

Steric hindrance of phenanthroline diamides permits to reach a hundredfold increase of Am(III) extraction efficiency

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Supplementary Materials

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1. Materials and Methods

1.1. Materials

Chemical reagents such as $\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$, $\text{Nd}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$, $\text{Eu}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$, $\text{Lu}(\text{NO}_3)_3 \cdot x\text{H}_2\text{O}$ and other inorganic/organic reagents and solvents were of analytical grade. Water content x in lutetium nitrate was determined as $x = 5$. Deuterated solvents CD_3CN , C_6D_6 and CDCl_3 for NMR spectra registration were purchased from commercial sources and used without further purification. All syntheses were performed in an argon inert atmosphere. Dichloromethane were purified by distillation over calcium hydride prior to use. Triethylamine was purified by simple distillation, previously held for 12 hours over sodium hydroxide. Acetonitrile and diethyl ether for the synthesis of complexes were purified according to known procedures. 1,10-phenanthroline-2,9-dicarbonyl dichloride for synthesis of ligands may be prepared according to knowning procedures [1].

Methods

NMR spectra were recorded using standard 5 mm sample tubes on Agilent 400-MR spectrometer with operating frequencies of 400.1 MHz (^1H) and 100.6 MHz (^{13}C) and on Bruker AV-600 spectrometer with operating frequencies of 600.2 MHz (^1H) and 150.9 MHz (^{13}C). The ROESY spectrum was recorded on an Agilent 400-MR spectrometer using a standard ROESYAD pulse sequence with a mixing time of 200 ms and an acquisition time of 150 ms.

IR spectra in the solid state were recorded on a Nicolet iS5 FTIR spectrometer (Thermo Scientific) using an internal reflectance attachment with diamond optical element–attenuated total reflection (ATR) with a 45° angle of incidence. The resolution is 4 cm^{-1} ; the number of scans is 32.

HRMS ESI mass spectra were recorded on a LCMS-IT-TOF (Shimadzu, Japan) in the positive ion mode. Resolution of the instrument is $>10,000$ according to the manufacturer. LabSolution software (version 3.80.410, Shimadzu, Kyoto, Japan) was used to acquire and process MS data.

Quantum chemical calculations were performed by the PRIODA-19 developed by Laikov [2]. Full electron relativistic L1 basis set [3] of TZ quality including one polarization function was used for all the atoms to provide the most reliable result. The CREST 3.0 program was used to find the most stable conformations of the ligand [4]. Additional calculations were also carried out using the Gaussian-16 [5] software at the B3LYP/6-31G(d,p) theoretical level, employing the PCM solvent model.

Single crystals of **L1** were obtained upon slow isothermal (25°C) recrystallization of corresponding substances from C_6H_6 . Single crystals of **L2** were obtained upon slow isothermal (25°C) recrystallization of corresponding substances from the mixture $\text{CH}_3\text{CN}/\text{CHCl}_3$.

General procedure for obtaining of crystals of complexes Nd(III) with **L1** and Eu(III) with **L1-L3**: The solvent evaporation method was used to prepare the single crystal of complexes formed by $\text{Ln}(\text{NO}_3)_3$ and **L1**, **L2** or **L3**. Ligand (0.01 mmol) was dissolved in 0.5 mL of chloroform, and to this mixture was added a solution of $\text{Ln}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ (0.01 mmol) in 0.5 mL acetonitrile. After stirring for 15 minutes,

the solution was left to evaporate slowly in air. Single crystals were obtained by recrystallization of complexes from CH₃CN:CHCl₃:C₆H₅CH₃ (1:1:1) mixture.

X-ray diffraction data for **L1** were collected at 295 K with a STOE STADI VARI diffractometer equipped with a Pilatus 100K detector using the Cu-K α radiation ($\lambda = 1.54186$ Å) monochromated by focusing mirrors.

X-ray diffraction data for **L2** were collected at 120 K with a Bruker APEXII CCD diffractometer, using graphite monochromated Mo-K α radiation ($\lambda = 0.71073$ Å). Using Olex2 [6], the structure was solved with the ShelXT [7] structure solution program using Intrinsic Phasing and refined with the XL [8] refinement package using Least Squares minimization against F^2_{hkl} in anisotropic approximation for non-hydrogen atoms. The positions of hydrogen atoms were calculated, and they were refined in the isotropic approximation in the riding model. Crystal data and structure refinement parameters are given in Table S1. CCDC 2393474 contains the supplementary crystallographic data for **L2**.

