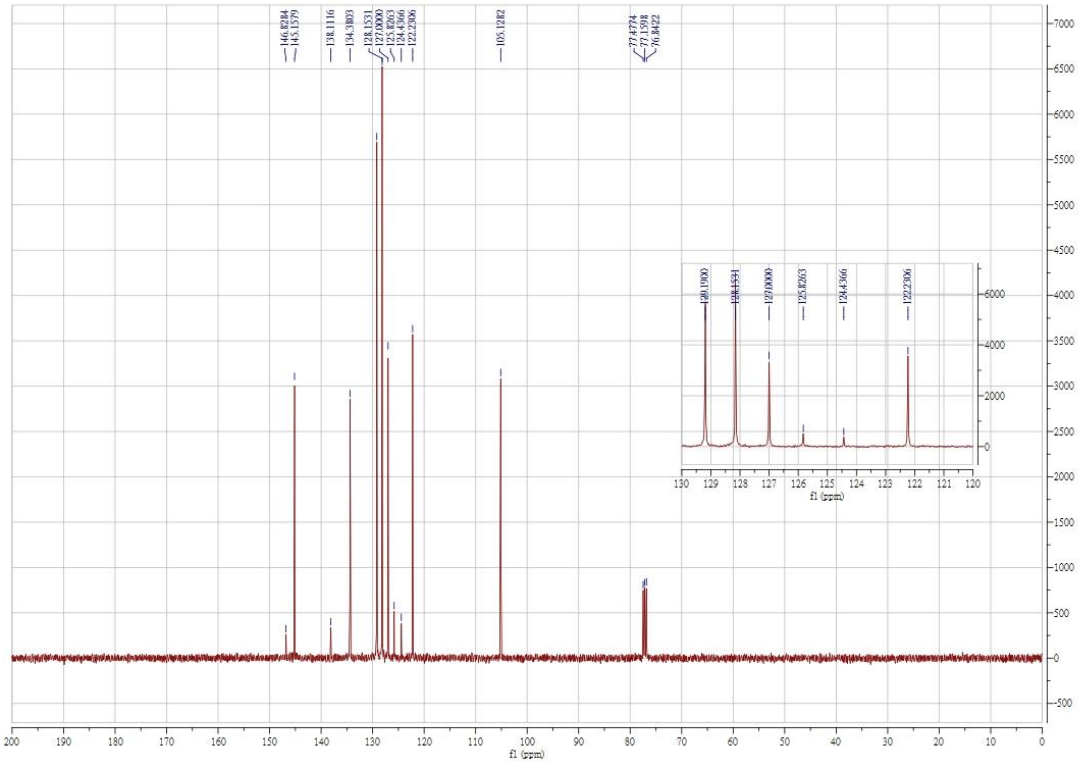


Fig. S29 ^{13}C NMR spectrum of 4-bromo-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine in $CDCl_3$.

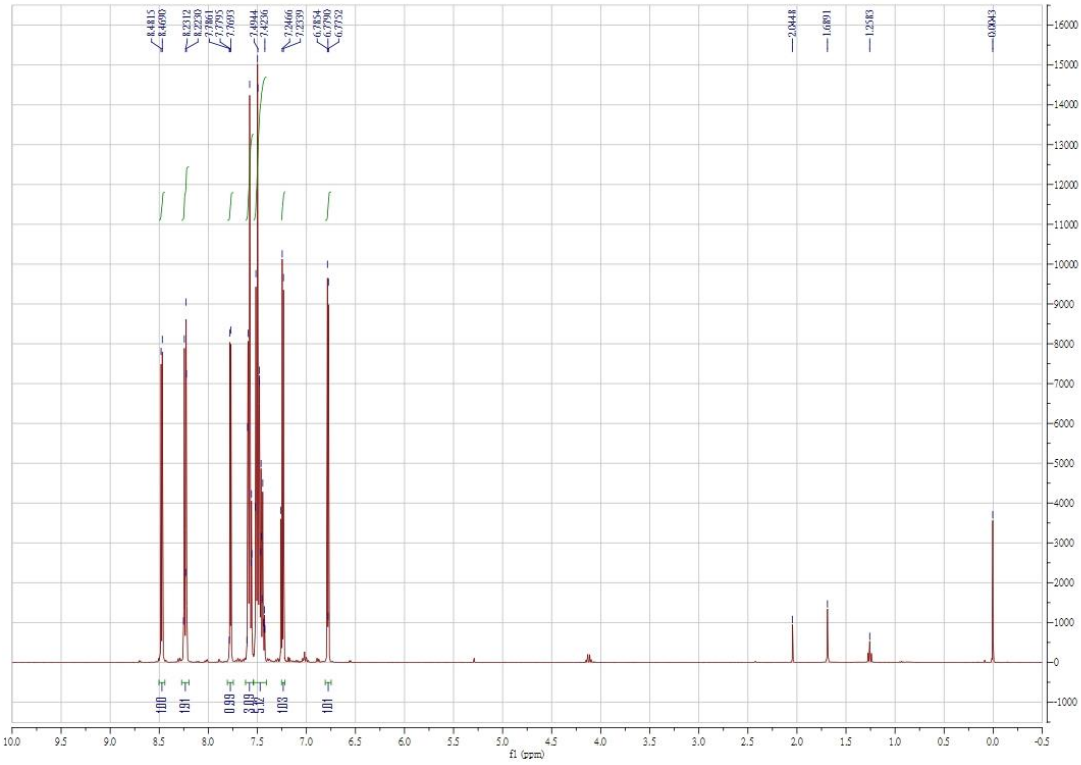


Fig. S30 ^{1}H NMR spectrum of 4-phenyl-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine in $CDCl_3$.

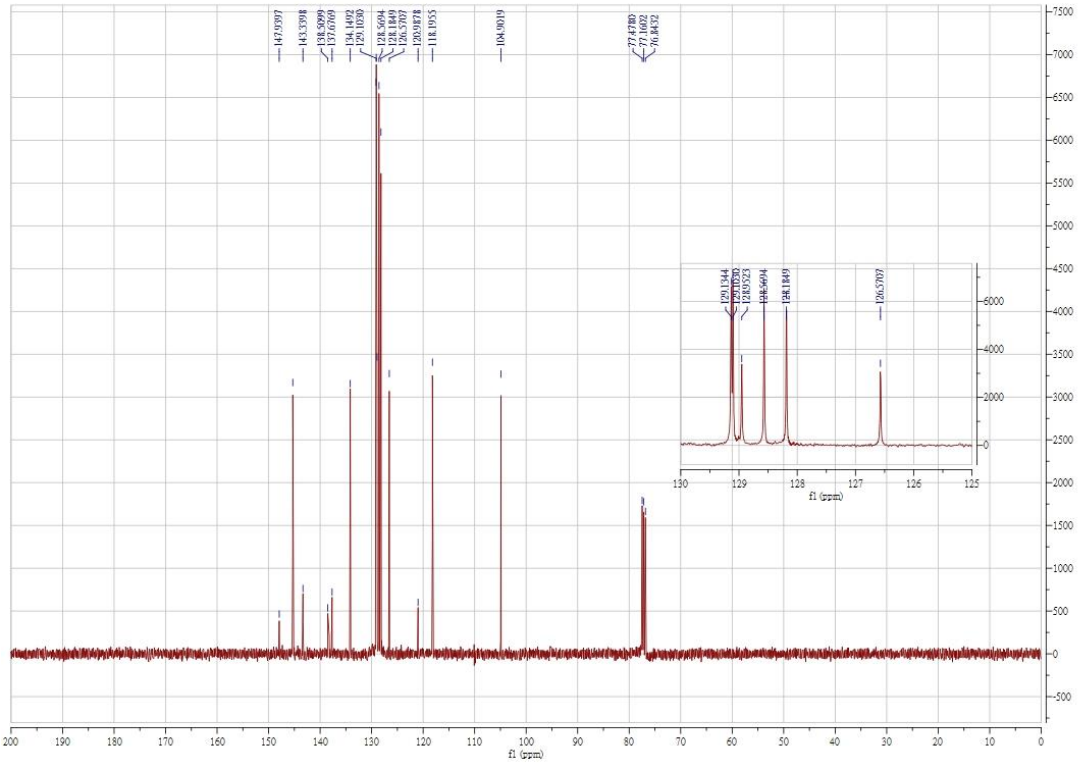


Fig. S31 ^{13}C NMR spectrum of 4-phenyl-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine in $CDCl_3$.

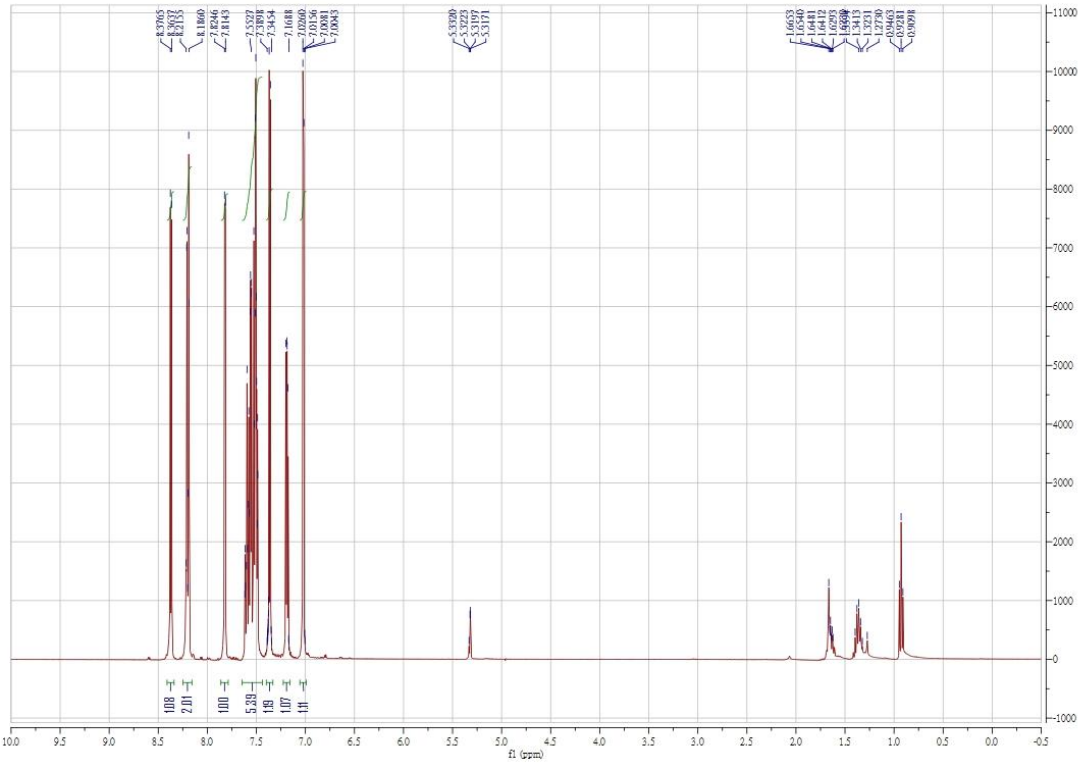


Fig. S32 ^{1}H NMR spectrum of 1-(phenylsulfonyl)-4-(thiophen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine in CD_2Cl_2.

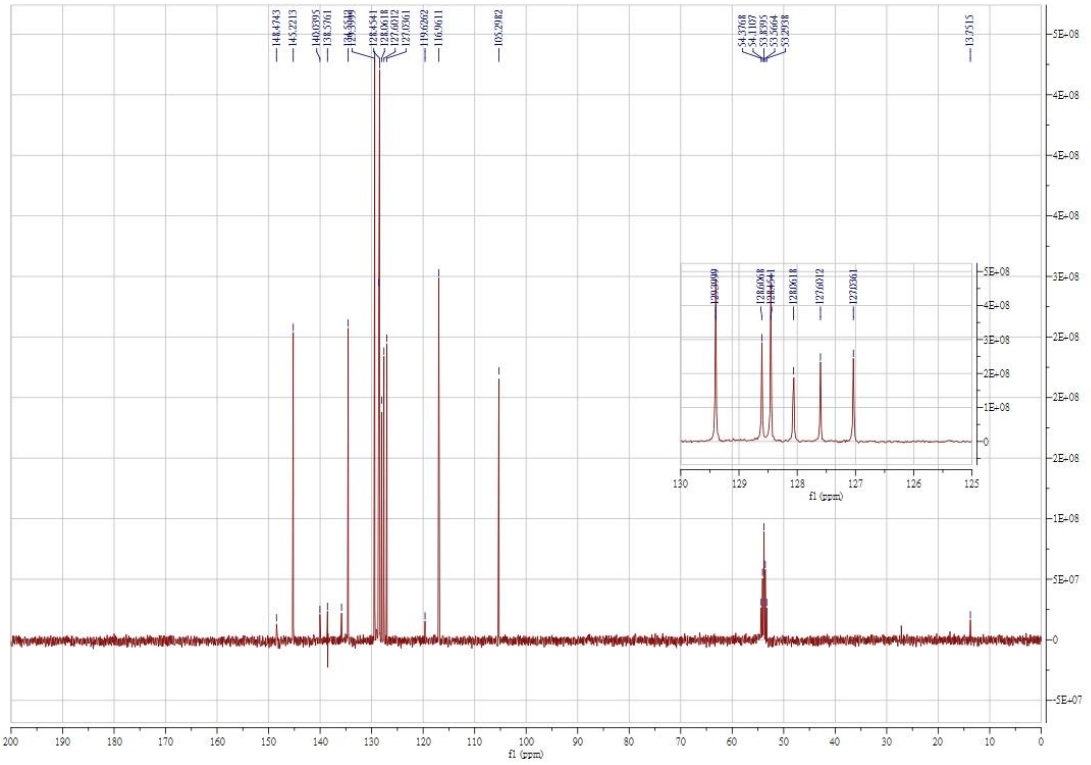


Fig. S33 ^{13}C NMR spectrum of 1-(phenylsulfonyl)-4-(thiophen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine in CD_2Cl_2.

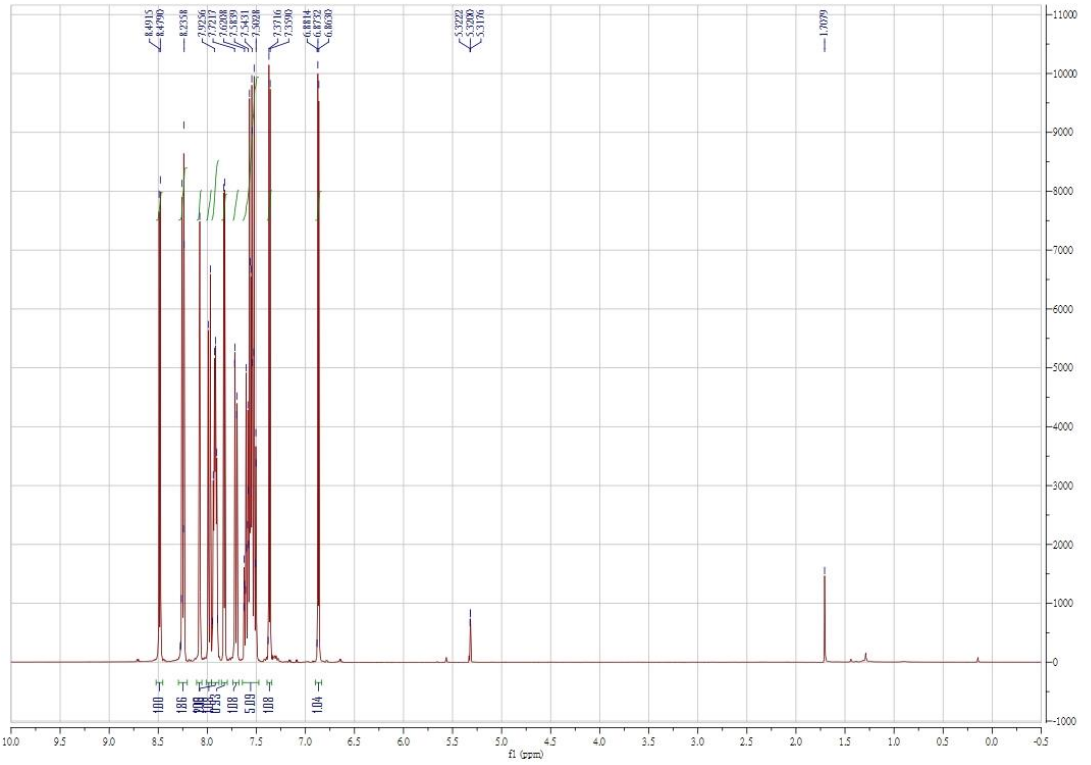


Fig. S34 ^{1}H NMR spectrum of 4-(naphthalen-2-yl)-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine in CD_2Cl_2.

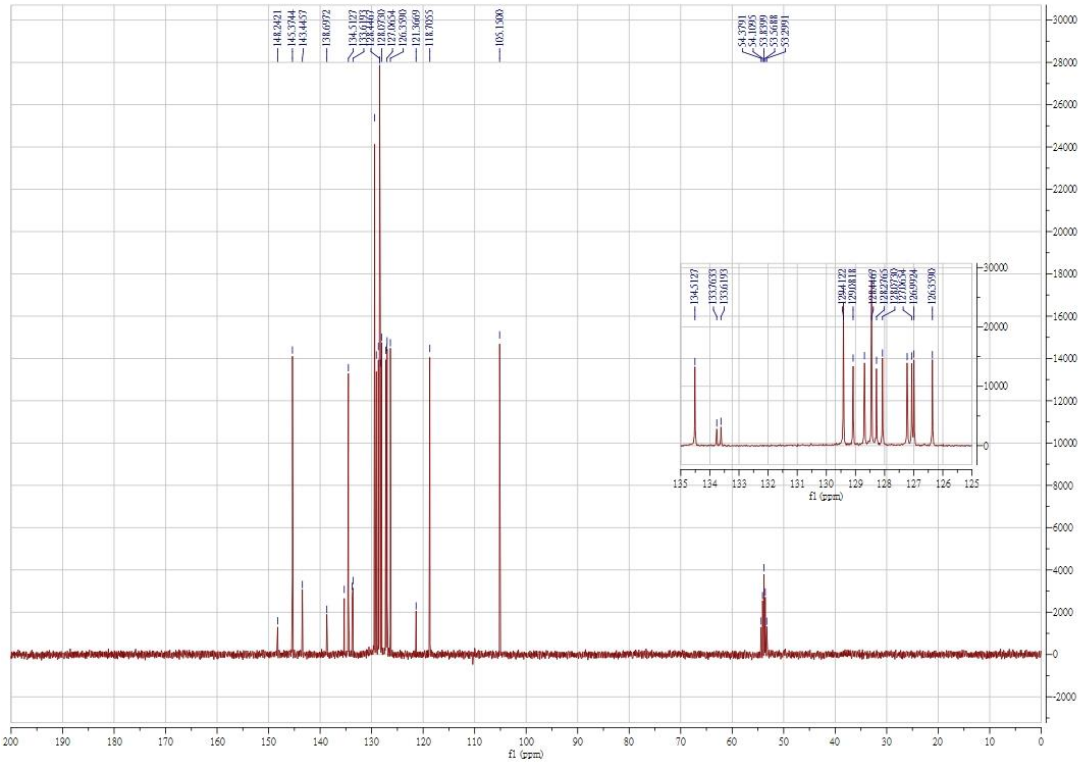


Fig. S35 ^{13}C NMR spectrum of 4-(naphthalen-2-yl)-1-(phenylsulfonyl)-1*H*-pyrrolo[2,3-*b*]pyridine in CD_2Cl_2.

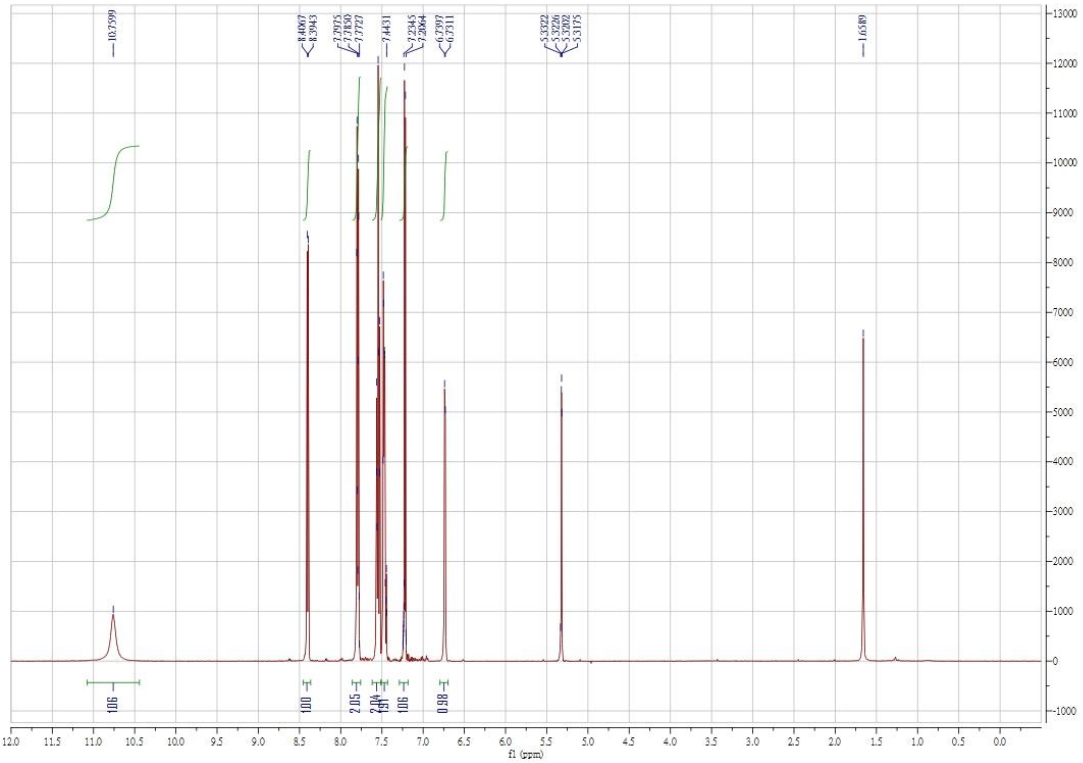


Fig. S36 ^{1}H NMR spectrum of 4-phenyl-1*H*-pyrrolo[2,3-*b*]pyridine in CD_2Cl_2.

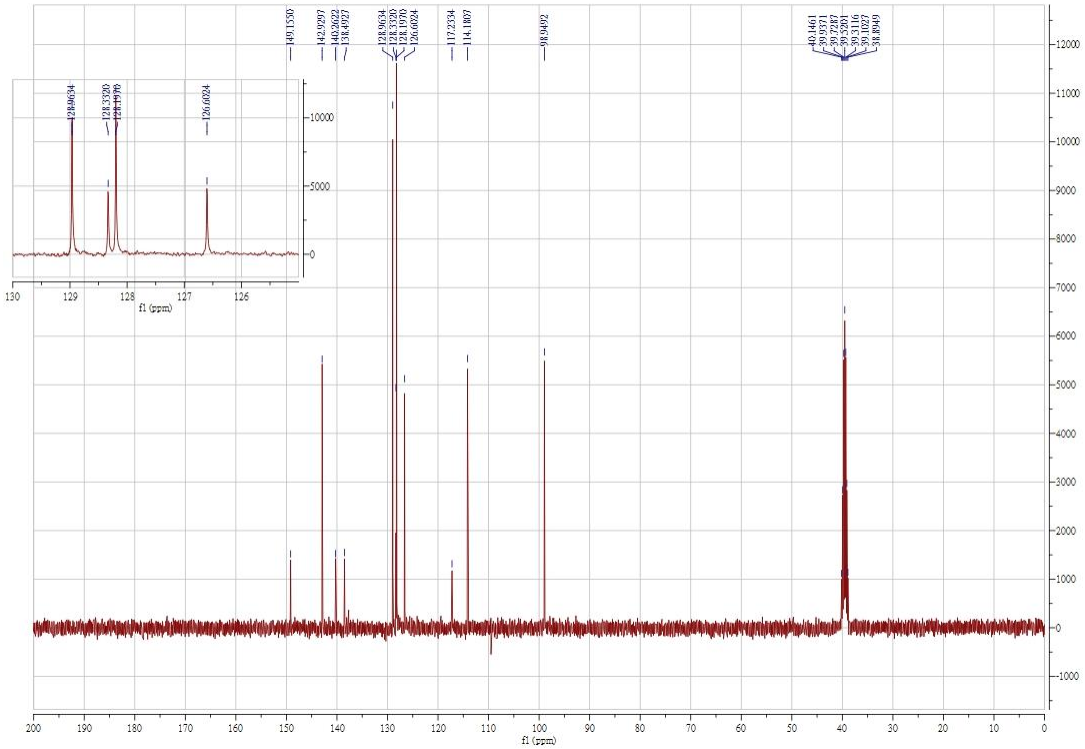


Fig. S37 ^{13}C NMR spectrum of 4-phenyl-1*H*-pyrrolo[2,3-*b*]pyridine in [D_6]DMSO.

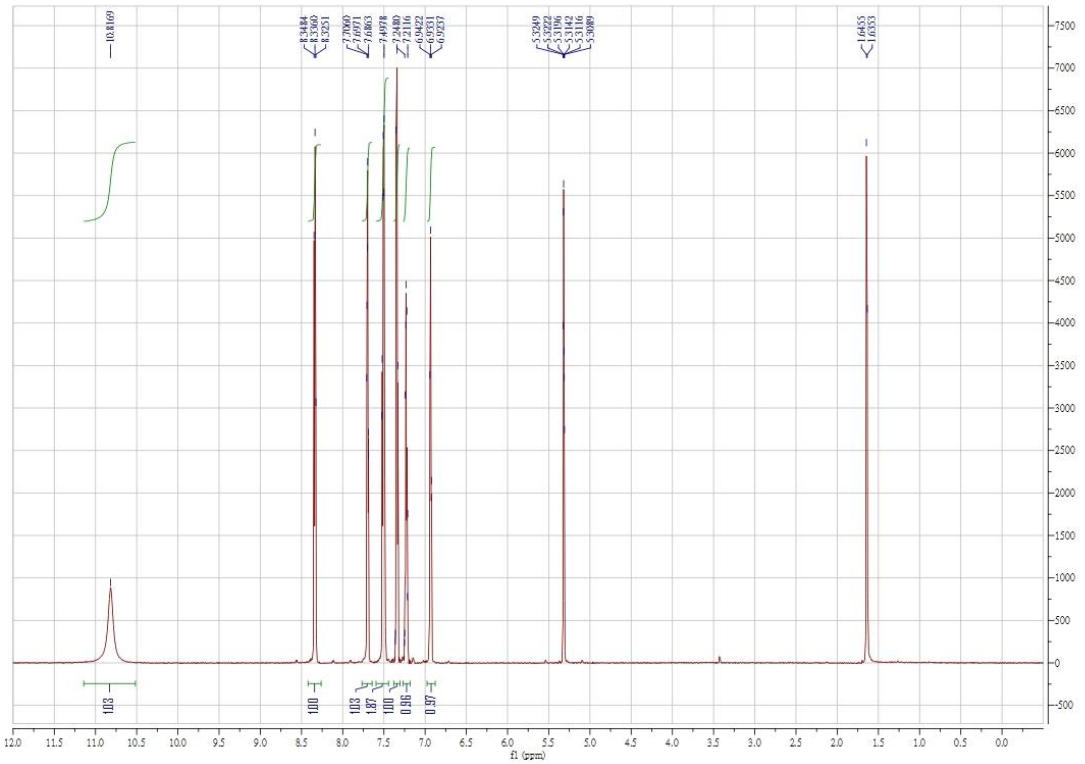


Fig. S38 ^{1}H NMR spectrum of 4-(thiophen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine in CD_2Cl_2.