The crystals of the complexes **L1•Nd(NO₃)₃**, **L1•Eu(NO₃)₃**, **L2•Nd(NO₃)₃**, **L2•Eu(NO₃)₃** and **L3•Eu(NO₃)₃** were analyzed on a Bruker SMART Photon II diffractometer at 150 K using graphite monochromatized MoK α radiation ($\lambda = 0.71073$ Å) in ω -scan mode. Cell refinement and data reduction for the structures were conducted using SAINT (V8.38A, Bruker). Absorption correction based on measurements of equivalent reflections (multi-scan) was applied (SADABS-2016/2, Bruker 2016/2). The structures were solved by direct methods (SHELXT 2018/2) [7] and refined by full matrix least-squares on F^2 (SHELXL 2018/3) [9] with anisotropic displacement parameters for all non-hydrogen atoms. Hydrogen atoms were placed in calculated positions and refined using the riding model. CCDC: 2394080 – 2394084.

Solvent extraction

For the extraction experiments, 0.5 ml of the organic solution (ligand L1-L3 in F-3) and 0.5 ml of the aqueous phase (HNO₃ with radionuclides or lanthanides) were treated on a vortex shaker for 30 min in a 1.5 ml polypropylene tube at 25 $\pm$ 1 °C. The samples were then centrifuged (5 min, 6000 rpm) and an aliquot of each phase was taken to determine the concentration of the radionuclide or lanthanide. The content of ²⁴¹Am and ¹⁵²Eu radionuclides in the initial aqueous phase was 1.5-2.5 kBq/ml. The total concentration of lanthanides in the initial aqueous phase was 10⁻³ mol/l. The content of ²⁴¹Am ($E_\gamma = 59.5$ keV) and ¹⁵²Eu ($E_\gamma = 121.8$ keV) was determined by γ -spectrometry (ORTEC DSPec50 radiometric complex with a coaxial gamma detector; Amptek, USA). The distribution ratios were calculated as the ratio of the count rates for the corresponding organic and aqueous phases. The separation coefficients of two elements were calculated as the ratio of the distribution ratios for these elements. The content of lanthanides was determined by ICP-MS (AnalytikJena PlasmaQuant MS Elite) in aqueous phases (initial and equilibrium after extraction). The concentration of lanthanides in

the organic phase was determined as the difference between the initial and equilibrium concentrations in the aqueous phases. Errors for $0.01 < D < 100$ are within 10%.

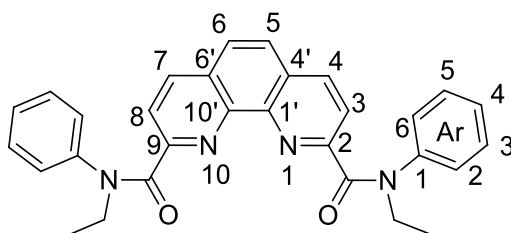
UV-vis titration

To determine the stability constants of the complexes with Eu(III) and the protonation constants of ligands **L1-L3**, UV-vis absorption spectra of ligand solutions were collected at the temperature 25.0 ± 0.1 °C on a Shimadzu UV 1800 spectrophotometer controlled by LabSolutions UV-Vis software with thermostatic attachment (Shimadzu TCC-100). Quartz cell cuvettes with a 10 mm optical path were used. For a typical titration, 2.0 mL of 10^{-5} mol/L ligand solution was put in the sample cuvette, into which 2-4 μ L aliquots of a titrant solution were added manually; after each addition, the solution was mixed, and auto zero calibration was performed before a spectrum was recorded. The titration continued until no noticeable change was observed in the spectra. The stability constants were calculated by the HypSpec2014 program [10]. First, the number of complex species formed was determined by factor analysis, and then models with different compositions of complexes were applied to fit the data. For the calculation of protonation constants, the pK_a of CF₃SO₃H was set to 0.7.

A ligand solution for titration was prepared by dissolving the respective ligand (5 μ mol) in CH₃CN (50 mL) and then diluting it 10 times to obtain the desired concentration of 10^{-5} mol/L. Eu(III) was chosen as a representative lanthanide to study the complexation behaviour of the ligands with lanthanides(III). A Eu(NO₃)₃ titrant solution (10^{-3} mol/L) was prepared by dissolving europium(III) nitrate hydrate Eu(NO₃)₃·6H₂O in CH₃CN. To study the protonation behaviour of the ligands, absolute CF₃SO₃H was dissolved in CH₃CN and used as a titrant. Acetonitrile (CH₃CN; 99.95%, HPLC grade, Panreac AppliChem) was dried over molecular sieves (zeolite KA, 3 Å, balls, diameter 1.6–2.5 mm, production HKC Corp., Hong Kong) prior to use.

1.2. Synthesis and Analytical Data

The diamides **L1-L3** were synthesized referring to the earlier described procedure [11].



N²,N⁹-bis(2,6-dimethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide (L1).

White powder. Yield 3.9g (74%). m.p. 238-241 °C; ¹H NMR (400 MHz, C₆D₆) δ 7.91 (d, J = 8.2 Hz, Phen-H^{3,8}, Form III), 7.75 (d, J = 8.2 Hz, Phen-H^{3,8}, Form II), 7.55 (d, J = 8.3 Hz, Phen-H^{4,7}, Form III), 7.49 (d, J = 8.2 Hz, Phen-H^{3,8}, Form II), 7.42 (d, J = 8.2 Hz, 2H, Phen-H^{3,8}, Form I), 7.40 (d, J = 8.2 Hz, Phen-H^{4,7}, Form II), 7.26 (d, J = 8.3 Hz, Phen-H^{4,7}, Form II), 7.15 (s, Phen-H^{5,6}, Form III), 7.10 – 7.08 (m, 2H, Phen-H^{4,7}, Form I), 7.08 – 7.06 (m, Ar-H⁴, Form II, Ar-H^{3,5}, Form III),

6.95 – 6.87 (m, Phen-H^{5,6}, Form II), 6.72 – 6.68 (m, 4H, Ar- H^{3,5}, Form I), 6.66 (s, 2H, Phen-H^{5,6}, Form I), 6.64 – 6.58 (m, Ar- H^{3,5}, Form II), 6.55 – 6.49 (m, 2H, Ar-H⁴, Form I), 6.49 – 6.45 (m, Ar-H⁴, Form II), 3.87 (q, $J = 7.2$ Hz, 4H, N-CH₂, Form I), 3.85 – 3.79 (m, N-CH₂, Form II), 3.72 (q, $J = 7.1$ Hz, N-CH₂, Form III), 3.54 (q, $J = 7.1$ Hz, N-CH₂, Form II), 2.51 (s, Ar-CH₃, Form II), 2.47 (s, 12H, Ar-CH₃, Form I), 2.43 (s, Ar-CH₃, Form II), 2.39 (s, Ar-CH₃, Form III), 1.27 (t, $J = 7.2$ Hz, 6H, N-CH₂-CH₃, Form I), 1.25 – 1.20 (m, N-CH₂-CH₃, Forms II, III); ¹³C NMR (101 MHz, C₆D₆) δ 168.9 (C=O, Form II), 168.8 (C=O, Form I), 167.7 (C=O, Form II), 167.6 (C=O, Form III), 155.7 (Phen-C^{2,9}, Form II), 155.2 (Phen-C^{2,9}, Form III), 155.1 (Phen-C^{2,9}, Form I), 154.9 (Phen-C^{2,9}, Form II), 144.8 (Phen-C^{1',10'}, Form II), 144.8 (Phen-C^{1',10'}, Form II), 144.7 (Phen-C^{1',10'}, Form I), 140.5 (Ar-C¹, Form I), 140.3 (Ar-C¹, Form II), 140.1 (Ar-C¹, Form III), 140.1 (Ar-C¹, Form II), 137.1 (Ar-C^{2,6}, Form II), 136.8 (Ar-C^{2,6}, Form I), 136.5 (Phen-C^{4,7}, Form III), 136.2 (Ar-C^{2,6}, Form II), 136.2 (Ar-C^{2,6}, Form III), 136.1 (Phen-C^{4,7}, Form II), 135.4 (Phen-C^{4,7}, Form II), 135.0 (Phen-C^{4,7}, Form I), 128.6 (Ar-C^{3,5}, Form II), 128.6 (Ar-C^{3,5}, Form III), 128.4 (Ar-C^{3,5}, Form I), 128.3 (Ar-C^{3,5}, Form II), Ar-C⁴, Phen-C^{4',6'}-under solvent, 126.7 (Phen-C^{5,6}, Form III), 126.5 (Phen-C^{5,6}, Form II), 126.2 (Phen-C^{5,6}, Form II), 126.0 (Phen-C^{5,6}, Form I), 123.1 (Phen-C^{3,8}, Form III), 122.4 (Phen-C^{3,8}, Form II), 120.2 (Phen-C^{3,8}, Form I), 46.6 (N-CH₂, Form II), 46.6 (N-CH₂, Form III), 44.1 (N-CH₂, Form I), 44.0 (N-CH₂, Form II), 19.2 (Ar-CH₃, Form II), 19.1 (Ar-CH₃, Form I), 18.4 (Ar-CH₃, Form II), 18.3 (Ar-CH₃, Form III), 14.5 (N-CH₂-CH₃, Form III), 14.1 (N-CH₂-CH₃, Form II), 13.0 (N-CH₂-CH₃, Form I), 12.9 (N-CH₂-CH₃, Form II); IR (ν , cm⁻¹) 2984, 2970, 2933, 2873 (C-H stretching vibrations), 1647, 1635 (C=O), 1590, 1546, 1497, 1470 (C=C, C=N); HRMS (ESI-TOF) (m/z) [M+H]⁺ calcd for [C₃₄H₃₅N₄O₂]⁺ 531.2755 found 531.2753.