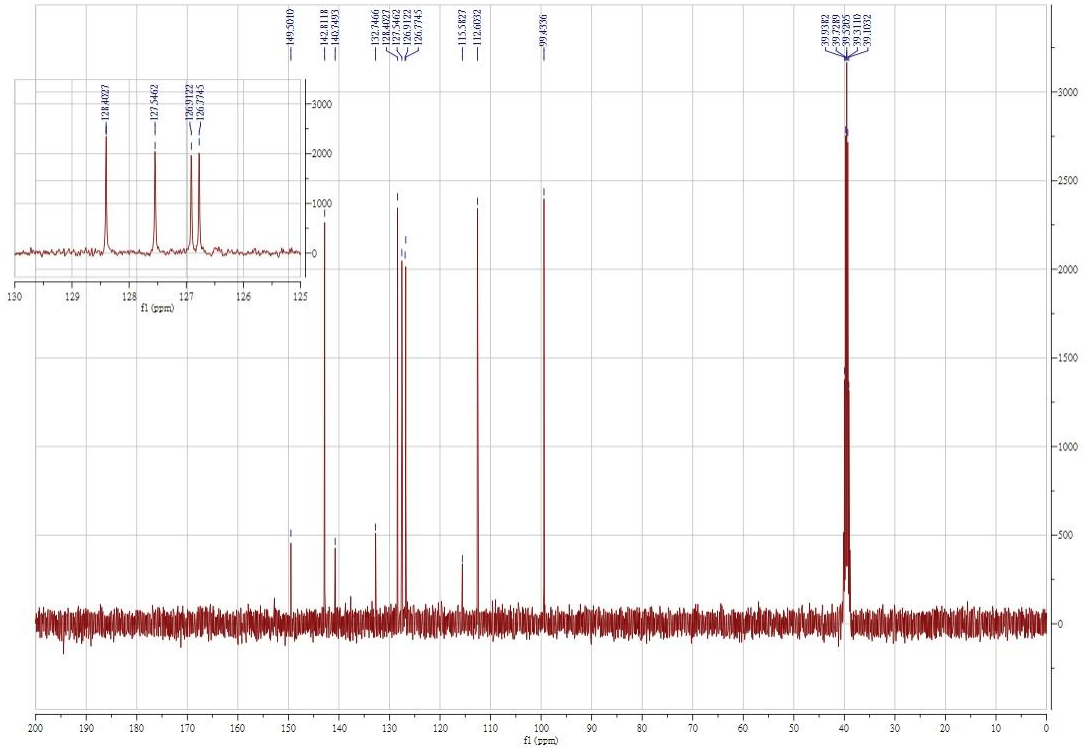


Fig. S39 ^{13}C NMR spectrum of 4-(thiophen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine in [D_6]DMSO.

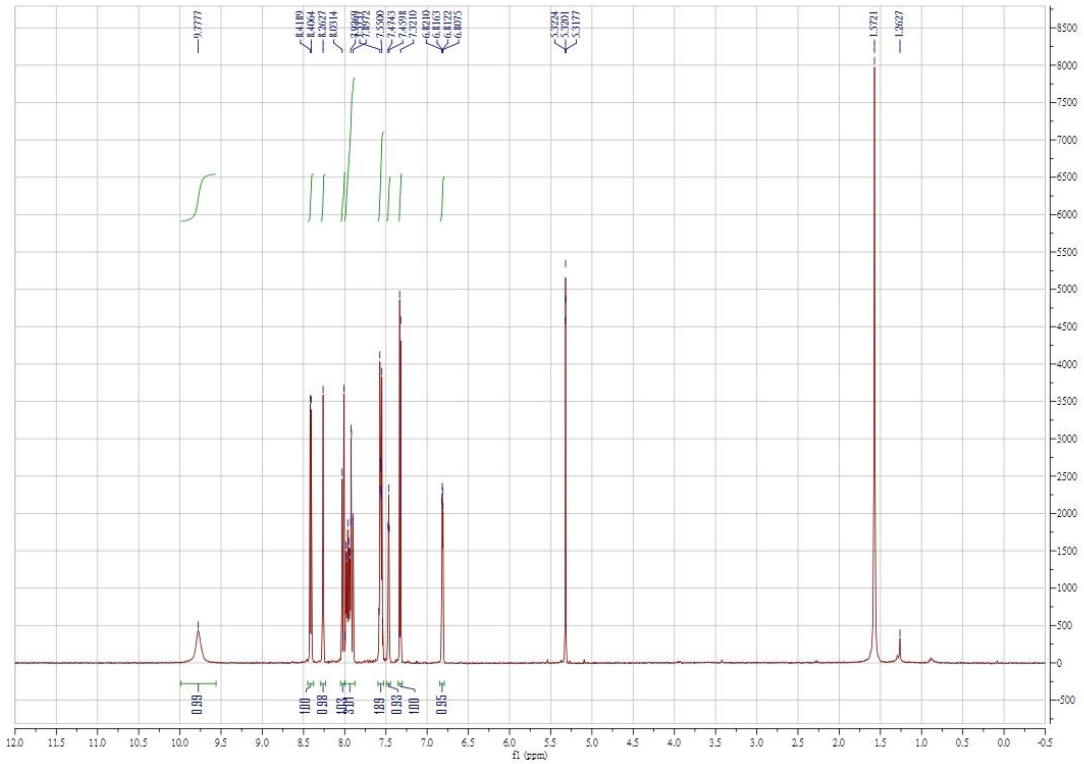


Fig. S40 ^{1}H NMR spectrum of 4-(naphthalen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine in CD_2Cl_2.

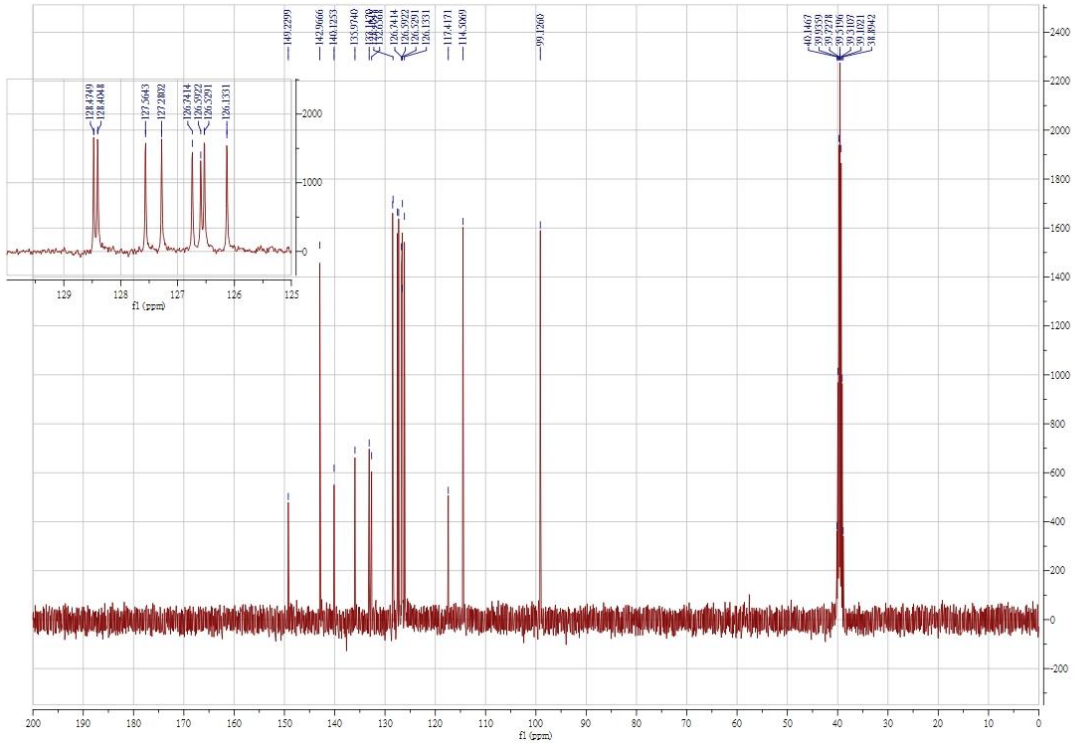


Fig. S41 ^{13}C NMR spectrum of 4-(naphthalen-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine in [D_6]DMSO.

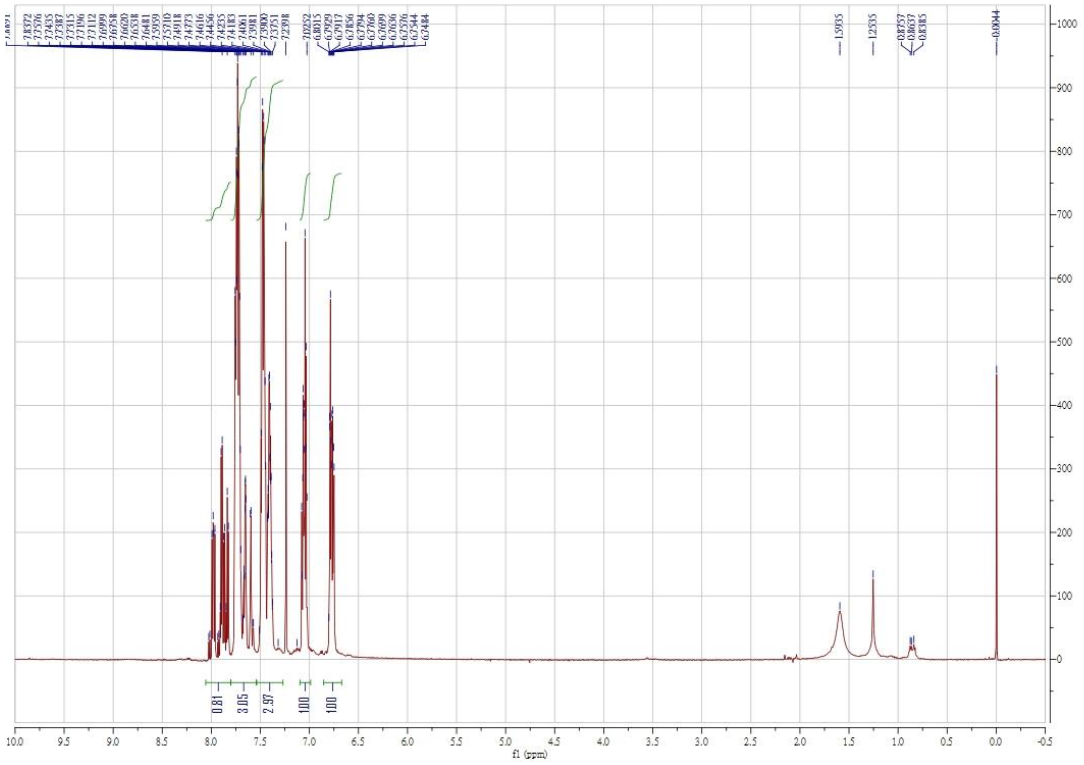


Fig. S42 ^{1}H NMR spectrum of [Zn_4O(AID-4-Phenyl)$_6$] (**Zn-1**) in $CDCl_3$.

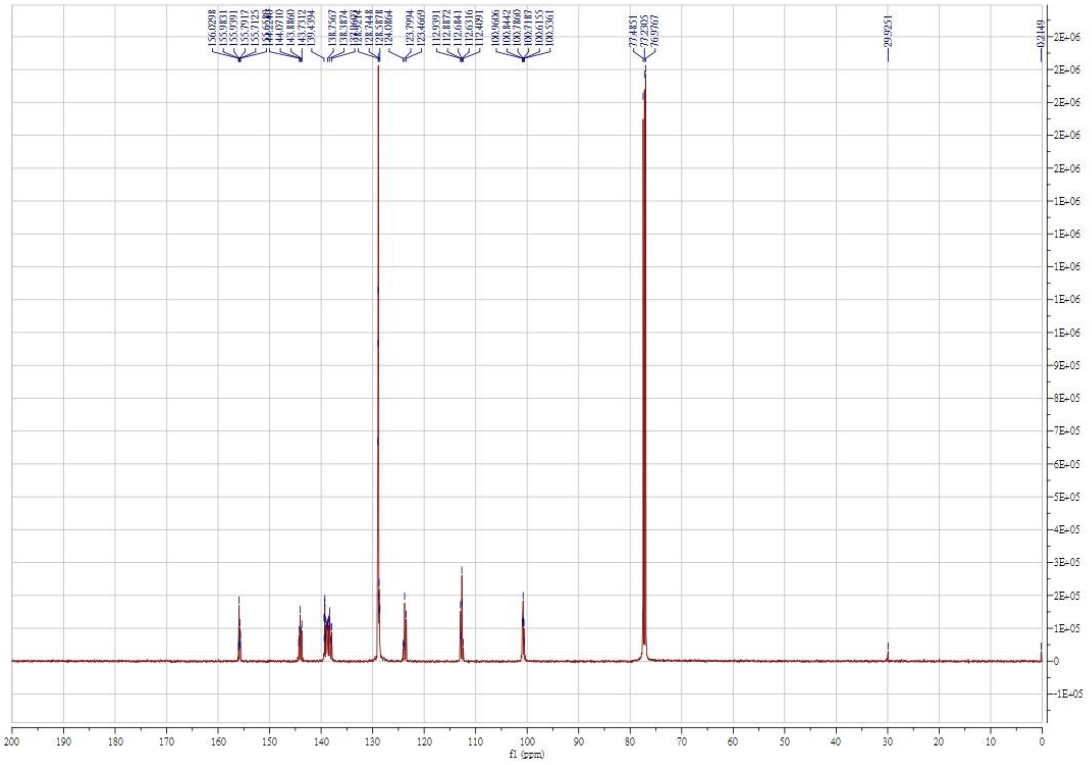


Fig. S43 ^{13}C NMR spectrum of $[Zn_4O(AID\text{-}4\text{-}Phenyl)_6]$ (**Zn-1**) in $CDCl_3$.

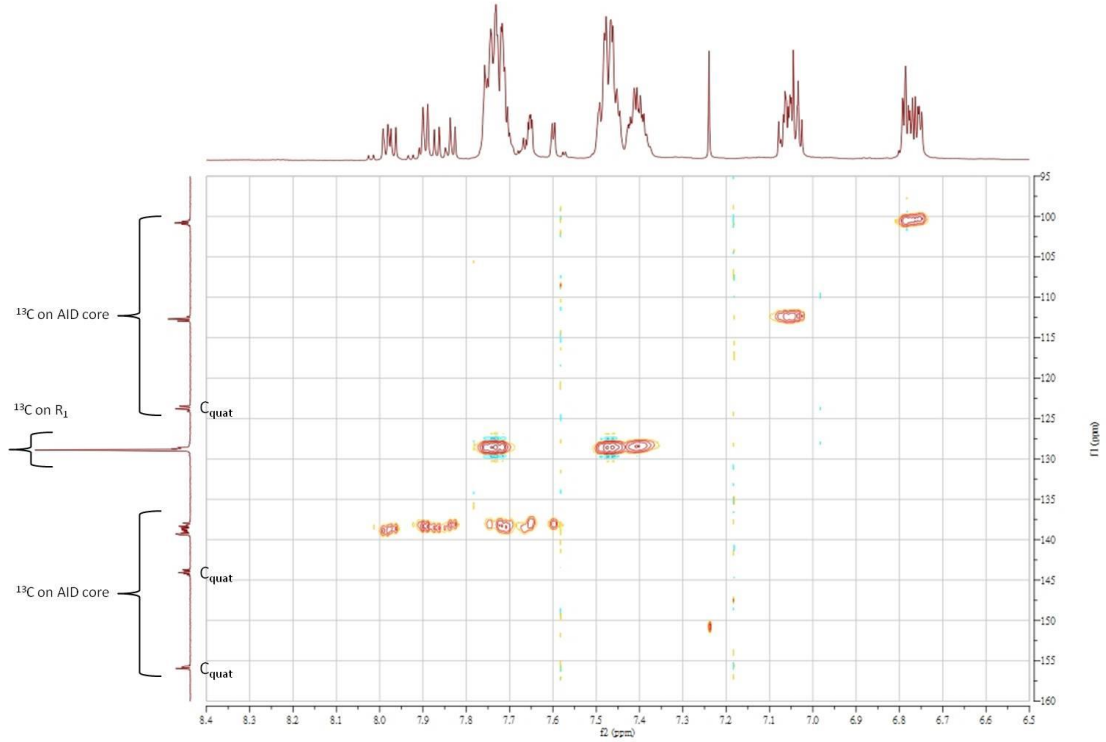


Fig. S44 ^{1}H-^{13}C HSQC NMR spectrum of $[Zn_4O(AID\text{-}4\text{-}Phenyl)_6]$ (**Zn-1**) in $CDCl_3$.

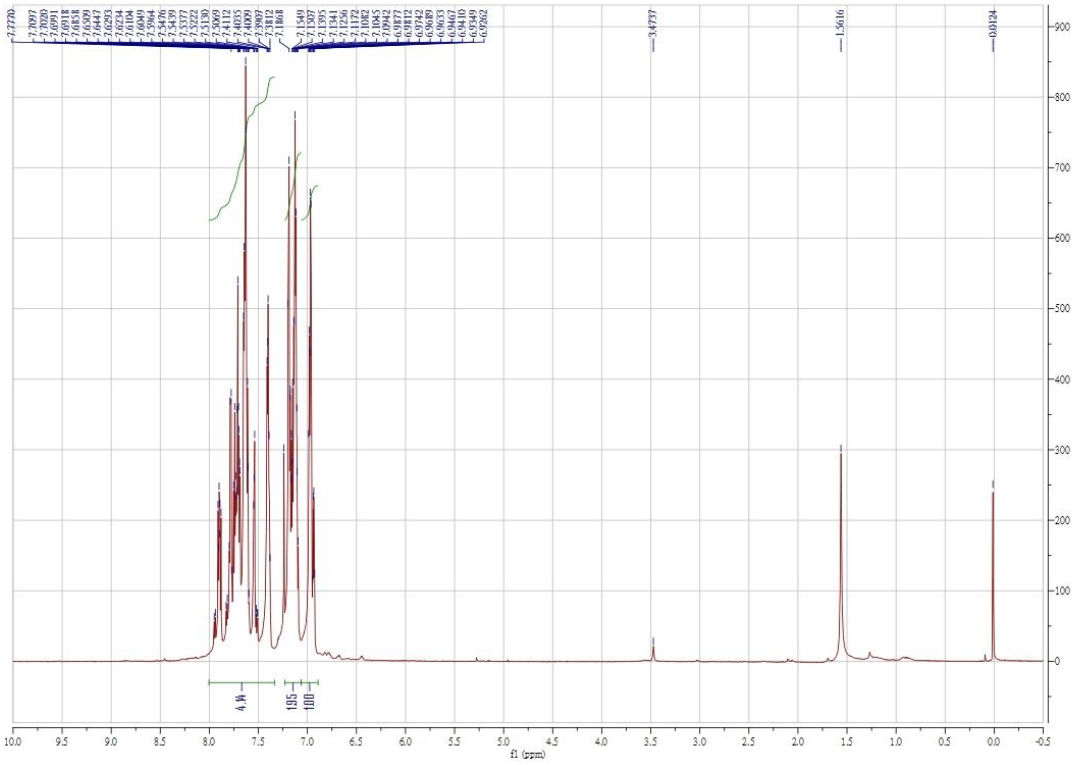


Fig. S45 ^{1}H NMR spectrum of [Zn_4O(AID-4-Thiophen-2-yl)$_6$] (**Zn-2**) in $CDCl_3$.

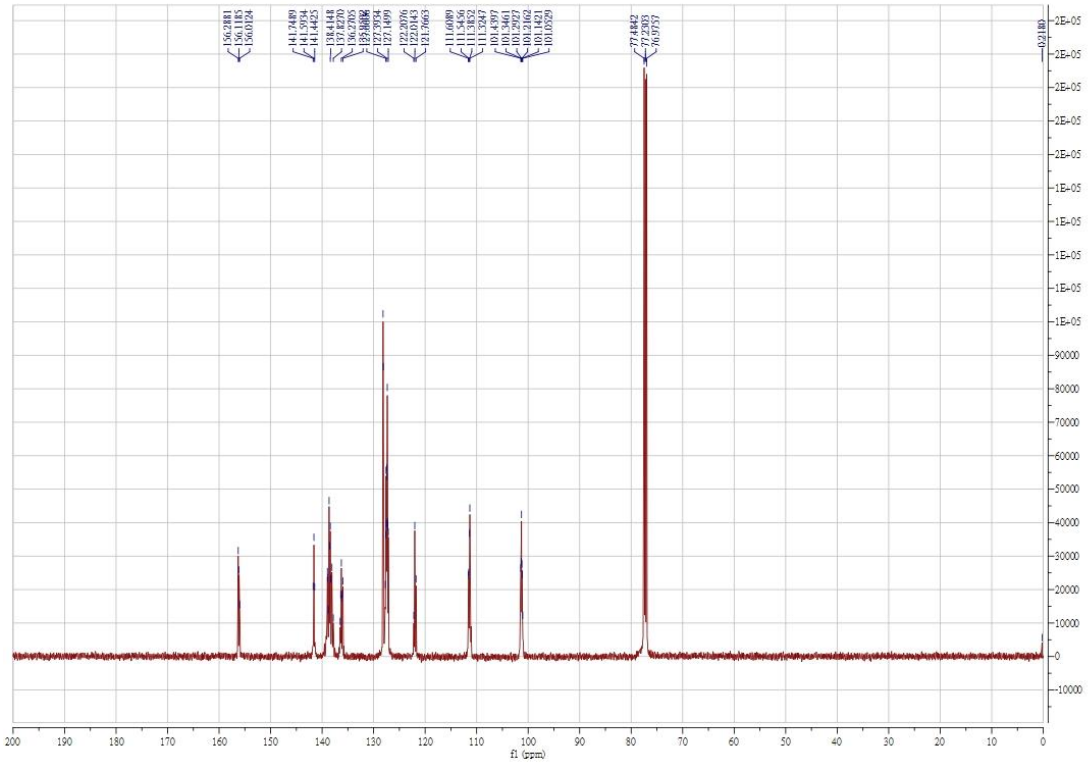


Fig. S46 ^{13}C NMR spectrum of [Zn_4O(AID-4-Thiophen-2-yl)$_6$] (**Zn-2**) in $CDCl_3$.

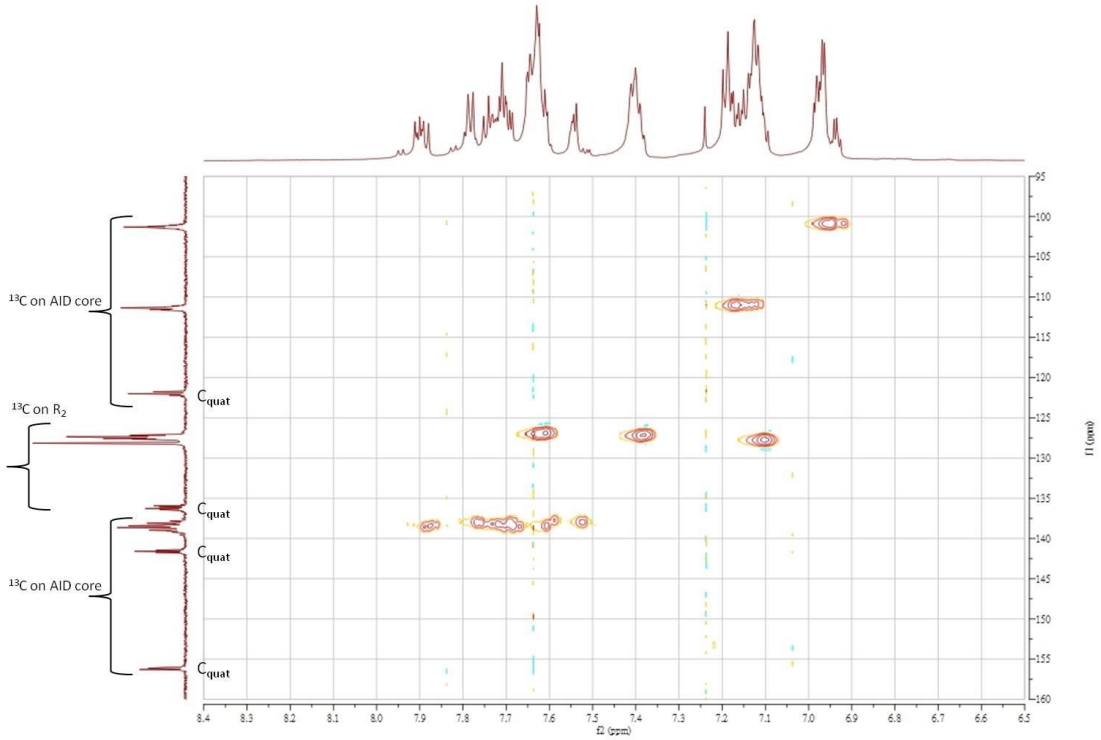


Fig. S47 ^{1}H-^{13}C HSQC NMR spectrum of [Zn_4O(AID-4-Thiophen-2-yl)$_6$] (**Zn-2**) in $CDCl_3$.