N²,N⁹-bis(2,6-diethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide (L2).

White powder. Yield 4.1 g (70%), m.p. 208-212°C (with decomp.); ¹H NMR (400 MHz, C₆D₆) δ 8.02 (d, $J = 8.3$ Hz, Phen-H^{3,8}), 7.94 (d, $J = 8.2$ Hz, Phen-H^{3,8}), 7.57 (d, $J = 8.3$ Hz, Phen-H^{4,7}), 7.43 (d, $J = 8.3$ Hz, Phen-H^{4,7}), 7.40 (d, $J = 8.2$ Hz, 2H, Phen-H^{3,8}, Form I), 7.24 – 7.14 (m, 5H, Phen-H^{5,6}, Ar-H⁴), 7.09 (d, $J = 8.3$ Hz, 2H, Phen-H^{4,7}, Form I), 6.97 – 6.87 (m, 1H, Phen-H^{5,6}, Form II), 6.75 (d, $J = 7.6$ Hz, 4H, Ar-H^{3,5}, Form I), 6.69 – 6.67 (m, 1H, Ar-H^{3,5}), 6.65 – 6.58 (m, 4H, Ar-H⁴, Phen-H^{5,6}), 3.90 (q, $J = 7.2$ Hz, 4H, N-CH₂, Form I), 3.87 – 3.81 (m, N-CH₂, Form II), 3.81 – 3.74 (m, N-CH₂, Form III), 3.26 – 3.14 (m, 4H, Ar-CH₂, Form I), 3.06 – 2.94 (m, 2H, Ar-CH₂), 2.93 – 2.81 (m, 4H, Ar-CH₂, Form I), 2.81 – 2.73 (m, Ar-CH₂), 2.73 – 2.61 (m, Ar-CH₂), 1.60 (t, $J = 7.0$ Hz, N-CH₂-CH₃), 1.38 – 1.32 (m, 8H, N-CH₂-CH₃), 1.35 – 1.30 (m, 10H, N-CH₂-CH₃), 1.28 (d, $J = 7.5$ Hz, 6H, N-CH₂-CH₃), 1.23 (t, $J = 7.5$ Hz, 12H, Ar-CH₂-CH₃, Form I), 1.09 (t, $J = 7.6$ Hz, 1H, Ar-CH₃); ¹³C NMR (101 MHz, C₆D₆) δ 169.2 (C=O, Form I), 168.7 (C=O, Form II), 168.4 (C=O, Form III), 167.8 (C=O, Form II), 155.6 (Phen-C^{2,9}, Form II), 155.2 (Phen-C^{2,9}, Form III), 155.2 (Phen-C^{2,9}, Form I), 154.3 (Phen-C^{2,9}, Form II), 145.4 (Phen-C^{1',10'}, Form II), 144.6 (Phen-C^{1',10'}, Form III), 144.5 (Phen-C^{1',10'}, Form II), 144.5 (Phen-C^{1',10'}, Form I), 142.2 (Ar-C^{2,6}, Form II), 142.1 (Ar-C^{2,6}, Form I), 141.8 (Ar-C^{2,6}, Form