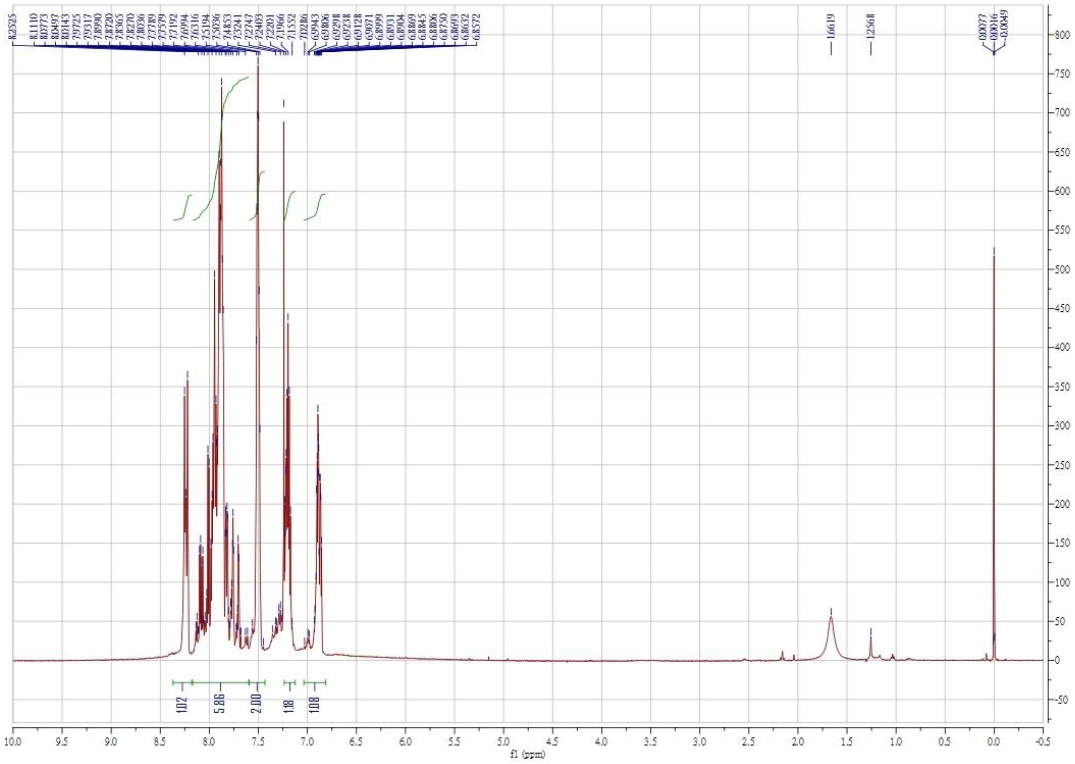


Fig. S48 ^{1}H NMR spectrum of [Zn_4O(AID-4-Naphthalen-2-yl)$_6$] (**Zn-3**) in $CDCl_3$.

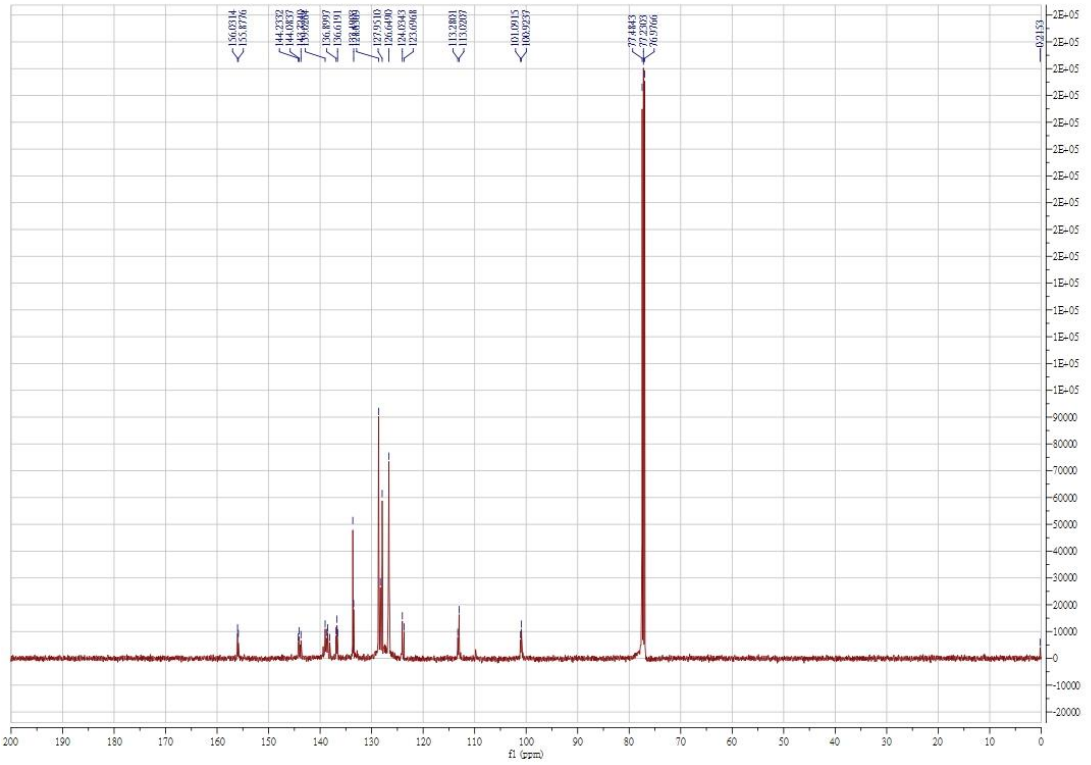


Fig. S49 ^{13}C NMR spectrum of [Zn_4O(AID-4-Naphthalen-2-yl)$_6$] (**Zn-3**) in $CDCl_3$.

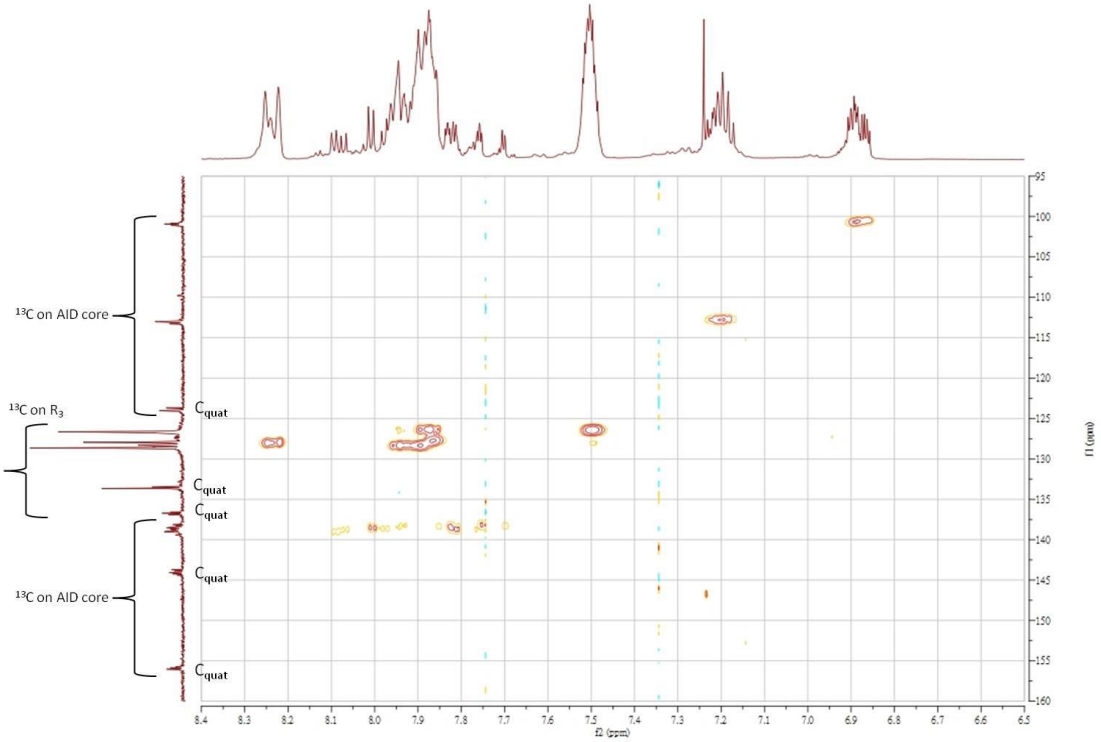


Fig. S50 ^{1}H-^{13}C HSQC NMR spectrum of [Zn_4O(AID-4-Naphthalen-2-yl)$_6$] (**Zn-3**) in $CDCl_3$.

20. Synthesis of Cu(I) complexes

Synethic procedures

1,10-Phenanthroline, 2,9-dimethylphenanthroline, 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline, 4,7-diphenylphenanthroline and 6,6'-dimethyl-2,2'-bipyridine were purchased from commercial sources and used as received. $[Me_4N][(PPh_2)_2C_2B_9H_{10}]$ was synthesized according to a literature method.[8]

Cu-1: A mixture of $[Me_4N][(PPh_2)_2C_2B_9H_{10}]$ (57.6 mg, 100 μmol) and $[Cu(MeCN)_4]PF_6$ (37.3 mg, 100 μmol) was stirred in EtOH (6 mL) for 1 h under Ar and afforded a white suspension. An ethanolic solution (5 mL) of 1,10-phenanthroline (18.4 mg, 102 μmol) degassed by bubbling with Ar was added to the white suspension and this mixture was then refluxed for 1 h. After cooling the reaction mixture to room temperature, the precipitates were filtered and washed with hexane. The copper complex was purified by column chromatography on silica gel using dichloromethane as eluent. Upon concentration under reduced pressure, hexane was added to induce precipitation and the product was filtered, washed with diethyl ether and air-dried. Yield: 52 mg (70%). ^{1}H NMR (400 MHz, [D$_6$]DMSO): δ 9.90 (d, *J* = 4.6 Hz, 1H), 8.92 (d, *J* = 8.0 Hz, 1H), 8.60 (d, *J* = 7.9 Hz, 1H), 8.33 (dd, *J* = 8.2, 4.8 Hz, 1H), 8.24 (d, *J* = 8.9 Hz, 1H), 8.17 (d, *J* = 8.9 Hz, 1H), 7.27–7.44 (m, 21H), 6.41 (d, *J* = 4.7 Hz, 1H), 0.60 (br, B–H), -1.91 (B–H). ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 150.6 (d, *J* = 8.2 Hz), 148.4, 142.6, 142.3, 137.9, 137.3, 134.9 (t, *J* = 19.0 Hz), 134.6 (t, *J* = 15.3 Hz), 134.0 (t, *J* = 7.2 Hz), 131.9 (t, *J* = 7.2 Hz), 130.3, 129.4, 128.7, 128.6, 128.2 (t, *J* = 5.3 Hz), 127.9 (t, *J* = 4.0 Hz), 127.2, 127.0, 125.9, 124.2. ^{31}P NMR (162 MHz, [D$_6$]DMSO): δ 18.1. FAB-MS (+ve): *m*/*z* 745.0 $[M]^+$. Elemental analyses calcd. for $C_{38}H_{38}B_9CuN_2P_2 \cdot 0.5C_6H_{14}$: C 62.33, H 5.75, N 3.55; found: C 61.85, H 5.63, N 3.46.

Cu-2: A mixture of $[Me_4N][(PPh_2)_2C_2B_9H_{10}]$ (45 mg, 78.1 μmol) and $[Cu(MeCN)_4]PF_6$ (29.1 mg, 78.1 μmol) was stirred in EtOH (4 mL) for 1 h under Ar and afforded a white suspension. A hot ethanolic solution (6 mL) of 2,9-dimethyl-1,10-phenanthroline (16.6 mg, 79.7 μmol) degassed by bubbling with Ar was added to the white suspension and this mixture was then refluxed for 1 h. After cooling the reaction mixture to room temperature, the precipitates were filtered and washed with hexane. The copper complex was purified by column chromatography on silica gel using dichloromethane as eluent. Upon concentration under reduced pressure, hexane was added to induce precipitation and the product was filtered, washed with diethyl ether and air-dried. Yield: 41 mg (68%). ^{1}H NMR (400 MHz, [D$_6$]DMSO): δ 8.82 (d, *J* = 8.3 Hz, 1H), 8.47 (d, *J* = 8.3 Hz, 1H), 8.16 (m, 2H), 8.07 (d, *J* = 8.8 Hz, 1H), 7.25–7.37 (m, 21H), 3.41 (s, 3H), 0.95 (br, B–H), 0.54 (s, 3H), -1.86 (B–H). ^{13}C NMR (126 MHz, [D$_6$]DMSO): δ 160.5, 160.2, 142.6, 142.1, 138.4, 138.2 (t, *J* = 15.4 Hz), 137.7, 135.4 (t, *J* = 10.2 Hz), 134.9 (t, *J* = 17.9 Hz), 131.9 (t, *J* = 6.6 Hz), 130.7, 128.4, 128.1, 128.1, 128.0, 127.6, 127.1, 126.2, 126.1, 126.0, 125.3, 29.7, 22.4. ^{31}P NMR (162 MHz, [D$_6$]DMSO): δ 15.3. FAB-MS (+ve): *m*/*z* 773.1 $[M]^+$. Elemental analysis calcd. for $C_{40}H_{42}B_9CuN_2P_2$: C 62.11, H 5.47, N 3.62; found: C 61.93, H 5.46, N 3.52.

Cu-3: A mixture of $[Me_4N][(PPh_2)_2C_2B_9H_{10}]$ (40 mg, 69.5 μmol) and $[Cu(MeCN)_4]PF_6$ (25.9 mg, 69.5 μmol) was stirred in EtOH (5 mL) for 1 h under Ar and afforded a white suspension. An ethanolic solution (5 mL) of 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (25.5 mg, 70.8 μmol) degassed by bubbling with Ar was added to the white suspension and this mixture was then refluxed for 1 h. After cooling the reaction mixture to room temperature, the precipitates were filtered and washed with hexane. The copper complex was purified by column chromatography on silica gel using dichloromethane as eluent. Upon concentration under reduced pressure, hexane was added to induce precipitation and the product was filtered, washed with diethyl ether and air-dried. Yield: 51 mg (79%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, *J* = 9.3 Hz, 1H), 7.88 (m, 2H), 7.62 (m, 5H), 7.45-7.53 (m, 11H), 7.37-7.40 (m, 2H), 7.31 (t, *J* = 7.2 Hz, 2H), 7.17-7.23 (m, 10H), 7.07 (s, 1H), 3.48 (s, 3H), 0.71 (s, 3H), -1.74 (br, B–H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 160.7, 159.7, 150.2, 149.2, 144.6, 144.0, 139.5 (t, *J* = 15.8 Hz), 136.7, 136.7, 136.2 (t, *J* = 10.0 Hz), 135.6 (t, *J* = 18.4 Hz), 132.6 (t, *J* = 6.7 Hz), 130.5, 129.6, 129.4, 129.1, 129.0, 128.9, 128.2, 127.9, 127.9, 127.8, 127.8, 126.0, 125.9, 125.4, 125.3, 123.9, 123.5, 30.8, 23.3. ^{31}P NMR (162 MHz, $CDCl_3$): δ 16.2. FAB-MS (+ve): 924.2 $[M - H]^+$. Elemental analysis calcd. for $C_{52}H_{50}B_9CuN_2P_2 \cdot H_2O$: C 66.18, H 5.55, N 2.97; found: C 66.50, H 5.62, N 2.84.

Cu-4: A mixture of $[Me_4N][(PPh_2)_2C_2B_9H_{10}]$ (46 mg, 80 μmol) and $[Cu(MeCN)_4]PF_6$ (29.8 mg, 80 μmol) was stirred in EtOH (5 mL) for 1 h under Ar and afforded a white suspension. An ethanolic solution (5 mL) of 4,7-diphenyl-1,10-phenanthroline (27.1 mg, 81.6 μmol) degassed by bubbling with Ar was added to the white suspension and this mixture was then refluxed for 1 h. After cooling the reaction mixture to room temperature, the precipitates were filtered and washed with hexane. The copper complex was purified by column chromatography on silica gel using dichloromethane as eluent. Upon concentration under reduced pressure, hexane was added to

induce precipitation and the product was filtered, washed with diethyl ether and air-dried. Yield: 49 mg (68%). ^{1}H NMR (400 MHz, [D_6]DMSO): δ 9.95 (d, *J* = 5.0 Hz, 1H), 8.29 (d, *J* = 5.0 Hz, 1H), 8.07 (d, *J* = 9.5 Hz, 1H), 8.02 (d, *J* = 9.5 Hz, 1H), 7.63–7.77 (m, 5H), 7.56 (m, 5H), 7.46 (m, 4H), 7.28–7.40 (m, 17H), 6.53 (d, *J* = 4.9 Hz, 1H), 0.63 (br, B–H), -1.91 (B–H). ^{13}C NMR (126 MHz, [D_6]DMSO): δ 150.2 (d, *J* = 7.5 Hz), 149.2, 148.6, 148.2, 143.4, 143.1, 136.0, 135.7, 134.9 (t, *J* = 18.9 Hz), 134.5 (t, *J* = 15.2 Hz), 134.1 (t, *J* = 9.3 Hz), 132.0 (t, *J* = 7.4 Hz), 130.3, 129.8, 129.7, 129.4, 129.3, 129.0, 128.9, 128.7, 128.2 (t, *J* = 5.3 Hz), 128.0 (t, *J* = 3.6 Hz), 126.9, 126.0, 124.8, 124.7, 124.3. ^{31}P NMR (162 MHz, [D_6]DMSO): δ 18.1. FAB-MS (+ve): *m*/*z* 896.5 $[M - H]^+$. Elemental analyses calcd. for $C_{50}H_{46}B_9CuN_2P_2 \cdot 0.5H_2O$: C 66.23, H 5.22, N 3.09; found: C 66.31, H 5.12, N 3.00.

Cu-5: A mixture of $[Me_4N][(PPh_2)_2C_2B_9H_{10}]$ (49 mg, 85 μmol) and $[Cu(MeCN)_4]PF_6$ (31.6 mg, 85 μmol) was stirred in EtOH (5 mL) for 1 h under Ar and afforded a white suspension. An ethanolic solution (5 mL) of 6,6'-dimethyl-2,2'-bipyridine (15.7 mg, 85 μmol) degassed by bubbling with Ar was added to the white suspension and this mixture was then refluxed for 1 h. After cooling the reaction mixture to room temperature, the precipitates were filtered and washed with hexane. The copper complex was purified by column chromatography on silica gel using dichloromethane as eluent. Upon concentration under reduced pressure, hexane was added to induce precipitation and the product was filtered, washed with diethyl ether and air-dried. Yield: 52 mg (82%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99-8.06 (m, 2H), 7.89 (d, *J* = 7.9 Hz, 1H), 7.66 (t, *J* = 8.0 Hz, 2H), 7.28-7.46 (m, 10H), 7.15-7.21 (m, 10H), 6.81 (d, *J* = 7.4 Hz, 1H), 3.19 (s, 3H), 0.50 (s, 3H), -1.79 (br, B–H). ^{13}C NMR could not be obtained due to low solubility in $CDCl_3$ and instability in [D_6]DMSO. ^{31}P NMR (162 MHz, [D_6]DMSO): δ 14.7. FAB-MS (+ve): *m*/*z* 749.1 $[M]^+$. Elemental analysis calcd. for $C_{38}H_{42}B_9CuN_2P_2 \cdot CH_2Cl_2$: C 56.13, H 5.31, N 3.36; found: C 56.52, H 5.30, N 3.44.

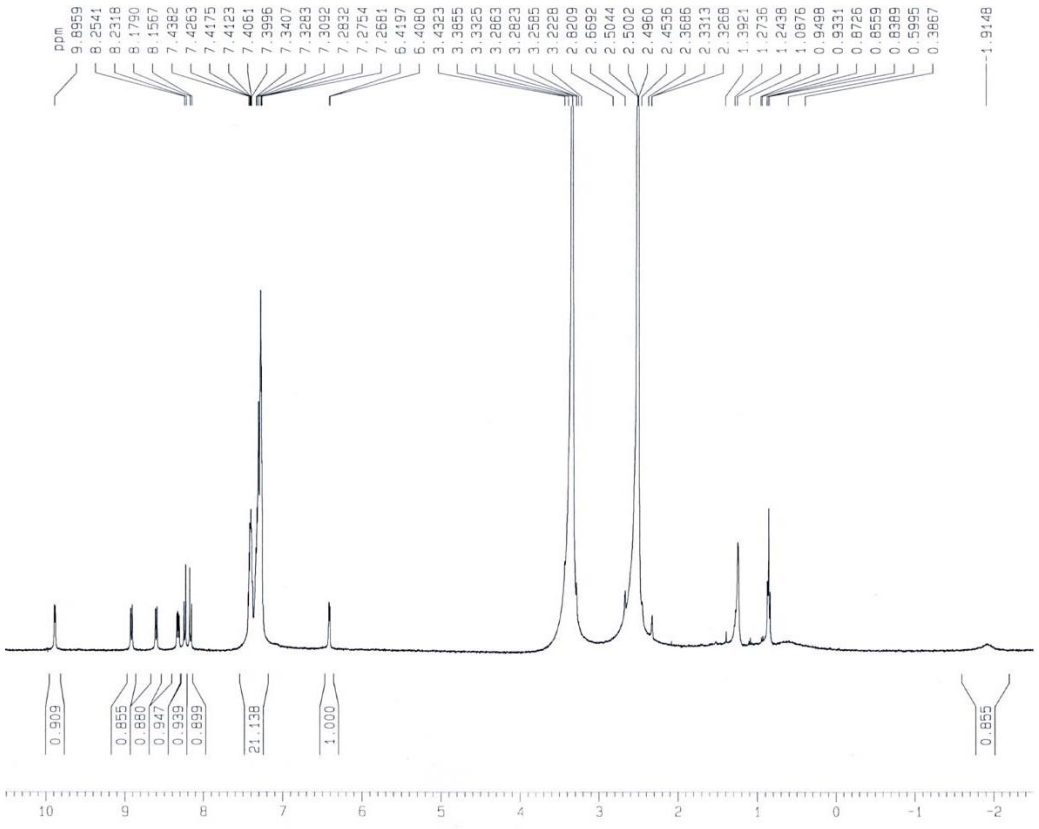


Fig. S51 ^{1}H NMR spectrum of **Cu-1** in [D_6]DMSO.

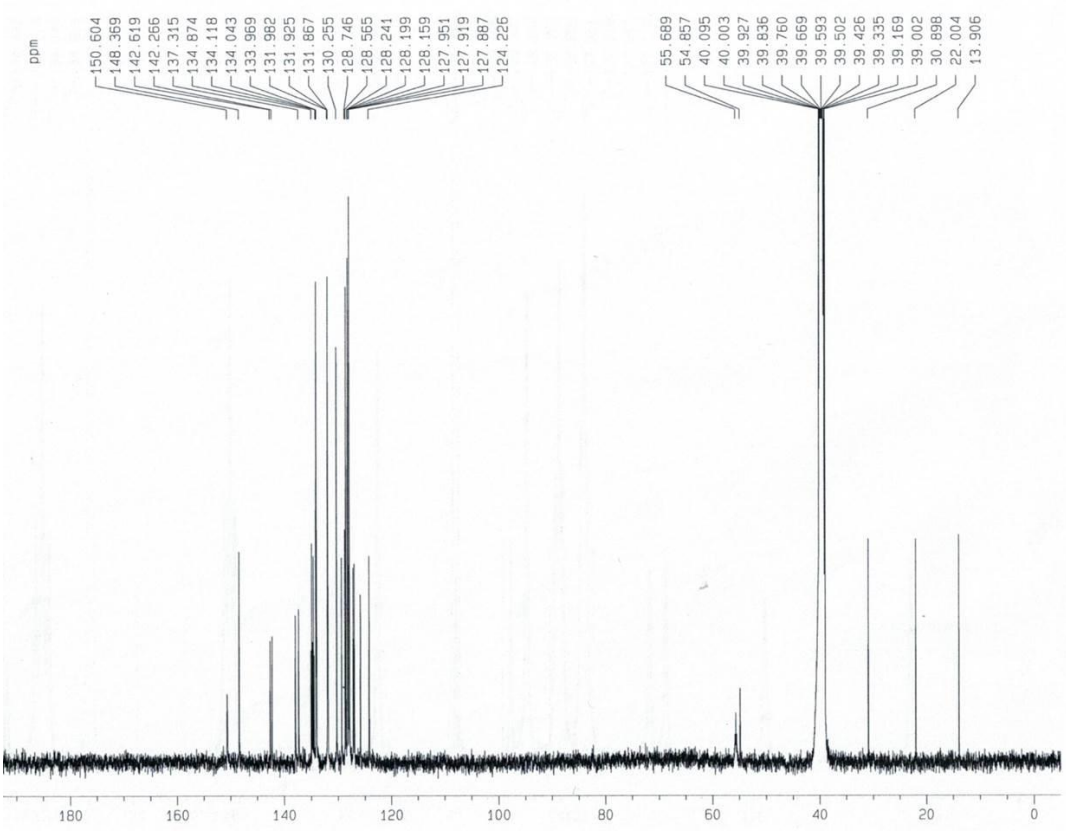


Fig. S52 ^{13}C NMR spectrum of **Cu-1** in [D_6]DMSO.

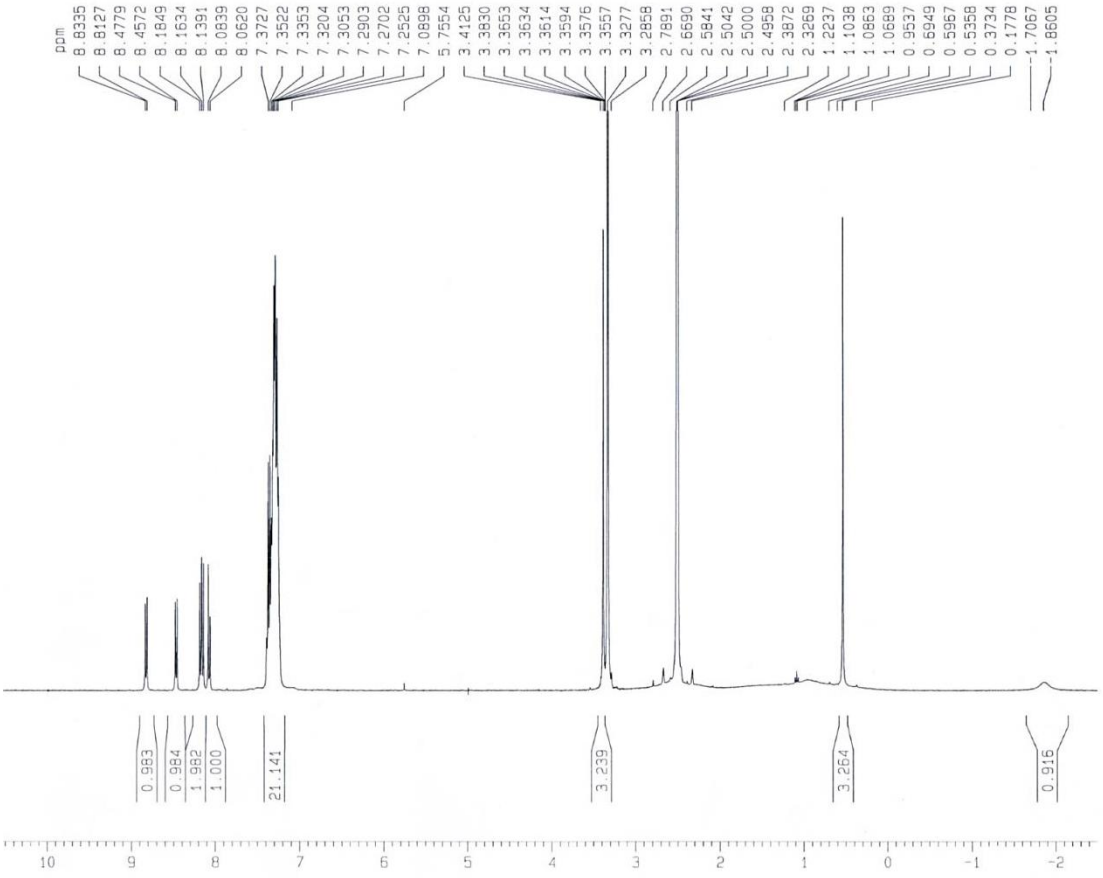


Fig. S53 ^{1}H NMR spectrum of **Cu-2** in [D_6]DMSO.

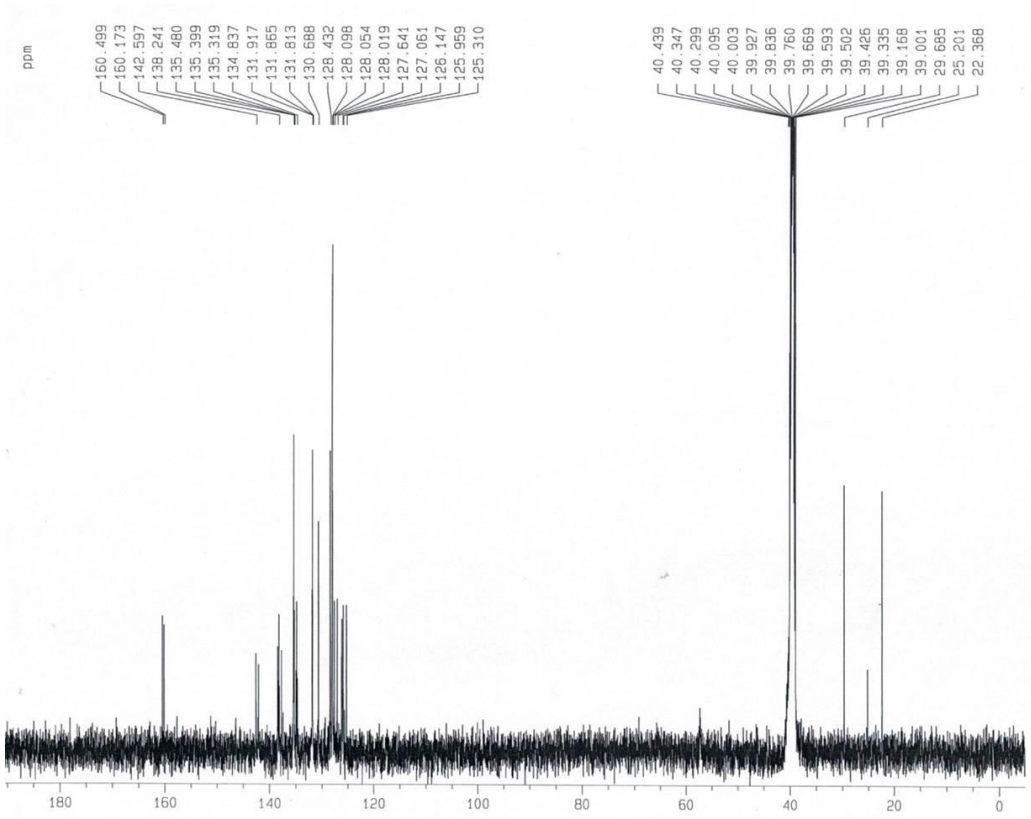


Fig. S54 ^{13}C NMR spectrum of **Cu-2** in [D_6]DMSO.

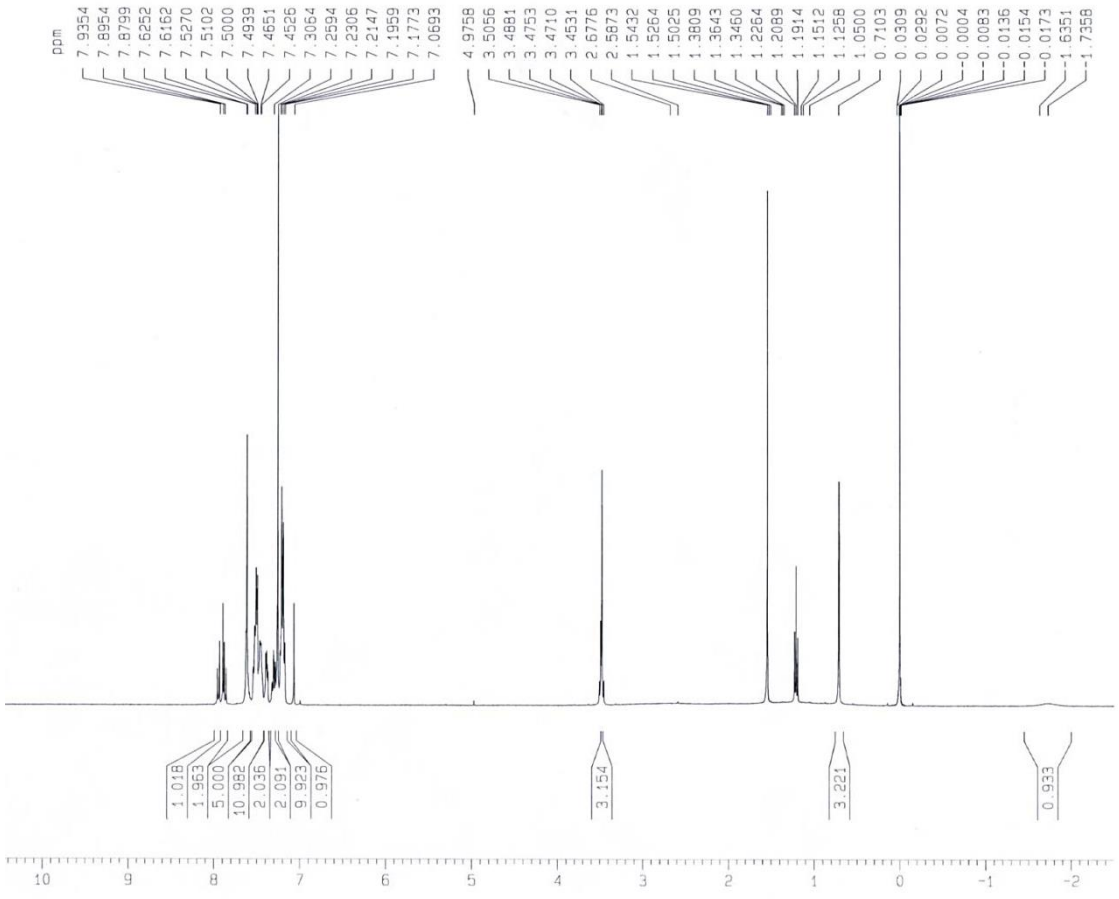


Fig. S55 ^{1}H NMR spectrum of **Cu-3** in $CDCl_3$.

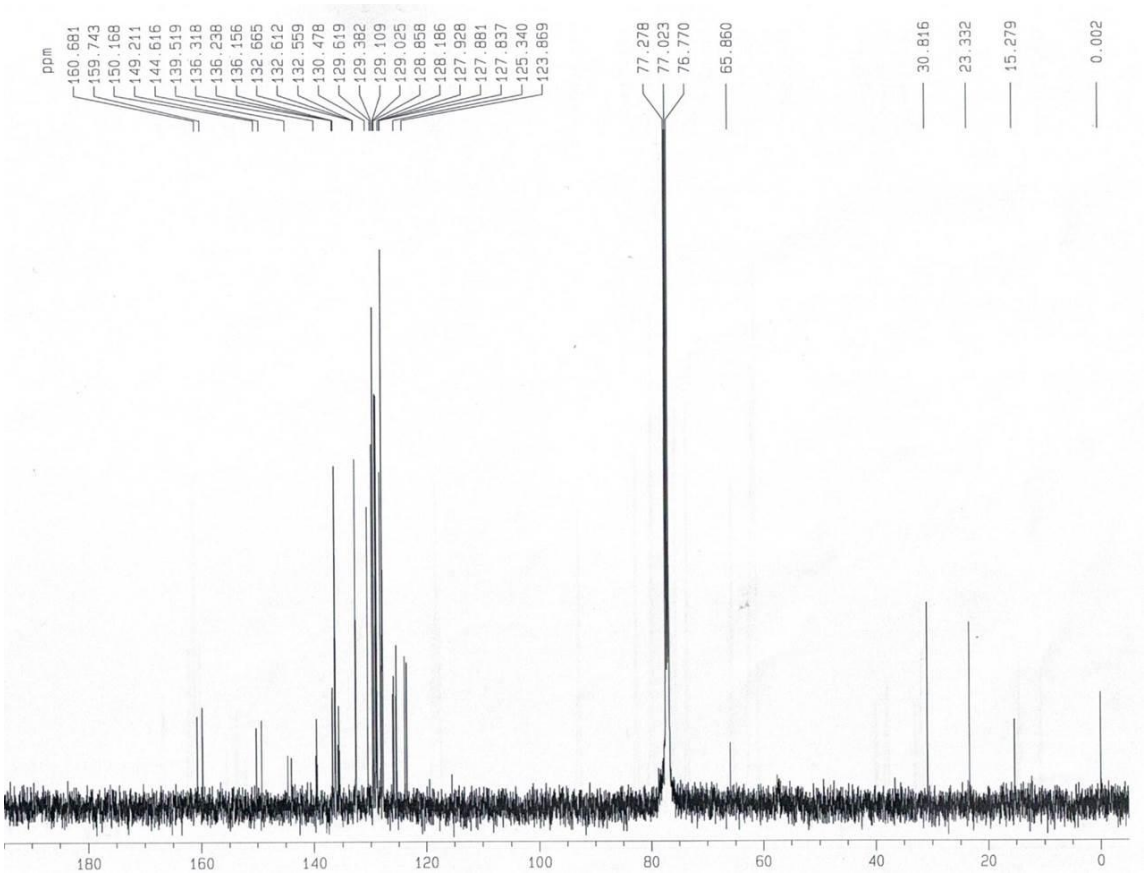


Fig. S56 ^{13}C NMR spectrum of **Cu-3** in $CDCl_3$.

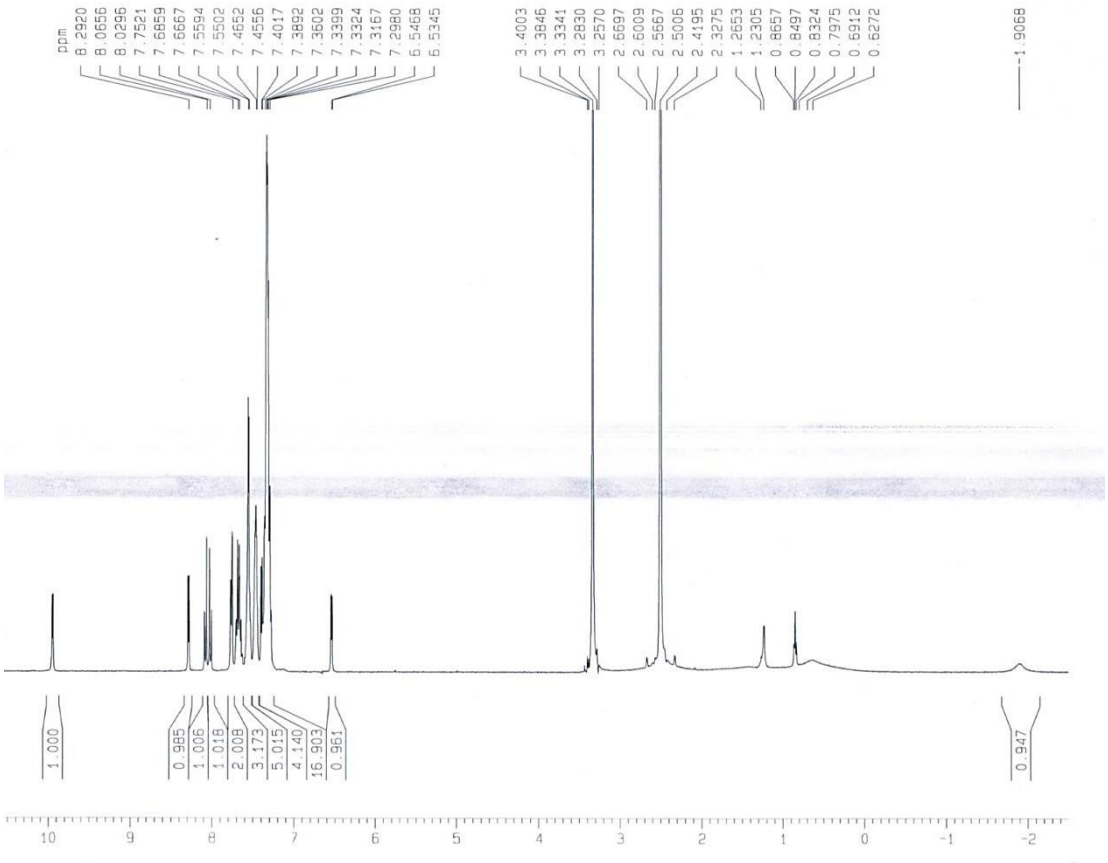


Fig. S57 ^{1}H NMR spectrum of **Cu-4** in $[D_6]DMSO$.

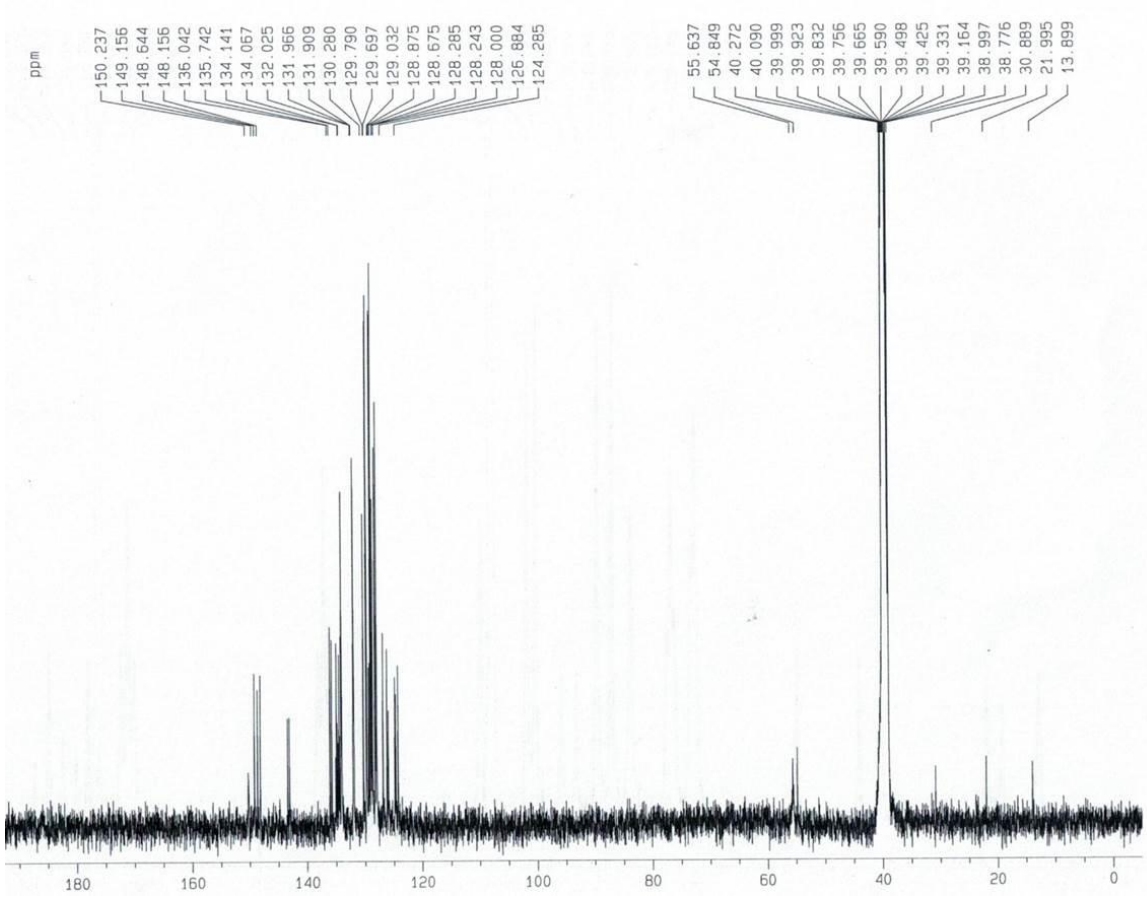


Fig. S58 ^{13}C NMR spectrum of **Cu-4** in [D_6]DMSO.

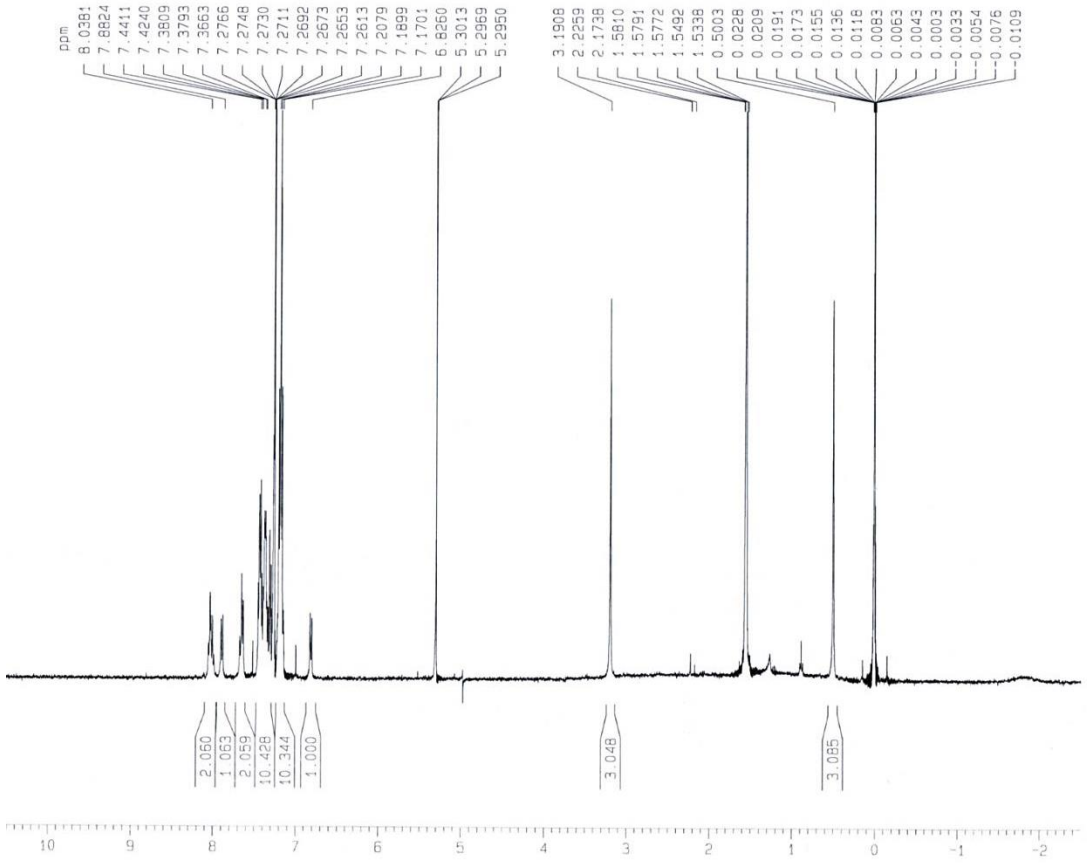


Fig. S59 ^{1}H NMR spectrum of **Cu-5** in $CDCl_3$.

21. X-ray crystal data of $Zn_4O(AID)_6$, Cu-1 and Cu-3

Table S3 Crystal data of $Zn_4O(AID)_6$, **Cu-1** and **Cu-3**

Complex	$Zn_4O(AID)_6$	**Cu-1**	**Cu-3**
Empirical formula	$C_{46}H_{40}N_{12}O_2Zn_4$	$C_{42}H_{48}B_9CuN_2OP_2$	$C_{53}H_{52}B_9Cl_2CuN_2P_2$
Formula weight	1054.46	819.59	1010.63
Temperature/K	293(2)	100	100
Crystal system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	$P2_1/c$
a/Å	10.283(2)	10.828(5)	15.5324(6)
b/Å	10.474(2)	13.677(5)	15.5957(6)
c/Å	20.857(4)	14.950(7)	20.6244(9)
α/°	95.09(3)	90.64(2)	90
β/°	94.25(3)	106.555(18)	98.7890(18)
γ/°	96.25(3)	95.534(17)	90
Volume/Å ^{3}	2216.3(8)	2110.5(16)	4937.4(3)
Z	2	2	4
ρcalcg/cm^3	1.58	1.29	1.36
μ/mm^{-1}	2.888	1.712	2.53
F(000)	1072	852	2088
Crystal size/mm^3	0.08 × 0.06 × 0.04	0.3 × 0.3 × 0.3	0.2 × 0.2 × 0.04
Radiation	CuKα (λ = 1.54178)	CuKα (λ = 1.54178)	CuKα (λ = 1.54178)
2θ range for data collection/°	4.26 to 134.34	6.172 to 133.976	5.758 to 135.5
Index ranges	-12 ≤ h ≤ 11, -12 ≤ k ≤ 12, -24 ≤ l ≤ 24	-12 ≤ h ≤ 12, -16 ≤ k ≤ 15, -17 ≤ l ≤ 17	-18 ≤ h ≤ 18, -18 ≤ k ≤ 18, -24 ≤ l ≤ 24
Reflections collected	24479	38050	67504
Independent reflections	6818 [R_{int} = 0.0642]	7368 [R_{int} = 0.0495]	8693 [R_{int} = 0.0596]
Data/restraints/parameters	6818/24/512	7368/3/532	8693/0/640
Goodness-of-fit on F^2	1.121	1.058	1.103
Final *R* indexes [I>=2σ (I)]	R_1 = 0.1133, wR_2 = 0.2773	R_1 = 0.0333, wR_2 = 0.0920	R_1 = 0.0603, wR_2 = 0.1666
Final *R* indexes [all data]	R_1 = 0.1253, wR_2 = 0.2831	R_1 = 0.0336, wR_2 = 0.0923	R_1 = 0.0670, wR_2 = 0.1720
Largest diff. peak/hole / e Å $^{-3}$	1.33/-1.63	1.08/-0.38	0.95/-1.15

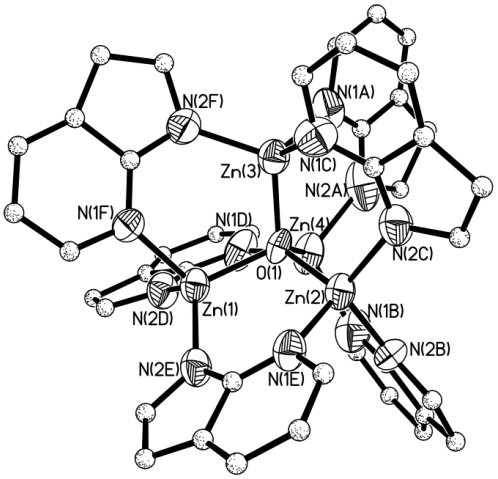


Fig. S60 Perspective view of $Zn_4O(AID)_6$ (all hydrogen atoms are omitted for clarity).

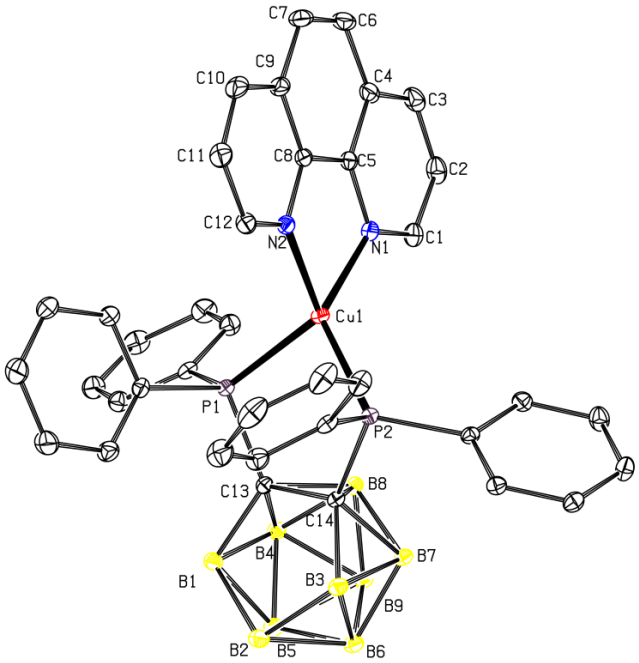


Fig. S61 Perspective view of **Cu-1** (all hydrogen atoms are omitted for clarity).

22. Computational details

Density functional theory (DFT) and time-dependent density functional theroy (TDDFT) calculations have been performed to understand the geometries and the electronic structures of copper(I) complexes (**Cu-1 to Cu-5)**, and Zn(II) complexes **(Zn-1 to Zn-3)** using Gaussian 09 package.[4] PBE0[5]/6-31G*(lanl2dz)[6] was used for the geometry optimization. PBE0 with triplet-zeta basis set (6-311G*) was used for TDDFT calculations of copper(I) complexes. Due to the very large size of the Zn(II) complexes, only double-zeta with pseudo potential basis set (6-31G*(lanl2dz) was employed for TDDFT calculations. The Solvent effects have been studied using self-consistent reaction field (SCRF) method based on PCM models.[7] The choice of solvents (dichloromethne, a dielectric constant ε = 8.93) was based on the solvent media for experiments.