III), 141.7 (Ar-C^{2,6}, Form II), 139.6 (Ar-C¹, Form II), 139.1 (Ar-C¹, Form II), 139.0 (Ar-C¹, Form I), 139.0 (Ar-C¹, Form III), 136.5 (Phen-C^{4,7}, Form III), 136.1 (Phen-C^{4,7}, Form II), 135.0 (Phen-C^{4,7}, Form I), 134.9 (Phen-C^{4,7}, Form II), 128.9 (Phen-C^{4',6'}, Form III), 128.7 (Phen-C^{4',6'}, Form II), 128.0 (Phen-C^{4',6'}, Form III), 127.8 (Ar-C⁴), 126.8 (Ar-C⁴), 126.6 (Ar-C^{3,5}), 126.5 (Ar-C⁴), 126.1 (Phen-C^{5,6}, Form II), 125.9 (Phen-C^{5,6}, Form I), 125.9 (Phen-C^{5,6}, Form III), 125.5 (Ar-C^{3,5}, Form I), 123.3 (Phen-C^{3,8}, Form III), 120.5 (Phen-C^{3,8}, Form I), 119.8 (Phen-C^{3,8}, Form II), 48.3 (N-CH₂, Form II), 47.6 (N-CH₂, Form III), 45.0 (N-CH₂, Form I), 44.9 (N-CH₂, Form II), 24.5 (Ar-CH₂, Form III), 24.4 (Ar-CH₂, Form II), 24.1 (Ar-CH₂, Form II), 24.1 (Ar-CH₂, Form I), 14.8 (Ar-CH₂-CH₃, Form III), 14.7 (Ar-CH₂-CH₃, Form II), 14.6 (N-CH₂-CH₃, Form II), 14.5 (N-CH₂-CH₃, Form III), 14.4 (Ar-CH₂-CH₃, Form II), 14.1 (Ar-CH₂-CH₃, Form I), 12.7 (N-CH₂-CH₃, Form I), 12.5 (N-CH₂-CH₃, Form II); IR (ν, cm⁻¹) 3061, 3030, 2970, 2935, 2877 (C-H stretching vibrations), 1642 (C=O), 1582, 1547, 1504, 1449 (C=C, C=N); HRMS (ESI-TOF) (*m/z*) [M+H]⁺ calcd for [C₃₈H₄₃N₄O₂]⁺ 587.3381 found 587.3386.

N²,N⁹-bis(2,6-diisopropylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide (L3).

White powder. Yield 4.18 g (65%). M.p. 232-234°C; ¹H NMR (400 MHz, C₆D₆) δ 8.20 (d, *J* = 8.2 Hz, Phen-H^{3,8}), 8.05 (d, *J* = 8.2 Hz, 2H, Phen-H^{3,8}, Form I), 8.01 (d, *J* = 8.2 Hz, Phen-H^{3,8}), 7.58 (d, *J* = 8.3 Hz, 2H, Phen-H^{4,7}, Form I), 7.49 (d, *J* = 8.3 Hz, Phen-H^{4,7}), 7.40 (d, *J* = 8.3 Hz, Phen-H^{4,7}), 7.33 – 7.23 (m, 3H, Ar-H⁴), 7.22 – 7.17 (m, 5H, Ar-H^{3,5}, Form I), 7.14 (s, 3H, Phen-H^{5,6}, Form I), 7.09-7.00 (m, 3H, Ar-H⁴), 6.92 (d, *J* = 8.7 Hz, Ar-H^{3,5}), 6.83 – 6.69 (m, Phen-H^{5,6}), 4.01 (q, *J* = 7.2 Hz, N-CH₂), 3.95 (q, *J* = 7.2 Hz, 4H, N-CH₂, Form I), 3.90 – 3.78 (m, N-CH₂), 3.75 (q, *J* = 7.2 Hz, N-CH₂), 3.57 – 3.48 (m, CH₃-CH-CH₃), 3.40 (hept, *J* = 6.8 Hz, 5H, CH₃-CH-CH₃, Form I), 1.92 (t, *J* = 7.0 Hz, N-CH₂-CH₃), 1.50 (t, *J* = 7.0 Hz, 8H, N-CH₂-CH₃, Form I), 1.44 – 1.34 (m, 18H, CH-CH₃, Form I), 1.26 (d, *J* = 6.8 Hz, 13H, CH-CH₃, Form I), 1.18 – 1.08 (m, CH-CH₃), 0.99 (d, *J* = 6.8 Hz, CH-CH₃); ¹³C NMR (101 MHz, C₆D₆) δ 168.7 (C=O), 168.5 (C=O), 168.5 (C=O), 168.5 (C=O, Form I), 168.4 (C=O), 168.0 (C=O), 155.3 (Phen-C^{2,9}), 155.2 (Phen-C^{2,9}, Form I), 155.1 (Phen-C^{2,9}), 155.0 (Phen-C^{2,9}), 153.9 (Phen-C^{2,9}), 147.0 (Ar-C^{2,6}), 146.8 (Ar-C^{2,6}), 146.4 (Ar-C^{2,6}), 146.4 (Ar-C^{2,6}), 146.4 (Ar-C^{2,6}), 146.4 (Ar-C^{2,6}, Form I), 146.3 (Ar-C^{2,6}), 146.0 (Ar-C^{2,6}), 145.1 (Ar-C^{1',10'}), 144.7 (Ar-C^{1',10'}), 144.7 (Ar-C^{1',10'}, Form I), 144.3 (Ar-C^{1',10'}), 140.1 (Ar-C^{1',10'}), 138.8 (Ar-C¹), 138.5 (Ar-C¹), 138.5 (Ar-C¹), 138.2 (Ar-C¹), 137.8 (Ar-C¹, Form I), 137.7 (Ar-C¹), 136.5 (Phen-C^{4,7}, Form I), 136.1 (Phen-C^{4,7}), 134.8 (Phen-C^{4,7}), 134.6 (Phen-C^{4,7}), 129.1 (Phen-C^{4',6'}), 129.1 (Phen-C^{4',6'}, Form I), 129.0 (Phen-C^{4',6'}), 128.8 (Phen-C^{4',6'}), 128.7 (Ar-C⁴), 128.5 (Phen-C^{4',6'}), 128.4 (Ar-C⁴, Form I), 128.2 (Ar-C⁴), 128.1 (Ar-C⁴), 127.2 (Phen-C^{5,6}), 126.9 (Phen-C^{5,6}), 126.9 (Phen-C^{5,6}, Form I), 126.7 (Phen-C^{5,6}), 126.6 (Phen-C^{5,6}), 126.2 (Phen-C^{5,6}), 126.2 (Phen-C^{5,6}), 124.3 (Ar-C^{3,5}), 124.2 (Ar-C^{3,5}), 124.1 (Ar-C^{3,5}, Form I), 124.1 (Ar-C^{3,5}), 124.0 (Ar-C^{3,5}), 123.8 (Phen-C^{3,8}, Form I), 123.7 (Phen-C^{3,8}), 123.6 (Phen-C^{3,8}), 121.9 (Phen-C^{3,8}), 120.1 (Phen-C^{3,8}), 49.6 (N-CH₂), 48.3 (N-CH₂, Form I), 48.2 (N-CH₂), 48.2