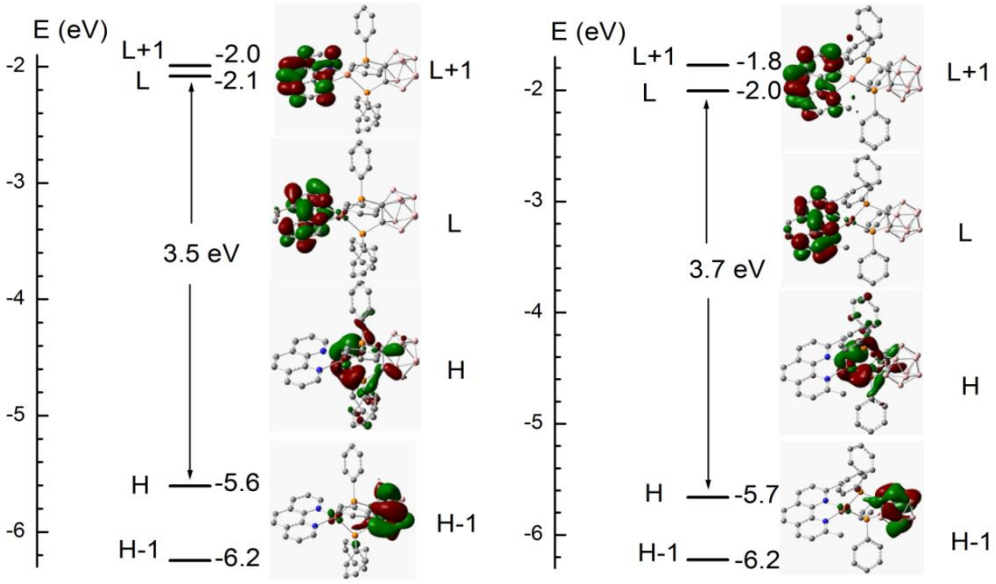
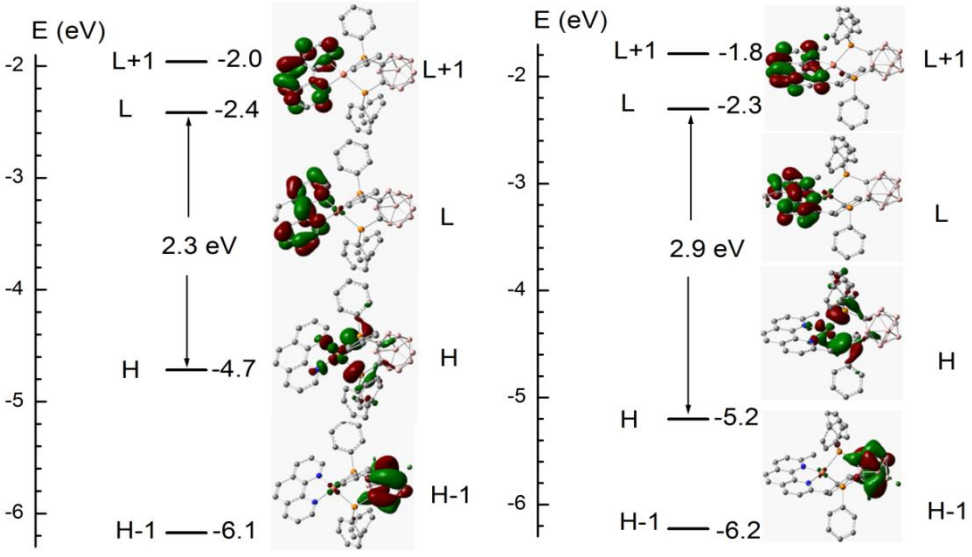


Fig. S62 Comparison of FMO diagram of **Cu-1** and **Cu-2** at ground state (S_0).



Cu-1 **Cu-2**

Fig. 63 Comparison of MO diagram of **Cu-1** and **Cu-2** at singlet excited state (S_1).

Geometries of the stationary points in mol2 format

Cu-1 S_0

@<TRIPOS>MOLECULE
Molecule Name
90 110
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 Cu1 -0.8105 0.2355 -0.1878 Cu
2 P2 0.4332 -1.7160 -0.1330 P
3 P3 1.1436 1.4510 -0.0391 P
4 N4 -2.3908 0.3586 1.2274 N
5 N5 -2.4432 0.6215 -1.4570 N
6 C6 -3.5848 0.6038 0.6445 C
7 C7 -2.3446 0.1910 2.5406 C
8 C8 -3.4853 0.2699 3.3554 C
9 H9 -3.3897 0.1247 4.4265 H
10 C10 -4.7071 0.5336 2.7746 C
11 H11 -5.6092 0.6055 3.3770 H
12 C12 -4.7871 0.7086 1.3790 C
13 C13 -6.0117 0.9807 0.6884 C
14 H14 -6.9269 1.0629 1.2687 H
15 C15 -6.0354 1.1328 -0.6627 C
16 H16 -6.9695 1.3387 -1.1787 H
17 C17 -4.8375 1.0196 -1.4390 C
18 C18 -4.8105 1.1526 -2.8408 C
19 H19 -5.7326 1.3587 -3.3784 H
20 C20 -3.6138 1.0154 -3.5116 C
21 H21 -3.5573 1.1082 -4.5912 H
22 C22 -2.4494 0.7465 -2.7769 C
23 C23 -3.6112 0.7542 -0.7880 C
24 C24 -0.0702 -3.2193 -1.0399 C
25 C25 0.5198 -4.4678 -0.8063 C
26 H26 1.3101 -4.5610 -0.0671 H
27 C27 0.1067 -5.5812 -1.5285 C
28 H28 0.5743 -6.5451 -1.3467 H
29 C29 -0.8957 -5.4610 -2.4905 C
30 H30 -1.2133 -6.3334 -3.0555 H
31 C31 -1.4888 -4.2244 -2.7261 C
32 H32 -2.2719 -4.1278 -3.4736 H
33 C33 -1.0803 -3.1086 -1.9992 C
34 H34 -1.5451 -2.1410 -2.1721 H
35 C35 0.6379 -2.3212 1.5814 C
36 C36 -0.3812 -3.1055 2.1425 C
37 H37 -1.2145 -3.4315 1.5244 H
38 C38 -0.3267 -3.4870 3.4788 C
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44 C44 1.7012 -1.9201 2.3939 C
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53 C53 0.7693 2.7126 3.8182 C
54 H54 -0.0067 3.2206 4.3855 H
55 C55 0.5649 2.4216 2.4738 C
56 H56 -0.3741 2.6989 1.9980 H
57 C57 1.3520 3.0900 -0.8186 C
58 C58 0.4886 3.4426 -1.8604 C
59 H59 -0.2810 2.7420 -2.1745 H
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4 N4 -2.3908 0.3586 1.2274 N
5 N5 -2.4432 0.6215 -1.4570 N
6 C6 -3.5848 0.6038 0.6445 C
7 C7 -2.3446 0.1910 2.5406 C
8 C8 -3.4853 0.2699 3.3554 C
9 H9 -3.3897 0.1247 4.4265 H
10 C10 -4.7071 0.5336 2.7746 C
11 H11 -5.6092 0.6055 3.3770 H
12 C12 -4.7871 0.7086 1.3790 C
13 C13 -6.0117 0.9807 0.6884 C
14 H14 -6.9269 1.0629 1.2687 H
15 C15 -6.0354 1.1328 -0.6627 C
16 H16 -6.9695 1.3387 -1.1787 H
17 C17 -4.8375 1.0196 -1.4390 C
18 C18 -4.8105 1.1526 -2.8408 C

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20	C20	-3.6138	1.0154	-3.5116 C
21	H21	-3.5573	1.1082	-4.5912 H
22	C22	-2.4494	0.7465	-2.7769 C
23	C23	-3.6112	0.7542	-0.7880 C
24	C24	-0.0702	-3.2193	-1.0399 C
25	C25	0.5198	-4.4678	-0.8063 C
26	H26	1.3101	-4.5610	-0.0671 H
27	C27	0.1067	-5.5812	-1.5285 C
28	H28	0.5743	-6.5451	-1.3467 H
29	C29	-0.8957	-5.4610	-2.4905 C
30	H30	-1.2133	-6.3334	-3.0555 H
31	C31	-1.4888	-4.2244	-2.7261 C
32	H32	-2.2719	-4.1278	-3.4736 H
33	C33	-1.0803	-3.1086	-1.9992 C
34	H34	-1.5451	-2.1410	-2.1721 H
35	C35	0.6379	-2.3212	1.5814 C
36	C36	-0.3812	-3.1055	2.1425 C
37	H37	-1.2145	-3.4315	1.5244 H
38	C38	-0.3267	-3.4870	3.4788 C
39	H39	-1.1172	-4.1075	3.8936 H
40	C40	0.7392	-3.0812	4.2809 C
41	H41	0.7823	-3.3799	5.3249 H
42	C42	1.7496	-2.2960	3.7344 C
43	H43	2.5866	-1.9753	4.3487 H
44	C44	1.7012	-1.9201	2.3939 C
45	H45	2.5003	-1.3158	1.9799 H
46	C46	1.5577	1.7796	1.7189 C
47	C47	2.7561	1.4256	2.3453 C
48	H48	3.5426	0.9445	1.7725 H
49	C49	2.9536	1.7072	3.6966 C
50	H50	3.8925	1.4285	4.1680 H
51	C51	1.9656	2.3505	4.4355 C
52	H52	2.1263	2.5722	5.4873 H
53	C53	0.7693	2.7126	3.8182 C
54	H54	-0.0067	3.2206	4.3855 H
55	C55	0.5649	2.4216	2.4738 C
56	H56	-0.3741	2.6989	1.9980 H
57	C57	1.3520	3.0900	-0.8186 C
58	C58	0.4886	3.4426	-1.8604 C
59	H59	-0.2810	2.7420	-2.1745 H
60	C60	0.6109	4.6769	-2.4915 C
61	H61	-0.0605	4.9387	-3.3051 H
62	C62	1.5898	5.5754	-2.0754 C
63	H63	1.6855	6.5411	-2.5648 H
64	C64	2.4440	5.2367	-1.0281 C
65	H65	3.2086	5.9362	-0.7011 H
66	C66	2.3278	4.0009	-0.4006 C
67	H67	2.9997	3.7396	0.4111 H
68	C68	2.4379	0.3448	-0.7469 C
69	C69	2.0880	-1.2080	-0.7577 C
70	B70	4.0186	0.6993	-0.6415 B
71	H71	4.3858	1.7162	-0.1264 H
72	B72	3.2324	0.8357	-2.2134 B
73	H73	2.9922	1.8844	-2.7239 H
74	B74	1.9423	-0.3764	-2.2401 B
75	H75	0.8529	-0.1774	-2.6945 H
76	B76	2.6994	-1.9676	-2.1725 B
77	H77	2.1218	-2.9098	-2.6110 H
78	B78	3.4605	-2.0897	-0.5503 B

79 H79 3.4370 -3.1534 -0.0036 H
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5 N5 -2.3505 1.4164 -0.5560 N
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7 C7 -2.4113 -1.7175 1.9648 C
8 C8 -3.5662 -2.2301 2.5215 C
9 H9 -3.5030 -3.0652 3.2107 H
10 C10 -4.8093 -1.6597 2.1810 C
11 H11 -5.7335 -2.0502 2.5975 H
12 C12 -4.8439 -0.5846 1.2984 C
13 C13 -6.0518 0.0720 0.8775 C
14 H14 -6.9972 -0.2911 1.2729 H
15 C15 -6.0284 1.1143 0.0048 C
16 H16 -6.9550 1.5894 -0.3077 H
17 C17 -4.7934 1.6179 -0.5299 C
18 C18 -4.7078 2.6706 -1.4351 C
19 H19 -5.6120 3.1676 -1.7757 H
20 C20 -3.4443 3.0753 -1.9032 C
21 H21 -3.3428 3.8858 -2.6163 H
22 C22 -2.3127 2.4298 -1.4385 C
23 C23 -3.5852 0.9893 -0.1073 C
24 C24 -0.3215 -2.7368 -1.4040 C
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27 C27 -0.4847 -4.8345 -2.5939 C
28 H28 -0.0598 -5.7970 -2.8633 H
29 C29 -1.7303 -4.4536 -3.0935 C
30 H30 -2.2780 -5.1234 -3.7505 H
31 C31 -2.2733 -3.2186 -2.7498 C
32 H32 -3.2445 -2.9209 -3.1342 H
33 C33 -1.5733 -2.3614 -1.9043 C
34 H34 -2.0082 -1.4038 -1.6290 H
35 C35 1.4131 -2.5614 0.9167 C
36 C36 0.7563 -3.6809 1.4493 C
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60 C60 -0.3001 5.2481 0.7756 C
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5 N5 -2.5368 0.0431 -1.3937 N
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7 C7 -2.2440 -0.0802 2.6533 C
8 C8 -3.3858 -0.1107 3.4868 C
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10 C10 -4.6403 -0.1013 2.9341 C
11 H11 -5.5292 -0.1241 3.5599 H
12 C12 -4.7784 -0.0592 1.5324 C
13 C13 -6.0527 -0.0453 0.8877 C
14 H14 -6.9471 -0.0697 1.5048 H
15 C15 -6.1430 -0.0025 -0.4671 C
16 H16 -7.1109 0.0080 -0.9612 H
17 C17 -4.9651 0.0290 -1.2748 C
18 C18 -5.0161 0.0731 -2.6804 C

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20	C20	-3.8459	0.1016	-3.3978 C
21	H21	-3.8564	0.1362	-4.4824 H
22	C22	-2.6053	0.0856	-2.7258 C
23	C23	-3.6847	0.0160	-0.6720 C
24	C24	-0.8835	-0.1133	3.2651 C
25	H25	-0.6697	-1.1102	3.6704 H
26	H26	-0.8043	0.6083	4.0853 H
27	H27	-0.1195	0.1210	2.5252 H
28	C28	-1.3289	0.1119	-3.4997 C
29	H29	-0.7065	0.9609	-3.1993 H
30	H30	-1.5167	0.1807	-4.5743 H
31	H31	-0.7393	-0.7906	-3.3079 H
32	C32	0.6629	-3.1483	-1.1526 C
33	C33	1.5970	-4.1931	-1.1610 C
34	H34	2.5160	-4.1002	-0.5895 H
35	C35	1.3536	-5.3422	-1.9038 C
36	H36	2.0879	-6.1431	-1.9113 H
37	C37	0.1754	-5.4672	-2.6402 C
38	H38	-0.0094	-6.3676	-3.2201 H
39	C39	-0.7645	-4.4423	-2.6257 C
40	H40	-1.6894	-4.5395	-3.1883 H
41	C41	-0.5214	-3.2890	-1.8809 C
42	H42	-1.2640	-2.4954	-1.8445 H
43	C43	1.1745	-2.3653	1.5197 C
44	C44	0.3486	-3.4188	1.9369 C
45	H45	-0.3651	-3.8544	1.2421 H
46	C46	0.4407	-3.9249	3.2294 C
47	H47	-0.2002	-4.7498	3.5302 H
48	C48	1.3568	-3.3848	4.1311 C
49	H49	1.4331	-3.7834	5.1392 H
50	C50	2.1789	-2.3370	3.7266 C
51	H51	2.9032	-1.9125	4.4166 H
52	C52	2.0870	-1.8306	2.4324 C
53	H53	2.7394	-1.0189	2.1332 H
54	C54	1.1904	2.3060	1.5900 C
55	C55	2.2371	1.8921	2.4174 C
56	H56	3.0108	1.2414	2.0242 H
57	C57	2.3220	2.3479	3.7321 C
58	H58	3.1501	2.0235	4.3568 H
59	C59	1.3680	3.2259	4.2363 C
60	H60	1.4410	3.5858	5.2592 H
61	C61	0.3250	3.6529	3.4146 C
62	H62	-0.4179	4.3506	3.7927 H
63	C63	0.2341	3.1929	2.1060 C
64	H64	-0.5826	3.5349	1.4738 H
65	C65	0.6524	3.1898	-1.0484 C
66	C66	-0.5748	3.3731	-1.6925 C
67	H67	-1.3254	2.5876	-1.6391 H
68	C68	-0.8482	4.5564	-2.3773 C
69	H69	-1.8063	4.6863	-2.8740 H
70	C70	0.1050	5.5681	-2.4172 C
71	H71	-0.1029	6.4919	-2.9508 H
72	C72	1.3271	5.3987	-1.7662 C
73	H73	2.0724	6.1888	-1.7939 H
74	C74	1.6010	4.2206	-1.0817 C
75	H75	2.5556	4.0916	-0.5807 H
76	C76	2.4608	0.8169	-0.6368 C
77	C77	2.4454	-0.7891	-0.6406 C
78	B78	3.9179	1.4812	-0.3473 B

79 H79 4.0055 2.5383 0.2084 H
80 B80 3.3221 1.4479 -2.0058 B
81 H81 2.9393 2.4147 -2.5846 H
82 B82 2.3150 -0.0016 -2.1459 B
83 H83 1.2853 -0.0327 -2.7362 H
84 B84 3.3694 -1.3989 -1.9547 B
85 H85 3.0568 -2.4327 -2.4507 H
86 B86 3.9424 -1.3604 -0.2582 B
87 H87 4.0776 -2.4018 0.3136 H
88 B88 4.9992 -0.8541 -1.5985 B
89 H89 5.9398 -1.4922 -1.9643 H
90 B90 5.0630 0.0977 -0.1015 B
91 H91 6.0762 0.0963 0.5324 H
92 H92 4.1366 -0.3252 0.6562 H
93 B93 3.9614 0.0037 -2.7923 B
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Cu-2 S_1
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4 N4 -2.2590 0.7609 -1.2335 N
5 N5 -2.4937 -0.6050 1.1577 N
6 C6 -3.5182 0.5396 -0.7049 C
7 C7 -2.1466 1.2716 -2.4688 C
8 C8 -3.2614 1.6587 -3.2170 C
9 H9 -3.1154 2.0817 -4.2052 H
10 C10 -4.5381 1.5296 -2.6680 C
11 H11 -5.4163 1.8562 -3.2193 H
12 C12 -4.6912 0.9589 -1.4082 C
13 C13 -5.9720 0.7693 -0.7954 C
14 H14 -6.8556 1.1033 -1.3340 H
15 C15 -6.0820 0.1921 0.4274 C
16 H16 -7.0555 0.0621 0.8942 H
17 C17 -4.9251 -0.2745 1.1363 C
18 C18 -5.0094 -0.8840 2.3826 C
19 H19 -5.9803 -1.0226 2.8507 H
20 C20 -3.8367 -1.3065 3.0221 C
21 H21 -3.8724 -1.7734 4.0005 H
22 C22 -2.6080 -1.1484 2.3899 C
23 C23 -3.6348 -0.1157 0.5386 C
24 C24 -0.7789 1.4633 -3.0454 C
25 H25 -0.4020 2.4687 -2.8265 H
26 H26 -0.8043 1.3487 -4.1330 H
27 H27 -0.0691 0.7398 -2.6380 H
28 C28 -1.3607 -1.5681 3.1040 C
29 H29 -0.6465 -2.0520 2.4350 H
30 H30 -1.5936 -2.2595 3.9184 H
31 H31 -0.8595 -0.6967 3.5428 H
32 C32 0.5879 2.4753 1.8761 C
33 C33 1.3704 3.5651 2.2852 C
34 H34 2.2715 3.8262 1.7376 H
35 C35 0.9936 4.3158 3.3927 C

36	H36	1.6068	5.1557	3.7065 H
37	C37	-0.1656	3.9916	4.0981 C
38	H38	-0.4572	4.5820	4.9622 H
39	C39	-0.9517	2.9173	3.6918 C
40	H40	-1.8600	2.6668	4.2321 H
41	C41	-0.5778	2.1611	2.5824 C
42	H42	-1.2059	1.3337	2.2607 H
43	C43	1.4976	2.6949	-0.8363 C
44	C44	0.8010	3.9133	-0.8710 C
45	H45	0.0736	4.1505	-0.1009 H
46	C46	1.0391	4.8312	-1.8894 C
47	H47	0.4994	5.7737	-1.8970 H
48	C48	1.9630	4.5429	-2.8919 C
49	H49	2.1484	5.2604	-3.6860 H
50	C50	2.6462	3.3281	-2.8733 C
51	H51	3.3668	3.0942	-3.6517 H
52	C52	2.4130	2.4084	-1.8568 C
53	H53	2.9522	1.4684	-1.8617 H
54	C54	1.1097	-1.6801	-2.0562 C
55	C55	2.2534	-1.1991	-2.7020 C
56	H56	3.1068	-0.8687	-2.1196 H
57	C57	2.3193	-1.1905	-4.0933 C
58	H58	3.2172	-0.8263	-4.5843 H
59	C59	1.2474	-1.6581	-4.8497 C
60	H60	1.3033	-1.6517	-5.9344 H
61	C61	0.1051	-2.1422	-4.2121 C
62	H62	-0.7312	-2.5146	-4.7965 H
63	C63	0.0321	-2.1507	-2.8244 C
64	H64	-0.8616	-2.5328	-2.3369 H
65	C65	0.4685	-3.3929	0.1396 C
66	C66	-0.8805	-3.6849	0.3753 C
67	H67	-1.6125	-2.8814	0.4115 H
68	C68	-1.2896	-5.0042	0.5612 C
69	H69	-2.3381	-5.2206	0.7445 H
70	C70	-0.3559	-6.0347	0.5154 C
71	H71	-0.6727	-7.0630	0.6649 H
72	C72	0.9874	-5.7485	0.2708 C
73	H73	1.7170	-6.5521	0.2271 H
74	C74	1.4024	-4.4360	0.0746 C
75	H75	2.4470	-4.2245	-0.1263 H
76	C76	2.4538	-1.1043	0.5231 C
77	C77	2.5345	0.4519	0.8246 C
78	B78	3.8721	-1.8173	0.1689 B
79	H79	3.9205	-2.7460	-0.5834 H
80	B80	3.1763	-2.0491	1.7782 B
81	H81	2.6931	-3.0761	2.1382 H
82	B82	2.2639	-0.5739	2.1545 B
83	H83	1.2027	-0.5650	2.6851 H
84	B84	3.4182	0.7491	2.2650 B
85	H85	3.1505	1.7027	2.9220 H
86	B86	4.0837	0.9821	0.6176 B
87	H87	4.3198	2.0995	0.2727 H
88	B88	5.0242	0.1554	1.8860 B
89	H89	5.9826	0.6434	2.4085 H
90	B90	5.1120	-0.5026	0.2417 B
91	H91	6.1615	-0.4658	-0.3310 H
92	H92	4.2724	0.1360	-0.4691 H
93	B93	3.8668	-0.8266	2.8525 B
94	H94	4.0036	-1.0270	4.0213 H
95	B95	4.8568	-1.6164	1.5933 B

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Cu-2 T_1
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96 114
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NO_CHARGES

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3 P3 0.7339 1.7026 0.2279 P
4 N4 -2.1999 -0.8893 1.2167 N
5 N5 -2.4790 0.3297 -1.2133 N
6 C6 -3.4725 -0.7606 0.6877 C
7 C7 -2.0595 -1.4111 2.4488 C
8 C8 -3.1500 -1.8575 3.1961 C
9 H9 -2.9792 -2.2669 4.1861 H
10 C10 -4.4362 -1.7843 2.6606 C
11 H11 -5.2946 -2.1446 3.2217 H
12 C12 -4.6217 -1.2255 1.3998 C
13 C13 -5.9121 -1.0801 0.7998 C
14 H14 -6.7799 -1.4426 1.3454 H
15 C15 -6.0509 -0.4978 -0.4191 C
16 H16 -7.0329 -0.3918 -0.8739 H
17 C17 -4.9156 -0.0024 -1.1428 C
18 C18 -5.0318 0.6033 -2.3902 C
19 H19 -6.0100 0.7246 -2.8466 H
20 C20 -3.8673 1.0402 -3.0466 C
21 H21 -3.9253 1.4915 -4.0316 H
22 C22 -2.6291 0.8893 -2.4496 C
23 C23 -3.6172 -0.1363 -0.5648 C
24 C24 -0.6839 -1.5305 3.0236 C
25 H25 -0.2479 -2.5078 2.7883 H
26 H26 -0.7138 -1.4355 4.1130 H
27 H27 -0.0192 -0.7599 2.6272 H
28 C28 -1.3947 1.3020 -3.1859 C
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30 H30 -1.6508 1.8426 -4.1010 H
31 H31 -0.8024 0.4238 -3.4687 H
32 C32 0.8076 -2.4753 -1.8457 C
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34 H34 2.6613 -3.5861 -1.7359 H
35 C35 1.4196 -4.2674 -3.3505 C
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37 C37 0.2079 -4.1152 -4.0253 C
38 H38 -0.0229 -4.7531 -4.8738 H
39 C39 -0.7074 -3.1539 -3.6074 C
40 H40 -1.6566 -3.0392 -4.1227 H
41 C41 -0.4105 -2.3360 -2.5187 C
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43 C43 1.7131 -2.5516 0.8805 C
44 C44 1.1876 -3.8514 0.9144 C
45 H45 0.5223 -4.1953 0.1287 H
46 C46 1.5180 -4.7146 1.9556 C
47 H47 1.1112 -5.7216 1.9647 H
48 C48 2.3645 -4.2904 2.9774 C
49 H49 2.6219 -4.9662 3.7880 H
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52 C52 2.5505 -2.1294 1.9197 C
53 H53 2.9511 -1.1222 1.9254 H
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59 C59 0.9657 1.8167 4.8378 C
60 H60 0.9917 1.8386 5.9235 H
61 C61 -0.2091 2.1443 4.1610 C
62 H62 -1.1008 2.4217 4.7155 H
63 C63 -0.2440 2.1157 2.7721 C
64 H64 -1.1656 2.3700 2.2538 H
65 C65 0.1728 3.3846 -0.1962 C
66 C66 -1.1822 3.5608 -0.4999 C
67 H67 -1.8420 2.6991 -0.5606 H
68 C68 -1.6898 4.8405 -0.7170 C
69 H69 -2.7424 4.9671 -0.9533 H
70 C70 -0.8492 5.9460 -0.6338 C
71 H71 -1.2435 6.9434 -0.8072 H
72 C72 0.4994 5.7749 -0.3208 C
73 H73 1.1561 6.6370 -0.2479 H
74 C74 1.0120 4.5027 -0.0934 C
75 H75 2.0595 4.3807 0.1608 H
76 C76 2.3576 1.2764 -0.5016 C
77 C77 2.5688 -0.2678 -0.8026 C
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80 B80 3.0370 2.2775 -1.7387 B
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83 H83 1.2136 0.6473 -2.6995 H
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Cu-3 S_0
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4 N4 -1.3154 -1.4391 -0.0196 N
5 N5 -1.1641 1.2590 -0.0669 N
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7 C7 3.6460 -0.6222 0.8749 C
8 C8 1.8220 -1.0460 3.2199 C
9 C9 0.6362 -1.7693 3.3743 C
10 H10 -0.0945 -1.7687 2.5687 H
11 C11 0.3765 -2.4637 4.5551 C
12 H12 -0.5489 -3.0235 4.6625 H
13 C13 1.3008 -2.4319 5.5937 C

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15	C15	2.4800	-1.6996	5.4547 C
16	H16	3.2019	-1.6707	6.2664 H
17	C17	2.7401	-1.0073	4.2781 C
18	H18	3.6594	-0.4381	4.1741 H
19	C19	2.3311	1.5931	2.3304 C
20	C20	1.4910	2.0492	3.3562 C
21	H21	0.7791	1.3681	3.8157 H
22	C22	1.5666	3.3639	3.8046 C
23	H23	0.9141	3.6956	4.6083 H
24	C24	2.4801	4.2490	3.2338 C
25	H25	2.5429	5.2747	3.5873 H
26	C26	3.3166	3.8057	2.2135 C
27	H27	4.0390	4.4828	1.7655 H
28	C28	3.2409	2.4895	1.7644 C
29	H29	3.9030	2.1601	0.9723 H
30	C30	1.9316	-1.2126	-3.1140 C
31	C31	0.7114	-1.8708	-3.2935 C
32	H32	-0.0550	-1.7879	-2.5261 H
33	C33	0.4648	-2.6066	-4.4518 C
34	H34	-0.4883	-3.1135	-4.5791 H
35	C35	1.4379	-2.6844	-5.4421 C
36	H36	1.2509	-3.2580	-6.3462 H
37	C37	2.6530	-2.0194	-5.2770 C
38	H38	3.4139	-2.0763	-6.0507 H
39	C39	2.9002	-1.2838	-4.1241 C
40	H40	3.8492	-0.7713	-3.9984 H
41	C41	2.4359	1.4645	-2.3426 C
42	C42	1.4972	1.9288	-3.2756 C
43	H43	0.6924	1.2744	-3.6033 H
44	C44	1.5910	3.2136	-3.7979 C
45	H45	0.8622	3.5512	-4.5305 H
46	C46	2.6189	4.0629	-3.3887 C
47	H47	2.6943	5.0671	-3.7976 H
48	C48	3.5551	3.6100	-2.4648 C
49	H49	4.3716	4.2561	-2.1530 H
50	C50	3.4673	2.3191	-1.9462 C
51	H51	4.2277	1.9639	-1.2592 H
52	C52	-2.4796	-0.7437	-0.0569 C
53	C53	-1.3616	-2.7720	-0.0088 C
54	C54	-2.5853	-3.4635	-0.0131 C
55	H55	-2.5744	-4.5482	0.0316 H
56	C56	-3.7914	-2.7906	-0.0316 C
57	C57	-3.7506	-1.3698	-0.0787 C
58	C58	-4.9234	-0.5636	-0.1987 C
59	H59	-5.8852	-1.0552	-0.2974 H
60	C60	-4.8463	0.7932	-0.2205 C
61	H61	-5.7468	1.3868	-0.3360 H
62	C62	-3.5896	1.4642	-0.1246 C
63	C63	-3.4667	2.8828	-0.1235 C
64	C64	-2.1933	3.4122	-0.1267 C
65	H65	-2.0560	4.4897	-0.1163 H
66	C66	-1.0545	2.5835	-0.0961 C
67	C67	-2.3993	0.7006	-0.0814 C
68	C68	-5.0557	-3.5605	-0.0022 C
69	C69	-6.0393	-3.3099	0.9636 C
70	H70	-5.8811	-2.5247	1.6982 H
71	C71	-7.1978	-4.0787	1.0067 C
72	H72	-7.9465	-3.8806	1.7687 H
73	C73	-7.3942	-5.1030	0.0833 C

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80 C80 -4.7487 4.8089 -1.0616 C
81 H81 -3.9927 4.8967 -1.8377 H
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84 C84 -6.7996 5.5717 -0.0451 C
85 H85 -7.6377 6.2625 -0.0205 H
86 C86 -6.6948 4.5652 0.9121 C
87 H87 -7.4456 4.4743 1.6922 H
88 C88 -5.6246 3.6775 0.8792 C
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90 B90 4.5778 -2.0660 -1.2904 B
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94 B94 3.5445 -2.1586 0.1438 B
95 H95 2.5210 -2.7590 0.1754 H
96 B96 4.5688 -1.9039 1.5530 B
97 H97 4.2416 -2.3632 2.5992 H
98 B98 5.1279 -0.2045 1.4585 B
99 H99 5.2384 0.4091 2.4790 H
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101 H101 5.3993 -3.9625 0.2784 H
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103 H103 7.1730 -2.0264 -1.3647 H
104 B104 6.2766 -0.0950 0.0177 B
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106 H106 5.3360 0.6703 0.3934 H
107 B107 6.2064 -1.5546 1.0262 B
108 H108 7.1370 -1.8865 1.6966 H
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111 H111 0.4984 -3.2770 0.9277 H
112 H112 -0.2441 -4.6057 0.0144 H
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Cu-3 S_1
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5 N5 -1.1076 1.2774 -0.1866 N
6 C6 3.7419 -0.8824 -0.5679 C
7 C7 3.7106 -0.4571 0.9544 C
8 C8 1.6756 -0.4745 3.1825 C
9 C9 0.4833 -1.1974 3.2837 C
10 H10 -0.1528 -1.3268 2.4110 H
11 C11 0.0967 -1.7378 4.5087 C
12 H12 -0.8318 -2.2969 4.5795 H
13 C13 0.8972 -1.5580 5.6319 C
14 H14 0.5972 -1.9822 6.5862 H
15 C15 2.0827 -0.8289 5.5376 C
16 H16 2.7075 -0.6867 6.4147 H
17 C17 2.4716 -0.2823 4.3208 C
18 H18 3.3927 0.2893 4.2514 H
19 C19 2.4104 2.0097 1.9842 C
20 C20 1.5844 2.6130 2.9437 C
21 H21 0.8511 2.0196 3.4818 H
22 C22 1.7053 3.9708 3.2204 C
23 H23 1.0658 4.4237 3.9728 H
24 C24 2.6444 4.7439 2.5405 C
25 H25 2.7417 5.8030 2.7619 H
26 C26 3.4588 4.1535 1.5771 C
27 H27 4.1956 4.7483 1.0448 H
28 C28 3.3401 2.7969 1.2963 C
29 H29 3.9815 2.3502 0.5461 H
30 C30 1.8728 -1.7541 -2.8078 C
31 C31 0.5678 -2.2385 -2.9461 C
32 H32 -0.2001 -1.9474 -2.2332 H
33 C33 0.2494 -3.0907 -4.0019 C
34 H34 -0.7656 -3.4643 -4.1017 H
35 C35 1.2294 -3.4614 -4.9165 C
36 H36 0.9824 -4.1302 -5.7365 H
37 C37 2.5286 -2.9719 -4.7856 C
38 H38 3.2944 -3.2577 -5.5010 H
39 C39 2.8535 -2.1143 -3.7414 C
40 H40 3.8646 -1.7314 -3.6462 H
41 C41 2.4093 1.0162 -2.4282 C
42 C42 1.3711 1.3687 -3.3042 C
43 H43 0.5200 0.7052 -3.4351 H
44 C44 1.4290 2.5590 -4.0175 C
45 H45 0.6237 2.8167 -4.6994 H
46 C46 2.5184 3.4155 -3.8612 C
47 H47 2.5655 4.3446 -4.4227 H
48 C48 3.5509 3.0714 -2.9936 C

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50	C50	3.5006	1.8775	-2.2780 C
51	H51	4.3320	1.5942	-1.6409 H
52	C52	-2.4213	-0.7189	-0.0100 C
53	C53	-1.3086	-2.7846	0.1981 C
54	C54	-2.5081	-3.4516	0.2565 C
55	H55	-2.5007	-4.5269	0.4029 H
56	C56	-3.7504	-2.7663	0.2119 C
57	C57	-3.6920	-1.3598	0.0390 C
58	C58	-4.8571	-0.5579	-0.1731 C
59	H59	-5.8165	-1.0574	-0.2529 H
60	C60	-4.7941	0.7947	-0.3143 C
61	H61	-5.6992	1.3625	-0.5024 H
62	C62	-3.5468	1.4755	-0.2655 C
63	C63	-3.4232	2.8768	-0.3987 C
64	C64	-2.1438	3.4144	-0.4763 C
65	H65	-2.0075	4.4869	-0.5744 H
66	C66	-1.0132	2.5911	-0.3664 C
67	C67	-2.3558	0.6935	-0.1498 C
68	C68	-4.9966	-3.5305	0.3432 C
69	C69	-6.0566	-3.1049	1.1650 C
70	H70	-5.9551	-2.1801	1.7262 H
71	C71	-7.2091	-3.8688	1.3053 C
72	H72	-8.0075	-3.5187	1.9549 H
73	C73	-7.3374	-5.0845	0.6361 C
74	H74	-8.2389	-5.6806	0.7471 H
75	C75	-6.2921	-5.5299	-0.1709 C
76	H76	-6.3780	-6.4755	-0.7003 H
77	C77	-5.1395	-4.7672	-0.3123 C
78	H78	-4.3395	-5.1153	-0.9608 H
79	C79	-4.5920	3.7824	-0.4584 C
80	C80	-4.6817	4.7524	-1.4652 C
81	H81	-3.9097	4.7950	-2.2293 H
82	C82	-5.7548	5.6363	-1.5080 C
83	H83	-5.8136	6.3740	-2.3038 H
84	C84	-6.7525	5.5736	-0.5381 C
85	H85	-7.5898	6.2654	-0.5701 H
86	C86	-6.6693	4.6211	0.4746 C
87	H87	-7.4373	4.5728	1.2420 H
88	C88	-5.5998	3.7325	0.5145 C
89	H89	-5.5283	3.0035	1.3170 H
90	B90	4.5933	-2.3720	-0.8110 B
91	H91	4.2074	-3.1815	-1.5929 H
92	B92	5.1992	-0.7833	-1.2909 B
93	H93	5.2803	-0.5282	-2.4571 H
94	B94	3.5791	-2.1248	0.6249 B
95	H95	2.5474	-2.6783	0.8130 H
96	B96	4.6259	-1.5468	1.9189 B
97	H97	4.2975	-1.7256	3.0467 H
98	B98	5.2049	0.0781	1.4257 B
99	H99	5.3221	0.9044	2.2795 H
100	B100	5.2254	-2.7358	0.7988 B
101	H101	5.4216	-3.8573	1.1499 H
102	B102	6.2240	-1.8879	-0.4162 B
103	H103	7.1891	-2.3761	-0.9206 H
104	B104	6.3317	-0.1667	-0.0174 B
105	H105	7.3458	0.4418	-0.1825 H
106	H106	5.4124	0.6886	0.1945 H
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108	H108	7.1917	-1.5262	2.0269 H

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109 C109    -0.0248   -3.5423    0.3281 C
110 H110     0.6708   -3.3078   -0.4830 H
111 H111     0.4837   -3.3000    1.2683 H
112 H112    -0.2059   -4.6205    0.3161 H
113 C113     0.3421    3.2220   -0.4283 C
114 H114     0.5460    3.7983    0.4815 H
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Cu-3 T_1
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8 C8 1.6965 -1.1735 3.1067 C
9 C9 0.5106 -1.9133 3.1405 C
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11 C11 0.1884 -2.6696 4.2667 C
12 H12 -0.7352 -3.2408 4.2848 H
13 C13 1.0451 -2.6841 5.3630 C
14 H14 0.7947 -3.2735 6.2406 H
15 C15 2.2210 -1.9327 5.3418 C
16 H16 2.8858 -1.9352 6.2009 H
17 C17 2.5451 -1.1743 4.2232 C
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20 C20 1.3469 1.9147 3.3556 C
21 H21 0.5867 1.2205 3.7032 H
22 C22 1.3995 3.1962 3.8934 C
23 H23 0.6812 3.4884 4.6540 H
24 C24 2.3718 4.0983 3.4625 C
25 H25 2.4148 5.0975 3.8863 H

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27	H27	4.0512	4.4065	2.1479 H
28	C28	3.2370	2.4304	1.9463 C
29	H29	3.9614	2.1470	1.1925 H
30	C30	1.9058	-1.0827	-3.0921 C
31	C31	0.6656	-1.7026	-3.2763 C
32	H32	-0.0939	-1.6373	-2.5007 H
33	C33	0.3917	-2.3847	-4.4612 C
34	H34	-0.5745	-2.8626	-4.5955 H
35	C35	1.3521	-2.4462	-5.4659 C
36	H36	1.1401	-2.9787	-6.3888 H
37	C37	2.5848	-1.8148	-5.2938 C
38	H38	3.3322	-1.8540	-6.0811 H
39	C39	2.8617	-1.1289	-4.1172 C
40	H40	3.8197	-0.6333	-3.9919 H
41	C41	2.4646	1.5654	-2.2162 C
42	C42	1.5402	2.0523	-3.1529 C
43	H43	0.7421	1.4106	-3.5177 H
44	C44	1.6433	3.3536	-3.6312 C
45	H45	0.9265	3.7148	-4.3633 H
46	C46	2.6639	4.1886	-3.1766 C
47	H47	2.7447	5.2047	-3.5523 H
48	C48	3.5830	3.7123	-2.2454 C
49	H49	4.3881	4.3520	-1.8950 H
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53	C53	-1.3076	-2.8064	-0.1933 C
54	C54	-2.5030	-3.4663	-0.2418 C
55	H55	-2.4904	-4.5514	-0.2585 H
56	C56	-3.7579	-2.7869	-0.1824 C
57	C57	-3.6943	-1.3487	-0.1904 C
58	C58	-4.8434	-0.5329	-0.3418 C
59	H59	-5.8024	-1.0115	-0.5064 H
60	C60	-4.7820	0.8430	-0.3123 C
61	H61	-5.6876	1.4257	-0.4400 H
62	C62	-3.5464	1.5005	-0.1480 C
63	C63	-3.4134	2.9179	-0.0851 C
64	C64	-2.1394	3.4442	-0.0405 C
65	H65	-1.9923	4.5183	0.0176 H
66	C66	-1.0062	2.6007	-0.0210 C
67	C67	-2.3557	0.7091	-0.1030 C
68	C68	-4.9913	-3.5605	-0.0986 C
69	C69	-6.0764	-3.1746	0.7192 C
70	H70	-5.9982	-2.2726	1.3192 H
71	C71	-7.2217	-3.9552	0.8128 C
72	H72	-8.0334	-3.6363	1.4618 H
73	C73	-7.3277	-5.1493	0.0978 C
74	H74	-8.2251	-5.7569	0.1716 H
75	C75	-6.2620	-5.5561	-0.7066 C
76	H76	-6.3295	-6.4822	-1.2719 H
77	C77	-5.1142	-4.7804	-0.8001 C
78	H78	-4.3055	-5.1027	-1.4507 H
79	C79	-4.5806	3.8278	-0.0603 C
80	C80	-4.6375	4.9173	-0.9394 C
81	H81	-3.8439	5.0556	-1.6691 H
82	C82	-5.7089	5.8045	-0.8991 C
83	H83	-5.7442	6.6377	-1.5954 H
84	C84	-6.7328	5.6236	0.0287 C
85	H85	-7.5676	6.3182	0.0620 H

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116 H116 0.4831 3.9502 -0.7570 H
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5	N5	1.1708	-1.2228	-0.3097 N
6	C6	-3.5854	0.9756	-0.4212 C
7	C7	-3.4249	0.6588	1.1288 C
8	C8	-1.5160	0.3550	3.3713 C
9	C9	-0.4534	1.2407	3.5707 C
10	H10	0.1291	1.5739	2.7150 H
11	C11	-0.1415	1.6920	4.8510 C
12	H12	0.6837	2.3845	4.9955 H
13	C13	-0.8851	1.2525	5.9421 C
14	H14	-0.6430	1.6023	6.9423 H
15	C15	-1.9414	0.3623	5.7520 C
16	H16	-2.5262	0.0215	6.6021 H
17	C17	-2.2576	-0.0852	4.4745 C
18	H18	-3.0886	-0.7691	4.3276 H
19	C19	-2.2589	-1.9683	1.8856 C
20	C20	-1.3349	-2.7577	2.5870 C
21	H21	-0.4762	-2.2887	3.0621 H
22	C22	-1.5159	-4.1320	2.6956 C
23	H23	-0.7982	-4.7271	3.2548 H
24	C24	-2.6156	-4.7432	2.0941 C
25	H25	-2.7579	-5.8173	2.1791 H
26	C26	-3.5304	-3.9692	1.3876 C
27	H27	-4.3914	-4.4345	0.9154 H
28	C28	-3.3548	-2.5909	1.2843 C
29	H29	-4.0798	-1.9994	0.7372 H
30	C30	-2.2006	1.4435	-2.9852 C
31	C31	-1.2458	2.4623	-3.0618 C
32	H32	-0.5389	2.5925	-2.2459 H
33	C33	-1.1993	3.3036	-4.1695 C
34	H34	-0.4580	4.0970	-4.2168 H
35	C35	-2.0994	3.1238	-5.2165 C
36	H36	-2.0633	3.7780	-6.0837 H
37	C37	-3.0442	2.1017	-5.1532 C
38	H38	-3.7479	1.9591	-5.9688 H
39	C39	-3.0963	1.2636	-4.0443 C
40	H40	-3.8382	0.4724	-3.9960 H
41	C41	-2.6867	-1.2598	-2.1763 C
42	C42	-1.6654	-1.9757	-2.8178 C
43	H43	-0.6708	-1.5389	-2.8902 H
44	C44	-1.9111	-3.2303	-3.3650 C
45	H45	-1.1109	-3.7674	-3.8682 H
46	C46	-3.1807	-3.7972	-3.2648 C
47	H47	-3.3748	-4.7798	-3.6867 H
48	C48	-4.1981	-3.0977	-2.6232 C
49	H49	-5.1924	-3.5302	-2.5464 H
50	C50	-3.9574	-1.8345	-2.0842 C
51	H51	-4.7628	-1.2877	-1.6040 H
52	C52	2.4528	0.7800	-0.1285 C
53	C53	1.2941	2.7508	0.1150 C
54	H54	0.3272	3.2388	0.2134 H
55	C55	2.4781	3.4930	0.1449 C
56	H56	2.4305	4.5690	0.2800 H
57	C57	3.7066	2.8560	0.0466 C
58	C58	3.7036	1.4416	-0.1131 C
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60	H60	5.8420	1.1729	-0.3783 H
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69 C69 2.3975 -0.6563 -0.2735 C
70 C70 4.9511 3.6545 0.1095 C
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77 C77 6.2501 5.5538 -0.6533 C
78 H78 6.3581 6.4100 -1.3131 H
79 C79 5.1033 4.7701 -0.7231 C
80 H80 4.3237 5.0093 -1.4418 H
81 C81 4.6702 -3.7084 -0.5010 C
82 C82 4.7844 -4.6895 -1.4936 C
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84 C84 5.8724 -5.5561 -1.5096 C
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97 H97 -1.9518 2.6405 0.6428 H
98 B98 -4.0292 1.9523 2.0876 B
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100 B100 -4.9043 0.4101 1.8030 B
101 H101 -5.0469 -0.3275 2.7338 H
102 B102 -4.5739 3.1458 0.9438 B
103 H103 -4.5499 4.3069 1.2173 H
104 B104 -5.8384 2.3940 -0.0702 B
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106 B106 -6.1574 0.7428 0.4844 B
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5 N5 1.1873 -1.2138 -0.3747 N
6 C6 -3.3481 1.3302 0.6958 C
7 C7 -3.2194 -0.0327 1.4948 C
8 C8 -1.2594 -2.0688 2.3428 C
9 C9 -0.0205 -1.6085 2.8034 C
10 H10 0.5102 -0.8310 2.2609 H
11 C11 0.5445 -2.1532 3.9540 C
12 H12 1.5058 -1.7898 4.3054 H
13 C13 -0.1192 -3.1634 4.6451 C
14 H14 0.3238 -3.5903 5.5406 H
15 C15 -1.3522 -3.6289 4.1886 C
16 H16 -1.8734 -4.4141 4.7286 H
17 C17 -1.9240 -3.0847 3.0441 C
18 H18 -2.8902 -3.4429 2.7012 H
19 C19 -2.9207 -2.5852 0.0247 C
20 C20 -2.3713 -3.8743 -0.0542 C
21 H21 -1.4489 -4.1108 0.4691 H
22 C22 -3.0176 -4.8715 -0.7782 C
23 H23 -2.5854 -5.8671 -0.8212 H
24 C24 -4.2149 -4.5962 -1.4354 C
25 H25 -4.7195 -5.3764 -1.9981 H
26 C26 -4.7628 -3.3173 -1.3666 C
27 H27 -5.6955 -3.0928 -1.8756 H
28 C28 -4.1198 -2.3162 -0.6455 C
29 H29 -4.5576 -1.3246 -0.6126 H
30 C30 -1.9932 3.1097 -1.3972 C
31 C31 -0.8636 3.2735 -2.2136 C
32 H32 -0.1641 2.4512 -2.3455 H
33 C33 -0.6247 4.4866 -2.8509 C
34 H34 0.2547 4.6004 -3.4783 H
35 C35 -1.5071 5.5503 -2.6751 C
36 H36 -1.3198 6.5001 -3.1679 H
37 C37 -2.6307 5.3928 -1.8671 C
38 H38 -3.3238 6.2179 -1.7299 H
39 C39 -2.8805 4.1788 -1.2317 C
40 H40 -3.7634 4.0695 -0.6143 H
41 C41 -3.0031 0.5380 -2.1384 C
42 C42 -2.2443 -0.4032 -2.8427 C
43 H43 -1.2280 -0.6345 -2.5273 H
44 C44 -2.7821 -1.0570 -3.9487 C
45 H45 -2.1846 -1.7865 -4.4875 H
46 C46 -4.0847 -0.7785 -4.3529 C
47 H47 -4.5080 -1.2907 -5.2124 H
48 C48 -4.8464 0.1602 -3.6566 C
49 H49 -5.8616 0.3816 -3.9735 H

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51	H51	-4.9047	1.5571	-2.0246 H
52	C52	2.4787	0.7610	-0.1003 C
53	C53	1.2886	2.7216	0.2810 C
54	H54	0.3231	3.2161	0.3356 H
55	C55	2.4503	3.4318	0.5343 C
56	H56	2.3845	4.4783	0.8108 H
57	C57	3.7061	2.7988	0.4341 C
58	C58	3.7224	1.4335	0.0875 C
59	C59	4.9101	0.6734	-0.1741 C
60	H60	5.8690	1.1803	-0.1457 H
61	C61	4.8620	-0.6458	-0.5040 C
62	H62	5.7831	-1.1660	-0.7451 H
63	C63	3.6255	-1.3744	-0.5620 C
64	C64	3.5203	-2.7484	-0.8622 C
65	C65	2.2159	-3.2858	-0.9948 C
66	H66	2.0808	-4.3375	-1.2238 H
67	C67	1.1102	-2.5035	-0.7400 C
68	H68	0.1115	-2.9269	-0.7962 H
69	C69	2.4327	-0.6249	-0.3539 C
70	C70	4.9318	3.5809	0.6941 C
71	C71	5.9337	3.1095	1.5560 C
72	H72	5.8093	2.1472	2.0451 H
73	C73	7.0654	3.8759	1.8175 C
74	H74	7.8260	3.4967	2.4947 H
75	C75	7.2179	5.1279	1.2249 C
76	H76	8.1022	5.7252	1.4288 H
77	C77	6.2255	5.6121	0.3739 C
78	H78	6.3357	6.5871	-0.0930 H
79	C79	5.0915	4.8492	0.1156 C
80	H80	4.3259	5.2275	-0.5571 H
81	C81	4.6828	-3.6353	-1.0531 C
82	C82	4.7061	-4.5364	-2.1302 C
83	H83	3.8862	-4.5323	-2.8440 H
84	C84	5.7721	-5.4115	-2.3088 C
85	H85	5.7727	-6.0923	-3.1559 H
86	C86	6.8375	-5.4130	-1.4098 C
87	H87	7.6697	-6.0977	-1.5476 H
88	C88	6.8235	-4.5333	-0.3286 C
89	H89	7.6405	-4.5373	0.3880 H
90	C90	5.7584	-3.6557	-0.1502 C
91	H91	5.7420	-2.9992	0.7155 H
92	B92	-3.5348	2.6790	1.7617 B
93	H93	-3.0041	3.7242	1.5488 H
94	B94	-4.8224	2.0062	0.7437 B
95	H95	-5.2433	2.6643	-0.1619 H
96	B96	-2.4712	1.3282	2.1923 B
97	H97	-1.2797	1.4090	2.2052 H
98	B98	-3.4028	0.2122	3.1852 B
99	H99	-2.8357	-0.5099	3.9402 H
100	B100	-4.6774	-0.4691	2.1185 B
101	H101	-4.9660	-1.6184	2.2668 H
102	B102	-3.6539	1.9256	3.3574 B
103	H103	-3.3096	2.5005	4.3454 H
104	B104	-5.1174	2.3578	2.4263 B
105	H105	-5.8702	3.2219	2.7695 H
106	B106	-5.8470	0.8988	1.7410 B
107	H107	-7.0362	0.7768	1.6941 H
108	H108	-5.3411	0.0101	0.9881 H
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5 N5 1.1364 -1.2197 -0.4201 N
6 C6 -3.3907 1.3610 0.5071 C
7 C7 -3.2918 0.0744 1.4283 C
8 C8 -1.3159 -1.8297 2.5495 C
9 C9 -0.0746 -1.3530 2.9852 C
10 H10 0.4801 -0.6377 2.3825 H
11 C11 0.4605 -1.7996 4.1911 C
12 H12 1.4245 -1.4257 4.5234 H
13 C13 -0.2369 -2.7260 4.9619 C
14 H14 0.1830 -3.0763 5.9006 H
15 C15 -1.4729 -3.2072 4.5300 C
16 H16 -2.0186 -3.9282 5.1316 H
17 C17 -2.0142 -2.7620 3.3295 C
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19 C19 -2.8390 -2.5861 0.2015 C
20 C20 -2.2629 -3.8624 0.2862 C
21 H21 -1.3751 -4.0246 0.8908 H
22 C22 -2.8383 -4.9373 -0.3849 C
23 H23 -2.3879 -5.9224 -0.3037 H
24 C24 -3.9887 -4.7516 -1.1484 C
25 H25 -4.4383 -5.5923 -1.6690 H
26 C26 -4.5620 -3.4853 -1.2408 C
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28 C28 -3.9902 -2.4065 -0.5738 C
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34 H34 0.6012 4.4608 -3.3939 H
35 C35 -1.3010 5.3725 -2.9474 C
36 H36 -1.0729 6.2974 -3.4697 H
37 C37 -2.5341 5.2120 -2.3190 C
38 H38 -3.2710 6.0095 -2.3514 H