(N-CH₂), 47.3 (N-CH₂), 47.2 (N-CH₂), 34.1, 31.6, 28.8 (CH₃-CH-CH₃, Form I), 28.7 (CH₃-CH-CH₃), 28.7 (CH₃-CH-CH₃), 28.4 (CH₃-CH-CH₃), 28.2 (CH₃-CH-CH₃), 25.9 (CH-CH₃), 25.7 (CH-CH₃), 25.3 (CH-CH₃), 25.1 (CH-CH₃, Form I), 23.8 (CH-CH₃), 23.6 (CH-CH₃), 23.6 (CH-CH₃), 23.5 (CH-CH₃), 23.5 (CH-CH₃, Form I), 23.4 (CH-CH₃), 23.1 (CH-CH₃), 22.6 (CH-CH₃), 14.7 (N-CH₂-CH₃), 14.6 (N-CH₂-CH₃), 14.5 (N-CH₂-CH₃), 14.5 (N-CH₂-CH₃, Form I), 14.4 (N-CH₂-CH₃), 13.9 (N-CH₂-CH₃), 12.7 (N-CH₂-CH₃), 12.5 (N-CH₂-CH₃); IR (ν, cm⁻¹) 2962, 2930, 2868 (C-H stretching vibrations), 1644 (C=O), 1586, 1544, 1505 (C=C, C=N); HRMS (ESI-TOF) (*m/z*) [M+H]⁺ calcd for [C₄₂H₅₁N₄O₂]⁺ 643.4007 found 643.4010.

General method for synthesis of complexes L•Ln(NO₃)₃

The complexes **L•Ln(NO₃)₃** were synthesized referring to the earlier described procedure [12].

N²,N⁹-bis(2,6-dimethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide

lanthanum trinitrate L1•La(NO₃)₃. White powder. Yield 78mg (91%). T_{decomp.} 339°C; ¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.31 (d, *J* = 8.6 Hz, 2H, Phen-H^{4,7}), 8.02 (s, 2H, Phen-H^{5,6}), 7.37 (t, *J* = 7.6 Hz, 2H, Ar-H⁴), 7.25 (d, *J* = 7.6 Hz, 4H, Ar-H^{3,5}), 6.97 (d, *J* = 8.5 Hz, 2H, Phen-H^{3,8}), 4.05 (q, *J* = 7.2 Hz, 4H, N-CH₂), 2.21 (s, 12H, Ar-CH₃), 1.36 (t, *J* = 7.2 Hz, 6H, N-CH₂-CH₃); IR (ν, cm⁻¹) 3063, 2971, 2938, 2877 (C-H stretching vibrations), 1602 (C=O), 1584, 1553, 1454 (C=C, C=N); HRMS (ESI-TOF) (*m/z*) [L•La(NO₃)₂]⁺ calcd for [C₃₄H₃₄LaN₆O₈]⁺ 793.1497, found 793.1490.

N²,N⁹-bis(2,6-dimethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide lutetium trinitrate L1•Lu(NO₃)₃. White powder. Yield 79mg (89%). T_{decomp.} 328°C; ¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.40 (d, *J* = 8.7 Hz, 2H, Phen-H^{4,7}), 8.09 (s, 2H, Phen-H^{5,6}), 7.54 – 7.43 (m, 2H, Ar-H⁴), 7.35 (d, *J* = 7.6 Hz, 4H, Ar-H^{3,5}), 6.79 (d, *J* = 8.7 Hz, 2H, Phen-H^{3,8}), 4.08 (q, *J* = 7.2 Hz, 4H, N-CH₂), 2.26 (s, 12H, Ar-CH₃), 1.40 (t, *J* = 7.2 Hz, 6H, N-CH₂-CH₃); IR (ν, cm⁻¹) 3057, 2978, 2939, 2877 (C-H stretching vibrations), 1601 (C=O), 1586, 1557, 1490 (C=C, C=N); HRMS (ESI-TOF) (*m/z*) [L•Lu(NO₃)₂]⁺ calcd for [C₃₄H₃₄LuN₆O₈]⁺ 829.1841, found 829.1839.

N²,N⁹-bis(2,6-diethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide lanthanum trinitrate L2•La(NO₃)₃. White powder. Yield 82 (90%). T_{decomp.} 361°C; ¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.30 (d, *J* = 8.6 Hz, 2H, Phen-H^{4,7}), 8.01 (s, 2H, Phen-H^{5,6}), 7.58 – 7.44 (m, 2H, Ar-H⁴), 7.35 (d, *J* = 7.7 Hz, 4H, Ar-H^{3,5}), 6.95 (d, *J* = 8.6 Hz, 2H, Phen-H^{3,8}), 4.04 (q, *J* = 7.2 Hz, 4H, N-CH₂), 2.77 – 2.60 (m, 4H, Ar-CH₂), 2.58 – 2.44 (m, 4H, Ar-CH₂), 1.34 (t, *J* = 7.2 Hz, 6H, N-CH₂-CH₃), 1.00 (t, *J* = 7.5 Hz, 12H, Ar-CH₂-CH₃); ¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 169.6 (C=O), 150.1 (Phen-C^{2,9}), 145.4 (Phen-C^{1',10'}), 141.9 (Ar-C¹), 140.6 (Phen-C^{4,7}), 138.4 (Ar-C^{2,6}), 131.8 (Phen-C^{4',6'}), 131.1 (Ar-C⁴), 129.7 (Phen-C^{5,6}), 128.7 (Ar-C^{3,5}), 125.4 (Phen-C^{3,8}), 50.3 (N-CH₂), 24.4 (Ar-CH₂), 14.3 (Ar-CH₂-CH₃), 11.6 (N-CH₂-CH₃); IR (ν, cm⁻¹) 3062, 2972, 2936, 2874 (C-H stretching vibrations), 1602 (C=O), 1585, 1553, 1430 (C=C, C=N); HRMS (ESI-TOF) (*m/z*) [L•La(NO₃)₂]⁺ calcd for [C₃₈H₄₂LaN₆O₈]⁺ 849.2123, found 849.2112.