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40	H40	-3.8031	3.9175	-1.1727 H
41	C41	-2.8869	0.3749	-2.2447 C
42	C42	-2.0574	-0.5582	-2.8777 C
43	H43	-1.0395	-0.7161	-2.5242 H
44	C44	-2.5255	-1.2937	-3.9636 C
45	H45	-1.8737	-2.0156	-4.4471 H
46	C46	-3.8275	-1.1061	-4.4195 C
47	H47	-4.1963	-1.6826	-5.2632 H
48	C48	-4.6580	-0.1756	-3.7952 C
49	H49	-5.6728	-0.0248	-4.1523 H
50	C50	-4.1916	0.5692	-2.7163 C
51	H51	-4.8428	1.2940	-2.2387 H
52	C52	2.4327	0.7234	-0.0131 C
53	C53	1.2328	2.6686	0.4556 C
54	H54	0.2637	3.1455	0.5701 H
55	C55	2.3929	3.3881	0.6482 C
56	H56	2.3281	4.4299	0.9433 H
57	C57	3.6570	2.7677	0.5033 C
58	C58	3.6738	1.4075	0.1417 C
59	C59	4.8604	0.6544	-0.1510 C
60	H60	5.8165	1.1673	-0.1427 H
61	C61	4.8166	-0.6676	-0.4702 C
62	H62	5.7380	-1.1844	-0.7173 H
63	C63	3.5824	-1.3997	-0.5226 C
64	C64	3.4780	-2.7703	-0.8287 C
65	C65	2.1736	-3.3113	-0.9550 C
66	H66	2.0410	-4.3626	-1.1872 H
67	C67	1.0648	-2.5241	-0.7397 C
68	H68	0.0658	-2.9427	-0.8230 H
69	C69	2.3892	-0.6484	-0.3166 C
70	C70	4.8792	3.5628	0.7347 C
71	C71	5.9211	3.0931	1.5497 C
72	H72	5.8309	2.1202	2.0252 H
73	C73	7.0493	3.8732	1.7846 C
74	H74	7.8405	3.4932	2.4254 H
75	C75	7.1594	5.1397	1.2139 C
76	H76	8.0406	5.7481	1.3978 H
77	C77	6.1274	5.6236	0.4112 C
78	H78	6.2032	6.6101	-0.0385 H
79	C79	4.9981	4.8459	0.1780 C
80	H80	4.2026	5.2248	-0.4586 H
81	C81	4.6425	-3.6529	-1.0331 C
82	C82	4.6669	-4.5351	-2.1253 C
83	H83	3.8443	-4.5237	-2.8359 H
84	C84	5.7377	-5.4005	-2.3225 C
85	H85	5.7398	-6.0664	-3.1814 H
86	C86	6.8061	-5.4104	-1.4271 C
87	H87	7.6422	-6.0872	-1.5796 H
88	C88	6.7905	-4.5497	-0.3310 C
89	H89	7.6105	-4.5604	0.3821 H
90	C90	5.7205	-3.6818	-0.1340 C
91	H91	5.7033	-3.0386	0.7416 H
92	B92	-3.6646	2.7932	1.4396 B
93	H93	-3.1410	3.8275	1.1649 H
94	B94	-4.8756	2.0082	0.4100 B
95	H95	-5.2519	2.5822	-0.5692 H
96	B96	-2.6068	1.5061	2.0454 B
97	H97	-1.4195	1.6051	2.1232 H
98	B98	-3.5787	0.4589	3.0754 B

99 H99 -3.0447 -0.1851 3.9199 H
100 B100 -4.7772 -0.3383 1.9989 B
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103 H103 -3.5927 2.8380 4.0383 H
104 B104 -5.2790 2.4945 2.0354 B
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106 B106 -5.9436 0.9680 1.4357 B
107 H107 -7.1257 0.8187 1.3302 H
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5 N5 1.0359 -2.2856 1.4577 N
6 C6 -1.5549 1.7983 -0.6936 C
7 C7 -0.0344 2.3011 -0.8317 C
8 C8 2.7223 1.3276 -1.4576 C
9 C9 3.1085 0.2179 -2.2148 C
10 H10 2.5656 -0.7175 -2.1042 H
11 C11 4.1957 0.2965 -3.0849 C
12 H12 4.4852 -0.5729 -3.6688 H
13 C13 4.9115 1.4847 -3.1936 C
14 H14 5.7609 1.5488 -3.8682 H
15 C15 4.5445 2.5927 -2.4279 C
16 H16 5.1069 3.5191 -2.5063 H
17 C17 3.4584 2.5161 -1.5635 C
18 H18 3.1793 3.3807 -0.9677 H
19 C19 2.0162 1.8237 1.2484 C
20 C20 3.3172 1.4475 1.6140 C
21 H21 3.9231 0.8532 0.9349 H
22 C22 3.8502 1.8362 2.8394 C
23 H23 4.8630 1.5416 3.1011 H
24 C24 3.0925 2.6030 3.7239 C
25 H25 3.5101 2.9085 4.6793 H
26 C26 1.7978 2.9759 3.3722 C
27 H27 1.1972 3.5746 4.0517 H

28	C28	1.2642	2.5860	2.1461 C
29	H29	0.2528	2.8808	1.8932 H
30	C30	-3.2575	-0.6873	-0.7251 C
31	C31	-3.1011	-1.9745	-1.2491 C
32	H32	-2.1223	-2.4468	-1.2240 H
33	C33	-4.1928	-2.6654	-1.7751 C
34	H34	-4.0561	-3.6649	-2.1787 H
35	C35	-5.4521	-2.0744	-1.7740 C
36	H36	-6.3053	-2.6089	-2.1827 H
37	C37	-5.6212	-0.7972	-1.2363 C
38	H38	-6.6059	-0.3378	-1.2250 H
39	C39	-4.5344	-0.1090	-0.7093 C
40	H40	-4.6729	0.8816	-0.2871 H
41	C41	-2.3858	0.3562	1.7553 C
42	C42	-2.8788	-0.7730	2.4265 C
43	H43	-2.9749	-1.7192	1.8985 H
44	C44	-3.2539	-0.6971	3.7632 C
45	H45	-3.6417	-1.5802	4.2640 H
46	C46	-3.1326	0.5069	4.4578 C
47	H47	-3.4229	0.5666	5.5031 H
48	C48	-2.6443	1.6320	3.8004 C
49	H49	-2.5564	2.5779	4.3282 H
50	C50	-2.2754	1.5584	2.4575 C
51	H51	-1.9273	2.4513	1.9503 H
52	C52	1.1825	-3.7664	-0.4426 C
53	C53	0.4632	-2.9839	-2.5102 C
54	C54	0.6280	-4.2488	-3.0773 C
55	H55	0.4053	-4.3955	-4.1289 H
56	C56	1.0639	-5.2999	-2.2850 C
57	C57	1.3466	-5.0570	-0.9492 C
58	C58	2.2326	-4.3393	1.7626 C
59	C59	2.4719	-4.0144	3.0923 C
60	C60	1.9659	-2.8269	3.5919 C
61	H61	2.1214	-2.5419	4.6277 H
62	C62	1.2509	-1.9729	2.7451 C
63	C63	1.4948	-3.4577	0.9743 C
64	B64	-2.5062	2.2727	-2.0641 B
65	H65	-3.3313	1.5530	-2.5338 H
66	B66	-2.6396	2.9862	-0.4583 B
67	H67	-3.6387	2.7936	0.1734 H
68	B68	-0.8171	1.7796	-2.2496 B
69	H69	-0.4764	0.7715	-2.7736 H
70	B70	0.1632	3.2383	-2.2538 B
71	H71	1.2133	3.2398	-2.8112 H
72	B72	0.0336	3.9305	-0.6097 B
73	H73	1.0004	4.4580	-0.1456 H
74	B74	-1.3996	3.2668	-3.0147 B
75	H75	-1.4987	3.3539	-4.2025 H
76	B76	-2.5531	4.0045	-1.8719 B
77	H77	-3.4757	4.6796	-2.2288 H
78	B78	-1.6999	4.5316	-0.4153 B
79	H79	-2.0002	5.5519	0.1352 H
80	H80	-0.9518	3.8763	0.3733 H
81	B81	-0.8655	4.6327	-1.9763 B
82	H82	-0.5934	5.6913	-2.4648 H
83	C83	-0.0075	-1.8391	-3.3472 C
84	H84	-0.9298	-1.4101	-2.9443 H
85	H85	0.7382	-1.0381	-3.3656 H
86	H86	-0.1958	-2.1572	-4.3755 H
87	C87	0.7012	-0.6886	3.2759 C

88 H88 1.4989 -0.0664 3.6957 H
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Cu-5 S_1

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5 N5 -1.7473 -1.9638 1.1923 N
6 C6 1.3384 2.1210 -0.4613 C
7 C7 2.2727 0.8650 -0.7296 C
8 C8 1.7821 -1.9009 -1.8066 C
9 C9 0.6458 -2.3896 -2.4605 C
10 H10 -0.3482 -2.1215 -2.1088 H
11 C11 0.7753 -3.2404 -3.5567 C
12 H12 -0.1141 -3.6138 -4.0558 H
13 C13 2.0404 -3.6122 -4.0019 C
14 H14 2.1428 -4.2752 -4.8563 H
15 C15 3.1780 -3.1421 -3.3454 C
16 H16 4.1661 -3.4382 -3.6855 H
17 C17 3.0534 -2.2937 -2.2511 C
18 H18 3.9439 -1.9429 -1.7378 H
19 C19 2.6164 -1.5599 0.9226 C
20 C20 2.8506 -2.9425 0.9086 C
21 H21 2.4837 -3.5524 0.0892 H
22 C22 3.5589 -3.5461 1.9444 C
23 H23 3.7402 -4.6166 1.9149 H
24 C24 4.0314 -2.7834 3.0094 C
25 H25 4.5844 -3.2560 3.8161 H
26 C26 3.7880 -1.4110 3.0383 C
27 H27 4.1495 -0.8087 3.8667 H
28 C28 3.0814 -0.8046 2.0063 C
29 H29 2.8917 0.2620 2.0517 H
30 C30 -1.5872 2.9652 -0.2567 C
31 C31 -2.8582 2.4946 -0.6082 C
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33 C33 -3.8968 3.3936 -0.8442 C
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35 C35 -3.6721 4.7619 -0.7310 C
36 H36 -4.4801 5.4635 -0.9187 H
37 C37 -2.4101 5.2337 -0.3694 C
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39 C39 -1.3704 4.3437 -0.1245 C
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42 C42 -1.4827 1.4802 2.6702 C
43 H43 -2.3860 1.2680 2.1030 H
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45 H45 -2.4580 1.2219 4.5641 H
46 C46 -0.3739 1.7258 4.7980 C
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50 C50 0.8658 2.0593 2.7508 C

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58 C58 -3.9124 -2.9874 1.5506 C
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62 C62 -1.4111 -2.2914 2.4590 C
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74 B74 2.8236 2.7114 -2.6842 B
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81 B81 4.2618 2.4963 -1.6269 B
82 H82 5.3636 2.6212 -2.0744 H
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Cu-5 T_1
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5 N5 -1.6740 1.9999 -1.1894 N
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7 C7 2.2275 -0.9486 0.7431 C
8 C8 1.8577 1.8413 1.8229 C
9 C9 0.7510 2.4038 2.4678 C
10 H10 -0.2563 2.1909 2.1159 H
11 C11 0.9303 3.2580 3.5545 C
12 H12 0.0641 3.6895 4.0476 H
13 C13 2.2145 3.5592 3.9978 C
14 H14 2.3551 4.2247 4.8448 H

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16	H16	4.3269	3.2579	3.6859 H
17	C17	3.1500	2.1644	2.2632 C
18	H18	4.0188	1.7583	1.7538 H
19	C19	2.6556	1.4620	-0.9093 C
20	C20	2.9344	2.8358	-0.8992 C
21	H21	2.5878	3.4599	-0.0817 H
22	C22	3.6602	3.4130	-1.9381 C
23	H23	3.8755	4.4773	-1.9130 H
24	C24	4.1067	2.6314	-3.0006 C
25	H25	4.6734	3.0831	-3.8097 H
26	C26	3.8207	1.2674	-3.0239 C
27	H27	4.1622	0.6508	-3.8502 H
28	C28	3.0960	0.6875	-1.9890 C
29	H29	2.8733	-0.3727	-2.0305 H
30	C30	-1.7093	-2.8773	0.2455 C
31	C31	-2.9541	-2.3615	0.6246 C
32	H32	-3.0921	-1.2879	0.7196 H
33	C33	-4.0225	-3.2221	0.8704 C
34	H34	-4.9839	-2.8123	1.1662 H
35	C35	-3.8537	-4.5968	0.7390 C
36	H36	-4.6849	-5.2683	0.9347 H
37	C37	-2.6182	-5.1133	0.3481 C
38	H38	-2.4859	-6.1857	0.2365 H
39	C39	-1.5495	-4.2616	0.0930 C
40	H40	-0.5956	-4.6716	-0.2206 H
41	C41	-0.3514	-1.7808	-2.0215 C
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43	H43	-2.4355	-1.2016	-2.1299 H
44	C44	-1.5820	-1.4522	-4.0821 C
45	H45	-2.5075	-1.2010	-4.5918 H
46	C46	-0.4393	-1.7710	-4.8155 C
47	H47	-0.4724	-1.7693	-5.9012 H
48	C48	0.7418	-2.0985	-4.1546 C
49	H49	1.6306	-2.3603	-4.7215 H
50	C50	0.7897	-2.1039	-2.7621 C
51	H51	1.7042	-2.3935	-2.2555 H
52	C52	-3.2774	2.0008	0.6024 C
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54	C54	-3.9036	1.1255	3.1600 C
55	H55	-4.1115	0.7768	4.1657 H
56	C56	-4.7638	2.0434	2.5124 C
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58	C58	-3.7082	3.2801	-1.4980 C
59	C59	-3.3082	3.6422	-2.7576 C
60	C60	-2.0754	3.1637	-3.2491 C
61	H61	-1.7306	3.4182	-4.2454 H
62	C62	-1.2951	2.3584	-2.4418 C
63	C63	-2.8892	2.4424	-0.6997 C
64	B64	1.3683	-3.3994	1.6603 B
65	H65	0.4051	-3.9750	2.0585 H
66	B66	1.9732	-3.5509	0.0065 B
67	H67	1.4336	-4.3138	-0.7401 H
68	B68	1.4974	-1.6827	2.0938 B
69	H69	0.6748	-1.0958	2.7108 H
70	B70	3.2046	-1.2683	2.1184 B
71	H71	3.5714	-0.3627	2.7938 H
72	B72	3.7834	-1.3995	0.4282 B
73	H73	4.6002	-0.6107	0.0637 H
74	B74	2.6997	-2.8374	2.6776 B

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76 B76 2.9775 -4.0043 1.3559 B
77 H77 3.2976 -5.1400 1.5513 H
78 B78 3.7459 -3.1884 -0.0146 B
79 H79 4.5890 -3.7392 -0.6597 H
80 H80 3.3838 -2.1586 -0.6662 H
81 B81 4.1499 -2.6626 1.6294 B
82 H82 5.2441 -2.8334 2.0801 H
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87 C87 0.0290 1.8744 -2.9384 C
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Zn-1 S_0
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5 O5 -0.1668 0.0263 -0.0497 O
6 N6 1.9405 -0.2427 -2.5762 N
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8 C8 2.4340 -0.0371 -3.8438 C
9 C9 3.6656 -0.6182 -4.0440 C
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11 C11 5.0662 -2.0061 -2.3085 C
12 C12 4.9443 -2.4636 -0.9898 C
13 C13 3.8088 -2.1874 -0.2357 C
14 C14 2.8788 -0.9941 -1.9497 C
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16 N16 1.6642 2.6630 -1.0377 N
17 C17 0.2625 4.2642 1.7126 C
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27 C27 -1.9553 2.8709 -4.4772 C
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41	C41	1.7027	-0.6815	3.0872 C
42	N42	-2.0655	-2.4046	-1.1726 N
43	N43	0.0398	-3.3266	-0.4649 N
44	C44	-3.1236	-2.9369	-1.8726 C
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46	C46	-1.6785	-4.6169	-1.6507 C
47	C47	-0.8785	-5.7689	-1.6341 C
48	C48	0.3788	-5.6465	-1.0308 C
49	C49	0.7899	-4.4404	-0.4771 C
50	C50	-1.1736	-3.4170	-1.0445 C
51	N51	-1.8985	1.1444	2.5455 N
52	N52	-3.1726	-0.4973	1.3400 N
53	C53	-2.1067	1.7749	3.7502 C
54	C54	-3.2809	1.4032	4.3607 C
55	C55	-3.8780	0.4527	3.4879 C
56	C56	-5.0301	-0.3471	3.5028 C
57	C57	-5.1921	-1.2321	2.4292 C
58	C58	-4.2660	-1.2759	1.3941 C
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61	H61	4.2380	-0.6180	-4.9609 H
62	H62	5.7547	-3.0216	-0.5316 H
63	H63	3.7256	-2.5415	0.7893 H
64	H64	-0.4398	4.2677	2.5390 H
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68	H68	0.2287	2.6678	-4.2379 H
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70	H70	-6.1135	1.6454	-2.5724 H
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73	H73	2.9492	1.9457	5.5223 H
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78	H78	-4.3999	-1.9672	0.5656 H
79	H79	1.7750	-4.3604	-0.0246 H
80	H80	1.0403	-6.5045	-0.9682 H
81	H81	-3.9639	-2.3026	-2.1341 H
82	H82	-3.6249	-4.8901	-2.7491 H
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84	C84	6.2718	-2.3122	-3.1042 C
85	C85	6.8662	-3.5792	-3.0368 C
86	C86	6.8594	-1.3403	-3.9250 C
87	C87	8.0102	-3.8686	-3.7722 C
88	H88	6.4089	-4.3490	-2.4206 H
89	C89	8.0076	-1.6284	-4.6549 C
90	H90	6.4239	-0.3462	-3.9657 H
91	C91	8.5857	-2.8936	-4.5836 C
92	H92	8.4507	-4.8605	-3.7157 H
93	H93	8.4561	-0.8590	-5.2777 H
94	H94	9.4805	-3.1188	-5.1576 H
95	C95	-5.1734	3.1144	-4.6619 C
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7	N7	2.8378	-1.3814	-0.4558 N
8	C8	2.3280	-0.6746	-3.8007 C
9	C9	3.5748	-1.3853	-3.9066 C
10	C10	3.9961	-1.6609	-2.6135 C
11	C11	5.1209	-2.3786	-2.0270 C
12	C12	4.9899	-2.5507	-0.6042 C
13	C13	3.9419	-2.0524	0.1029 C
14	C14	2.9449	-1.1773	-1.7747 C
15	N15	0.2860	3.3128	0.3985 N
16	N16	1.5988	2.5779	-1.4683 N
17	C17	0.1196	4.5452	0.9877 C
18	C18	0.9016	5.5250	0.4209 C
19	C19	1.6316	4.8785	-0.6160 C
20	C20	2.5773	5.2584	-1.5811 C
21	C21	3.0095	4.2580	-2.4611 C
22	C22	2.5063	2.9647	-2.3775 C
23	C23	1.1903	3.5143	-0.5913 C
24	N24	-0.9667	1.0926	-3.0868 N
25	N25	-2.9341	0.4077	-1.8850 N
26	C26	-0.7938	1.7152	-4.3017 C
27	C27	-1.9771	1.9641	-4.9545 C
28	C28	-2.9967	1.4720	-4.0937 C
29	C29	-4.3990	1.4358	-4.1111 C
30	C30	-5.0243	0.9009	-2.9783 C
31	C31	-4.2764	0.4090	-1.9155 C
32	C32	-2.3078	0.9475	-2.9489 C
33	N33	1.4071	-1.1957	2.5655 N
34	N34	1.3346	1.1947	2.7464 N
35	C35	1.9025	-2.1762	3.3941 C
36	C36	2.5064	-1.6723	4.5226 C
37	C37	2.3983	-0.2569	4.4153 C
38	C38	2.7795	0.8519	5.1873 C
39	C39	2.4264	2.1115	4.6882 C
40	C40	1.7208	2.2381	3.4963 C
41	C41	1.6903	-0.0250	3.1908 C
42	N42	-1.9258	-2.6076	-0.7475 N
43	N43	0.2097	-3.2926	0.1195 N
44	C44	-2.9596	-3.3056	-1.3279 C
45	C45	-2.7329	-4.6605	-1.3760 C
46	C46	-1.4519	-4.8540	-0.7881 C
47	C47	-0.6088	-5.9498	-0.5485 C
48	C48	0.6425	-5.6628	0.0087 C
49	C49	1.0049	-4.3566	0.3155 C
50	C50	-0.9961	-3.5416	-0.4276 C
51	N51	-1.9720	1.5444	2.2930 N
52	N52	-3.1484	-0.3402	1.3786 N
53	C53	-2.2343	2.3675	3.3637 C
54	C54	-3.4058	2.0566	4.0120 C
55	C55	-3.9424	0.9407	3.3130 C
56	C56	-5.0605	0.1048	3.4515 C
57	C57	-5.1595	-0.9626	2.5500 C
58	C58	-4.2085	-1.1465	1.5538 C
59	C59	-3.0058	0.6690	2.2588 C
60	H60	1.7216	-0.2780	-4.6058 H
61	H61	4.0438	-1.6811	-4.8356 H
62	H62	5.7963	-3.0150	-0.0462 H
63	H63	3.9153	-2.1331	1.1864 H

64	H64	-0.5918	4.6573	1.7987 H
65	H65	0.9246	6.5709	0.6921 H
66	H66	3.7664	4.4797	-3.2066 H
67	H67	2.8504	2.1948	-3.0639 H
68	H68	0.2061	1.9727	-4.6339 H
69	H69	-2.0991	2.4618	-5.9059 H
70	H70	-6.1064	0.8325	-2.9337 H
71	H71	1.7745	-3.2186	3.1241 H
72	H72	2.9420	-2.2420	5.3312 H
73	H73	2.7252	3.0100	5.2186 H
74	H74	1.4602	3.2221	3.1135 H
75	H75	-1.5307	3.1510	3.6223 H
76	H76	-3.8081	2.5439	4.8887 H
77	H77	-6.0048	-1.6414	2.5990 H
78	H78	-4.2930	-1.9797	0.8603 H
79	H79	1.9871	-4.1518	0.7336 H
80	H80	1.3374	-6.4654	0.2332 H
81	H81	-3.8221	-2.7670	-1.7058 H
82	H82	-3.3812	-5.4101	-1.8069 H
83	H83	-4.7745	-0.0068	-1.0434 H
84	C84	6.2813	-2.8105	-2.7503 C
85	C85	7.1110	-3.8507	-2.2546 C
86	C86	6.6694	-2.2170	-3.9791 C
87	C87	8.2286	-4.2768	-2.9509 C
88	H88	6.8397	-4.3548	-1.3318 H
89	C89	7.7924	-2.6466	-4.6669 C
90	H90	6.1121	-1.3659	-4.3557 H
91	C91	8.5816	-3.6843	-4.1666 C
92	H92	8.8302	-5.0882	-2.5487 H
93	H93	8.0681	-2.1561	-5.5972 H
94	H94	9.4602	-4.0207	-4.7093 H
95	C95	-5.1953	1.9328	-5.2508 C
96	C96	-6.3696	2.6652	-5.0333 C
97	C97	-4.8069	1.6650	-6.5702 C
98	C98	-7.1308	3.1217	-6.1036 C
99	H99	-6.6703	2.8990	-4.0152 H
100	C100	-5.5733	2.1152	-7.6398 C
101	H101	-3.9116	1.0771	-6.7508 H
102	C102	-6.7361	2.8471	-7.4109 C
103	H103	-8.0326	3.6985	-5.9161 H
104	H104	-5.2634	1.8887	-8.6566 H
105	H105	-7.3317	3.2025	-8.2474 H
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108	C108	-2.2937	-7.7996	-0.5843 C
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110	H110	0.9268	-7.8840	-1.6538 H
111	C111	-2.6509	-9.1160	-0.8557 C
112	H112	-3.0120	-7.1233	-0.1303 H
113	C113	-1.7239	-9.9940	-1.4125 C
114	H114	0.2929	-10.2238	-2.1333 H
115	H115	-3.6562	-9.4589	-0.6260 H
116	H116	-2.0052	-11.0213	-1.6279 H
117	C117	-6.0889	0.3158	4.4897 C
118	C118	-6.6395	-0.7722	5.1795 C
119	C119	-6.5503	1.6038	4.7926 C
120	C120	-7.6189	-0.5785	6.1475 C
121	H121	-6.2742	-1.7746	4.9714 H
122	C122	-7.5350	1.7958	5.7557 C
123	H123	-6.1484	2.4532	4.2479 H

124 C124 -8.0711 0.7064 6.4384 C
125 H125 -8.0257 -1.4336 6.6807 H
126 H126 -7.8886 2.8009 5.9703 H
127 H127 -8.8372 0.8581 7.1940 H
128 C128 3.5234 0.7235 6.4563 C
129 C129 3.2024 1.5324 7.5544 C
130 C130 4.5765 -0.1919 6.5845 C
131 C131 3.9089 1.4256 8.7472 C
132 H132 2.3735 2.2309 7.4758 H
133 C133 5.2872 -0.2930 7.7756 C
134 H134 4.8522 -0.8068 5.7326 H
135 C135 4.9548 0.5129 8.8620 C
136 H136 3.6379 2.0534 9.5919 H
137 H137 6.1082 -1.0009 7.8536 H
138 H138 5.5080 0.4299 9.7936 H
139 C139 3.1118 6.6314 -1.6778 C
140 C140 3.3198 7.2292 -2.9277 C
141 C141 3.4425 7.3567 -0.5254 C
142 C142 3.8378 8.5161 -3.0233 C
143 H143 3.0468 6.6866 -3.8291 H
144 C144 3.9671 8.6409 -0.6222 C
145 H145 3.3105 6.8946 0.4485 H
146 C146 4.1643 9.2265 -1.8706 C
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4 Zn4 2.1106 0.3999 -0.1470 Zn
5 O5 0.1904 -0.0250 -0.0313 O
6 N6 -1.6751 1.0501 -2.5295 N
7 N7 -2.5516 1.8654 -0.4581 N
8 C8 -2.0828 1.1956 -3.8343 C
9 C9 -3.2487 1.9174 -3.9582 C
10 C10 -3.6275 2.2639 -2.6308 C
11 C11 -4.6799 2.9646 -2.0157 C
12 C12 -4.6309 3.0660 -0.6162 C
13 C13 -3.5747 2.5270 0.1064 C
14 C14 -2.6010 1.7129 -1.7942 C
15 N15 -0.6917 -3.2061 0.1273 N
16 N16 -1.7946 -2.1409 -1.7112 N
17 C17 -0.7293 -4.4899 0.6180 C
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20 C20 -3.1404 -4.6338 -2.0908 C
21 C21 -3.3978 -3.5033 -2.8812 C
22 C22 -2.7158 -2.3115 -2.6724 C
23 C23 -1.5639 -3.1978 -0.9111 C
24 N24 1.0754 -0.9705 -3.0625 N
25 N25 3.0284 -0.6629 -1.6964 N
26 C26 0.8992 -1.4931 -4.3216 C
27 C27 2.0739 -1.8976 -4.9095 C
28 C28 3.0910 -1.6202 -3.9562 C
29 C29 4.4829 -1.7941 -3.8804 C
30 C30 5.0977 -1.4064 -2.6801 C
31 C31 4.3554 -0.8655 -1.6410 C

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33	N33	-1.3471	1.2591	2.5823 N
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35	C35	-1.7652	2.2340	3.4571 C
36	C36	-2.5415	1.7415	4.4808 C
37	C37	-2.6376	0.3403	4.2490 C
38	C38	-3.2621	-0.7566	4.8684 C
39	C39	-3.0686	-2.0081	4.2650 C
40	C40	-2.2717	-2.1441	3.1354 C
41	C41	-1.8613	0.1003	3.0680 C
42	N42	2.3668	2.4038	-0.4134 N
43	N43	0.3008	3.3335	0.3850 N
44	C44	3.5302	2.9775	-0.8680 C
45	C45	3.5001	4.3516	-0.8396 C
46	C46	2.2126	4.6946	-0.3431 C
47	C47	1.5179	5.8837	-0.0655 C
48	C48	0.2149	5.7424	0.4348 C
49	C49	-0.3399	4.4871	0.6359 C
50	C50	1.5550	3.4411	-0.0951 C
51	N51	1.6136	-1.8958	2.3027 N
52	N52	3.1051	-0.1440	1.6191 N
53	C53	1.6728	-2.8184	3.3198 C
54	C54	2.8176	-2.7205	4.0750 C
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56	C56	4.7675	-0.9915	3.7829 C
57	C57	5.0882	0.1021	2.9639 C
58	C58	4.2516	0.4863	1.9259 C
59	C59	2.7561	-1.1759	2.4106 C
60	H60	-1.4828	0.7710	-4.6318 H
61	H61	-3.7433	2.1806	-4.8820 H
62	H62	-5.4383	3.5505	-0.0780 H
63	H63	-3.5473	2.6129	1.1902 H
64	H64	-0.0850	-4.7657	1.4456 H
65	H65	-1.7887	-6.3502	0.1264 H
66	H66	-4.1557	-3.5427	-3.6560 H
67	H67	-2.9246	-1.4435	-3.2932 H
68	H68	-0.0997	-1.5647	-4.7381 H
69	H69	2.1797	-2.3557	-5.8821 H
70	H70	6.1723	-1.4959	-2.5641 H
71	H71	-1.4558	3.2615	3.3006 H
72	H72	-2.9597	2.3107	5.2984 H
73	H73	-3.5629	-2.8868	4.6649 H
74	H74	-2.1314	-3.1202	2.6773 H
75	H75	0.8522	-3.5123	3.4643 H
76	H76	3.0721	-3.3232	4.9346 H
77	H77	6.0168	0.6420	3.1140 H
78	H78	4.5078	1.3406	1.3041 H
79	H79	-1.3632	4.4004	0.9918 H
80	H80	-0.3928	6.6193	0.6290 H
81	H81	4.3408	2.3439	-1.2118 H
82	H82	4.2987	5.0161	-1.1353 H
83	H83	4.8458	-0.5737	-0.7157 H
84	C84	-4.0799	-0.6566	6.0739 C
85	C85	-4.2701	-1.6234	7.0357 C
86	S86	-5.0117	0.7576	6.4594 S
87	C87	-5.1527	-1.2259	8.0711 C
88	H88	-3.7628	-2.5817	7.0088 H
89	C89	-5.6343	0.0410	7.8892 C
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91	H91	-6.3206	0.5935	8.5175 H

92 C92 5.6750 -1.3756 4.8602 C
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95 C95 7.3083 -1.2478 6.5271 C
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99 H99 7.4856 -3.3496 7.1787 H
100 C100 2.0705 7.2202 -0.2649 C
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102 S102 3.2315 7.5815 -1.5049 S
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106 H106 2.3331 10.5019 0.4119 H
107 H107 3.9186 9.9241 -1.6144 H
108 C108 5.2947 -2.3537 -4.9572 C
109 C109 6.4733 -3.0557 -4.8361 C
110 S110 4.8878 -2.1578 -6.6343 S
111 C111 7.0370 -3.4333 -6.0804 C
112 H112 6.9027 -3.3165 -3.8749 H
113 C113 6.2866 -3.0115 -7.1431 C
114 H114 7.9563 -3.9993 -6.1835 H
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116 C116 -3.8549 -5.8787 -2.3585 C
117 C117 -4.3586 -6.3101 -3.5654 C
118 S118 -4.2285 -7.0299 -1.1125 S
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7 N7 -2.8503 1.3406 -0.7029 N
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9 C9 -3.5975 0.4721 -4.0826 C
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11 C11 -5.1441 1.7242 -2.3623 C
12 C12 -5.0908 2.1553 -1.0269 C
13 C13 -3.9543 1.9593 -0.2538 C
14 C14 -2.8953 0.8745 -1.9642 C
15 N15 -0.2006 -3.1396 0.9401 N
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25 N25 3.0323 -0.5760 -1.6333 N
26 C26 0.9986 -2.3114 -3.8613 C
27 C27 2.2085 -2.6766 -4.4023 C
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29 C29 4.5952 -1.9863 -3.5654 C
30 C30 5.1693 -1.2351 -2.5283 C
31 C31 4.3755 -0.5689 -1.6066 C
32 C32 2.4538 -1.3066 -2.6062 C
33 N33 -1.5084 1.6377 2.3234 N
34 N34 -1.4354 -0.6992 2.8503 N
35 C35 -2.0548 2.7211 2.9703 C
36 C36 -2.7189 2.3796 4.1258 C
37 C37 -2.5971 0.9657 4.2343 C
38 C38 -3.0236 -0.0292 5.1312 C
39 C39 -2.6463 -1.3462 4.8288 C
40 C40 -1.8658 -1.6299 3.7159 C
41 C41 -1.8212 0.5668 3.0962 C

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46	C46	1.4147	4.7668	-1.5276 C
47	C47	0.5448	5.8695	-1.5073 C
48	C48	-0.7085	5.6646	-0.9113 C
49	C49	-1.0528	4.4298	-0.3814 C
50	C50	0.9699	3.5299	-0.9467 C
51	N51	1.9034	-1.0369	2.6121 N
52	N52	3.0967	0.6997	1.4615 N
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54	C54	3.2630	-1.2490	4.4498 C
55	C55	3.8181	-0.2461	3.6091 C
56	C56	4.9254	0.6172	3.6559 C
57	C57	5.0566	1.5246	2.5936 C
58	C58	4.1434	1.5375	1.5488 C
59	C59	2.9284	-0.1593	2.4846 C
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61	H61	-4.1399	0.4364	-5.0163 H
62	H62	-5.9550	2.6289	-0.5740 H
63	H63	-3.9243	2.2991	0.7789 H
64	H64	0.7184	-4.2331	2.5041 H
65	H65	-0.6370	-6.3638	1.5606 H
66	H66	-3.5598	-4.8531	-2.6103 H
67	H67	-2.8159	-2.5596	-2.6382 H
68	H68	0.0135	-2.6253	-4.1886 H
69	H69	2.3618	-3.3390	-5.2418 H
70	H70	6.2473	-1.1410	-2.4554 H
71	H71	-1.9164	3.7152	2.5597 H
72	H72	-3.2029	3.0601	4.8115 H
73	H73	-2.9835	-2.1656	5.4541 H
74	H74	-1.5801	-2.6554	3.4947 H
75	H75	1.4195	-2.4227	4.1580 H
76	H76	3.6269	-1.5916	5.4075 H
77	H77	5.8976	2.2087	2.5614 H
78	H78	4.2520	2.2520	0.7365 H
79	H79	-2.0425	4.2820	0.0428 H
80	H80	-1.4440	6.4614	-0.9003 H
81	H81	3.8742	2.6216	-1.9235 H
82	H82	3.4074	5.1919	-2.4923 H
83	H83	4.8352	0.0045	-0.8056 H
84	C84	-3.8188	0.2360	6.3266 C
85	C85	-3.8311	-0.4877	7.4981 C
86	S86	-4.9549	1.5462	6.4243 S
87	C87	-4.7420	0.0119	8.4621 C
88	H88	-3.1790	-1.3378	7.6666 H
89	C89	-5.4229	1.1111	8.0169 C
90	H90	-4.8823	-0.4213	9.4463 H
91	H91	-6.1741	1.6903	8.5379 H
92	C92	5.9086	0.6237	4.7352 C
93	C93	6.6525	1.6934	5.1811 C
94	S94	6.3325	-0.8080	5.6224 S
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96	H96	6.5320	2.6956	4.7844 H
97	C97	7.4866	0.0388	6.5688 C
98	H98	8.2076	2.0745	6.7112 H
99	H99	8.0552	-0.4852	7.3260 H
100	C100	0.8726	7.1800	-2.0611 C
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Zn-3 S_0
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4 Zn4 -2.2059 0.1902 -0.3390 Zn
5 O5 -0.2670 -0.0440 -0.0588 O
6 N6 1.2416 2.4421 1.4925 N
7 N7 2.3101 2.0485 -0.6144 N
8 C8 1.4749 3.3515 2.4979 C
9 C9 2.5664 4.1546 2.2558 C
10 C10 3.0814 3.7314 0.9979 C
11 C11 4.1435 4.0986 0.1561 C
12 C12 4.2520 3.4015 -1.0548 C
13 C13 3.3398 2.4090 -1.3963 C
14 C14 2.2042 2.6816 0.5687 C
15 N15 0.7433 -2.6459 1.7172 N
16 N16 1.5863 -0.6206 2.6812 N
17 C17 0.8827 -3.9694 2.0662 C
18 C18 1.7089 -4.1569 3.1507 C
19 C19 2.1381 -2.8549 3.5340 C
20 C20 2.9599 -2.3074 4.5322 C
21 C21 3.0674 -0.9111 4.5571 C
22 C22 2.3821 -0.1220 3.6393 C
23 C23 1.4891 -1.9615 2.6199 C
24 N24 -1.4511 0.8068 2.9034 N
25 N25 -3.2549 0.1191 1.4700 N
26 C26 -1.3940 1.0883 4.2486 C
27 C27 -2.6117 0.9783 4.8765 C
28 C28 -3.5288 0.5896 3.8619 C
29 C29 -4.8942 0.2715 3.8039 C
30 C30 -5.3866 -0.1461 2.5607 C
31 C31 -4.5579 -0.2048 1.4478 C
32 C32 -2.7472 0.4939 2.6605 C
33 N33 1.5408 -0.3415 -2.8026 N
34 N34 1.8994 -2.2273 -1.3639 N
35 C35 2.0437 -0.0073 -4.0392 C
36 C36 2.9600 -0.9181 -4.5116 C
37 C37 3.0613 -1.9180 -3.5033 C
38 C38 3.7809 -3.1107 -3.3242 C
39 C39 3.5288 -3.8205 -2.1440 C
40 C40 2.6051 -3.3579 -1.2125 C
41 C41 2.1436 -1.5148 -2.4793 C
42 N42 -2.5632 1.9528 -1.2917 N
43 N43 -0.4661 2.4277 -2.3681 N
44 C44 -3.7874 2.5796 -1.3245 C
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50	C50	-1.7638	2.6819	-2.1078 C
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54	C54	-2.3223	-4.8342	-2.0217 C
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57	C57	-4.8249	-2.1255	-2.8754 C
58	C58	-4.1220	-1.1362	-2.1985 C
59	C59	-2.5072	-2.6206	-1.5458 C
60	H60	0.8097	3.3815	3.3540 H
61	H61	2.9281	4.9582	2.8814 H
62	H62	5.0732	3.6121	-1.7323 H
63	H63	3.4381	1.8668	-2.3341 H
64	H64	0.3465	-4.7284	1.5070 H
65	H65	1.9472	-5.0978	3.6262 H
66	H66	3.7143	-0.4275	5.2821 H
67	H67	2.4794	0.9609	3.6617 H
68	H68	-0.4428	1.3455	4.7016 H
69	H69	-2.8117	1.1239	5.9283 H
70	H70	-6.4360	-0.3968	2.4442 H
71	H71	1.6879	0.8884	-4.5363 H
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74	H74	2.4272	-3.9106	-0.2930 H
75	H75	-0.3886	-4.9381	-0.9648 H
76	H76	-2.4611	-5.8372	-2.3992 H
77	H77	-5.7532	-1.8602	-3.3710 H
78	H78	-4.4809	-0.1098	-2.2002 H
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82	H82	-4.6500	4.3250	-2.3454 H
83	H83	-4.9538	-0.5284	0.4885 H
84	C84	-5.7875	0.3607	4.9749 C
85	C85	-6.7880	-0.6278	5.1849 C
86	C86	-5.6928	1.4095	5.8692 C
87	C87	-7.6430	-0.5524	6.2535 C
88	H88	-6.8501	-1.4681	4.4988 H
89	C89	-6.5658	1.5191	6.9771 C
90	H90	-4.9517	2.1882	5.7083 H
91	C91	-7.5630	0.5183	7.1786 C
92	H92	-8.3938	-1.3240	6.4079 H
93	C93	-6.4829	2.5973	7.8946 C
94	C94	-8.4333	0.6285	8.2902 C
95	C95	-7.3419	2.6778	8.9632 C
96	H96	-5.7245	3.3608	7.7374 H
97	C97	-8.3264	1.6836	9.1637 C
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103	C103	-5.2894	-5.7620	-3.0040 C
104	C104	-6.5140	-5.2048	-5.4508 C
105	H105	-5.6491	-3.2640	-5.2686 H

106	C106	-6.0491	-6.7744	-3.6356 C
107	H107	-4.8337	-5.9746	-2.0403 H
108	C108	-6.6747	-6.4955	-4.8877 C
109	H109	-6.9803	-4.9891	-6.4095 H
110	C110	-6.2105	-8.0607	-3.0608 C
111	C111	-7.4299	-7.5128	-5.5205 C
112	C112	-6.9501	-9.0267	-3.6976 C
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119	C119	-2.2146	6.1484	-5.5303 C
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121	C121	-2.7937	7.2447	-6.1151 C
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138	C138	6.5112	7.0171	-0.1854 C
139	H139	5.1884	5.9752	-1.4942 H
140	C140	6.5678	6.2493	2.1347 C
141	H141	5.2797	4.5698	2.5613 H
142	C142	7.0300	7.1482	1.1270 C
143	H143	6.8520	7.7060	-0.9551 H
144	C144	7.0879	6.3678	3.4486 C
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147	H147	6.7375	5.6790	4.2138 H
148	C148	8.4691	8.2262	2.7542 C
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154	C154	4.3222	-4.3055	5.1205 C
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157	C157	5.0626	-5.0872	6.0383 C
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Zn-3 S_1
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4	Zn4	-2.1161	0.4525	-0.4076 Zn
5	O5	-0.2253	-0.0077	-0.0890 O
6	N6	1.4900	2.2049	1.6485 N
7	N7	2.5848	1.8157	-0.4452 N
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9	C9	2.9696	3.7084	2.5557 C
10	C10	3.4796	3.3039	1.2898 C
11	C11	4.6056	3.5959	0.5039 C
12	C12	4.6803	2.9615	-0.7438 C
13	C13	3.6765	2.1005	-1.1727 C
14	C14	2.5064	2.3872	0.7710 C
15	N15	0.4279	-2.8193	1.5472 N
16	N16	1.4417	-0.9495	2.6449 N
17	C17	0.2845	-4.1110	1.8664 C
18	C18	0.9921	-4.4234	3.0725 C
19	C19	1.6283	-3.2589	3.4809 C
20	C20	2.4418	-2.8803	4.6296 C
21	C21	2.6761	-1.4592	4.6988 C
22	C22	2.2297	-0.5965	3.7503 C
23	C23	1.2111	-2.2624	2.5432 C
24	N24	-1.4177	0.8077	2.8743 N
25	N25	-3.2342	0.3931	1.3554 N
26	C26	-1.3771	1.0100	4.2346 C
27	C27	-2.6202	0.9980	4.8212 C
28	C28	-3.5381	0.7634	3.7612 C
29	C29	-4.9259	0.5934	3.6473 C
30	C30	-5.4174	0.2969	2.3693 C
31	C31	-4.5626	0.2107	1.2781 C
32	C32	-2.7301	0.6487	2.5787 C
33	N33	1.6247	-0.3454	-2.7908 N
34	N34	1.7197	-2.3573	-1.4871 N
35	C35	2.1909	0.0090	-3.9942 C
36	C36	3.0015	-0.9713	-4.5174 C
37	C37	2.9598	-2.0428	-3.5812 C
38	C38	3.5250	-3.3241	-3.4795 C
39	C39	3.1602	-4.0802	-2.3584 C
40	C40	2.2774	-3.5750	-1.4107 C
41	C41	2.0748	-1.6019	-2.5436 C
42	N42	-2.2538	2.2864	-1.2783 N
43	N43	-0.0728	2.6072	-2.2398 N
44	C44	-3.4038	3.0409	-1.3114 C
45	C45	-3.2695	4.1934	-2.0480 C
46	C46	-1.9266	4.1923	-2.5165 C
47	C47	-1.1349	5.0389	-3.3070 C
48	C48	0.1775	4.6160	-3.5515 C
49	C49	0.6592	3.4335	-3.0046 C
50	C50	-1.3474	2.9801	-2.0092 C
51	N51	-1.5978	-2.8228	-1.1937 N
52	N52	-3.0083	-0.9450	-1.6990 N
53	C53	-1.6480	-4.1455	-1.5688 C
54	C54	-2.7308	-4.4429	-2.3615 C
55	C55	-3.4330	-3.2166	-2.5212 C
56	C56	-4.5682	-2.7870	-3.2258 C
57	C57	-4.8601	-1.4182	-3.1655 C
58	C58	-4.0782	-0.5532	-2.4099 C
59	C59	-2.6794	-2.2486	-1.7757 C
60	H60	1.1002	3.0755	3.5522 H
61	H61	3.3965	4.4265	3.2414 H

62	H62	5.5444	3.1166	-1.3819 H
63	H63	3.7478	1.6047	-2.1381 H
64	H64	-0.3101	-4.7814	1.2578 H
65	H65	0.9680	-5.3796	3.5777 H
66	H66	3.3104	-1.0573	5.4814 H
67	H67	2.4924	0.4570	3.7953 H
68	H68	-0.4197	1.1372	4.7282 H
69	H69	-2.8394	1.1090	5.8734 H
70	H70	-6.4828	0.1645	2.2103 H
71	H71	1.9559	0.9732	-4.4314 H
72	H72	3.5285	-0.9389	-5.4604 H
73	H73	3.5878	-5.0654	-2.2023 H
74	H74	2.0078	-4.1685	-0.5403 H
75	H75	-0.8634	-4.8234	-1.2506 H
76	H76	-2.9691	-5.4024	-2.7976 H
77	H77	-5.7269	-1.0210	-3.6837 H
78	H78	-4.3138	0.5076	-2.3715 H
79	H79	1.6947	3.1459	-3.1664 H
80	H80	0.8527	5.2366	-4.1317 H
81	H81	-4.2822	2.7004	-0.7736 H
82	H82	-4.0341	4.9337	-2.2345 H
83	H83	-4.9574	-0.0171	0.2912 H
84	C84	-5.8432	0.7105	4.7971 C
85	C85	-6.9373	-0.1883	4.9286 C
86	C86	-5.6788	1.7003	5.7468 C
87	C87	-7.8138	-0.0858	5.9773 C
88	H88	-7.0560	-0.9836	4.1978 H
89	C89	-6.5727	1.8380	6.8349 C
90	H90	-4.8621	2.4108	5.6469 H
91	C91	-7.6637	0.9262	6.9581 C
92	H92	-8.6374	-0.7898	6.0720 H
93	C93	-6.4201	2.8584	7.8078 C
94	C94	-8.5545	1.0632	8.0503 C
95	C95	-7.3016	2.9674	8.8553 C
96	H96	-5.5900	3.5542	7.7102 H
97	C97	-8.3787	2.0606	8.9787 C
98	H98	-9.3829	0.3644	8.1416 H
99	H99	-7.1734	3.7529	9.5951 H
100	H100	-9.0690	2.1568	9.8124 H
101	C101	-5.4236	-3.7039	-4.0034 C
102	C102	-5.9522	-3.2916	-5.2575 C
103	C103	-5.7508	-4.9576	-3.5240 C
104	C104	-6.7679	-4.1176	-5.9861 C
105	H105	-5.6767	-2.3166	-5.6501 H
106	C106	-6.5987	-5.8288	-4.2479 C
107	H107	-5.3755	-5.2777	-2.5553 H
108	C108	-7.1192	-5.4044	-5.5074 C
109	H109	-7.1532	-3.7938	-6.9503 H
110	C110	-6.9522	-7.1118	-3.7583 C
111	C111	-7.9649	-6.2791	-6.2320 C
112	C112	-7.7764	-7.9374	-4.4831 C
113	H113	-6.5575	-7.4314	-2.7965 H
114	C114	-8.2872	-7.5176	-5.7324 C
115	H115	-8.3571	-5.9522	-7.1924 H
116	H116	-8.0395	-8.9187	-4.0977 H
117	H117	-8.9382	-8.1801	-6.2964 H
118	C118	-1.6271	6.3197	-3.8496 C
119	C119	-1.2704	6.7223	-5.1658 C
120	C120	-2.4112	7.1629	-3.0863 C
121	C121	-1.6981	7.9196	-5.6784 C

122	H122	-0.6722	6.0520	-5.7773 H
123	C123	-2.8602	8.4086	-3.5839 C
124	H124	-2.6676	6.8836	-2.0675 H
125	C125	-2.5003	8.7988	-4.9087 C
126	H126	-1.4286	8.2077	-6.6919 H
127	C127	-3.6553	9.2855	-2.8032 C
128	C128	-2.9543	10.0449	-5.4053 C
129	C129	-4.0793	10.4887	-3.3116 C
130	H130	-3.9240	8.9875	-1.7924 H
131	C131	-3.7263	10.8718	-4.6256 C
132	H132	-2.6798	10.3375	-6.4162 H
133	H133	-4.6889	11.1521	-2.7042 H
134	H134	-4.0679	11.8263	-5.0167 H
135	C135	5.6778	4.5075	0.9473 C
136	C136	6.2781	5.4051	0.0221 C
137	C137	6.1386	4.4900	2.2495 C
138	C138	7.2901	6.2453	0.4075 C
139	H139	5.9030	5.4380	-0.9972 H
140	C140	7.1888	5.3372	2.6750 C
141	H141	5.7093	3.7904	2.9622 H
142	C142	7.7785	6.2378	1.7380 C
143	H143	7.7294	6.9365	-0.3082 H
144	C144	7.6780	5.3162	4.0058 C
145	C145	8.8267	7.0877	2.1675 C
146	C146	8.6976	6.1510	4.3924 C
147	H147	7.2300	4.6258	4.7167 H
148	C148	9.2770	7.0463	3.4648 C
149	H149	9.2715	7.7743	1.4507 H
150	H150	9.0635	6.1262	5.4153 H
151	H151	10.0829	7.7021	3.7828 H
152	C152	3.0226	-3.7986	5.5485 C
153	C153	3.4557	-3.3623	6.8491 C
154	C154	3.2160	-5.1617	5.2420 C
155	C155	3.9905	-4.2263	7.7562 C
156	H156	3.3018	-2.3268	7.1362 H
157	C157	3.7782	-6.0698	6.1602 C
158	H158	2.9948	-5.5209	4.2421 H
159	C159	4.1736	-5.6093	7.4545 C
160	H160	4.2799	-3.8677	8.7418 H
161	C161	3.9803	-7.4383	5.8399 C
162	C162	4.7306	-6.5190	8.3714 C
163	C163	4.5313	-8.3054	6.7560 C
164	H164	3.6889	-7.7928	4.8536 H
165	C165	4.9079	-7.8474	8.0343 C
166	H166	5.0257	-6.1585	9.3545 H
167	H167	4.6774	-9.3500	6.4940 H
168	H168	5.3406	-8.5394	8.7514 H
169	C169	4.4669	-3.8651	-4.4782 C
170	C170	4.3890	-5.2306	-4.8672 C
171	C171	5.4552	-3.0728	-5.0295 C
172	C172	5.2698	-5.7576	-5.7757 C
173	H173	3.5984	-5.8508	-4.4537 H
174	C174	6.3852	-3.5902	-5.9615 C
175	H175	5.5459	-2.0342	-4.7219 H
176	C176	6.2931	-4.9611	-6.3477 C
177	H177	5.1887	-6.8004	-6.0741 H
178	C178	7.4116	-2.7882	-6.5217 C
179	C179	7.2234	-5.4757	-7.2833 C
180	C180	8.3009	-3.3161	-7.4253 C
181	H181	7.4824	-1.7451	-6.2221 H

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185 H185 8.9149 -5.0786 -8.5267 H
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