N²,N⁹-bis(2,6-diethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide lutetium trinitrate L2•Lu(NO₃)₃. White powder. Yield 74 mg (80%). T_{decomp.} 338°C; ¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.38 (d, *J* = 8.7, 2.4 Hz, 2H, Phen-H^{4,7}), 8.06 (d, *J* = 2.3 Hz, 2H, Phen-H^{5,6}), 7.59 (t, *J* = 7.7 Hz, 2H, Ar-H⁴), 7.43 (d, *J* = 7.7 Hz, 4H, Ar-H^{3,5}), 6.75 (d, *J* = 8.8, 2.4 Hz, 2H, Phen-H^{3,8}), 4.06 (q, *J* = 7.3 Hz, 4H, N-CH₂), 2.80 – 2.62 (m, 4H, Ar-CH₂), 2.63 – 2.48 (m, 4H, Ar-CH₂), 1.37 (t, *J* = 7.2 Hz, 6H, N-CH₂-CH₃), 1.03 (t, *J* = 7.6 Hz, 12H, Ar-CH₂-CH₃); IR (ν, cm⁻¹) 3123, 3062, 2972, 2936, 2875 (C-H stretching vibrations), 1601 (C=O), 1586, 1557, 1514, 1483 (C=C, C=N); HRMS (ESI-TOF) (*m/z*) [L•Lu(NO₃)₂]⁺ calcd for [C₃₈H₄₂LuN₆O₈]⁺ 885.2467, found 885.2466.

N²,N⁹-bis(2,6-diisopropylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide

lanthanum trinitrate L3•La(NO₃)₃. White powder. Yield 80mg (83%). T_{decomp.} 362°C; ¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.33 (d, *J* = 8.6 Hz, 2H, Phen-H^{4,7}), 8.01 (s, 2H, Phen-H^{5,6}), 7.61 – 7.50 (m, 2H, Ar-H⁴), 7.39 (d, *J* = 7.8 Hz, 4H, Ar-H^{3,5}), 6.96 (d, *J* = 8.6 Hz, 2H, Phen-H^{3,8}), 4.04 (q, *J* = 7.2 Hz, 4H, N-CH₂), 3.13 (p, *J* = 6.8 Hz, 4H, Ar-CH), 1.44 (t, *J* = 7.2 Hz, 6H, N-CH₂-CH₃), 1.26 (d, *J* = 6.8 Hz, 12H, Ar-CH-CH₃), 0.69 (d, *J* = 6.7 Hz, 12H, Ar-CH-CH₃); ¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 169.7 (C=O), 150.1 (Phen-C^{2,9}), 146.7 (Phen-C^{1',10'}), 145.4 (Ar-C¹), 140.6 (Phen-C^{4,7}), 137.1 (Phen-C^{4',6'}), 131.8 (Ar-C⁴), 131.7 (Ar-C⁴), 129.8 (Phen-C^{5,6}), 127.1 (Ar-C^{3,5}), 125.9 (Phen-C^{3,8}), 51.6 (N-CH₂), 29.2 (Ar-CH), 25.1 (Ar-CH-CH₃), 24.0 (Ar-CH-CH₃), 11.7 (N-CH₂-CH₃); IR (ν, cm⁻¹) 3063, 2967, 2930, 2870 (C-H stretching vibrations), 1600 (C=O), 1584, 1554, 1444, 1416 (C=C, C=N); HRMS (ESI-TOF) (*m/z*) [L•La(NO₃)₂]⁺ calcd for [C₄₂H₅₀LaN₆O₈]⁺ 905.2749, found 905.2760

N²,N⁹-bis(2,6-diisopropylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide

lutetium trinitrate L3•Lu(NO₃)₃. White powder. Yield 90mg (90%). T_{decomp.} 367°C; ¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.41 (d, *J* = 8.7 Hz, 2H, Phen-H^{4,7}), 8.08 (s, 2H, Phen-H^{5,6}), 7.66 (t, *J* = 7.8 Hz, 2H, Ar-H⁴), 7.49 (d, *J* = 7.8 Hz, 4H, Ar-H^{3,5}), 6.72 (d, *J* = 8.7 Hz, 2H, Phen-H^{3,8}), 4.07 (q, *J* = 7.2 Hz, 4H, N-CH₂), 3.15 (p, *J* = 6.8 Hz, 4H, Ar-CH), 1.47 (t, *J* = 7.6 Hz, 6H, N-CH₂-CH₃), 1.29 (d, *J* = 6.8 Hz, 12H, Ar-CH-CH₃), 0.80 (d, *J* = 6.7 Hz, 12H, Ar-CH-CH₃); IR (ν, cm⁻¹) 3063, 2966, 2930, 2870 (C-H stretching vibrations), 1600 (C=O), 1584, 1557, 1494, 1462 (C=C, C=N); HRMS (ESI-TOF) (*m/z*) [L•Lu(NO₃)₂]⁺ calcd for [C₄₂H₅₀LuN₆O₈]⁺ 941.3093, found 941.3092.

2. NMR and IR spectra of synthesized compounds

N²,N⁹-bis(2,6-dimethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide (L1)

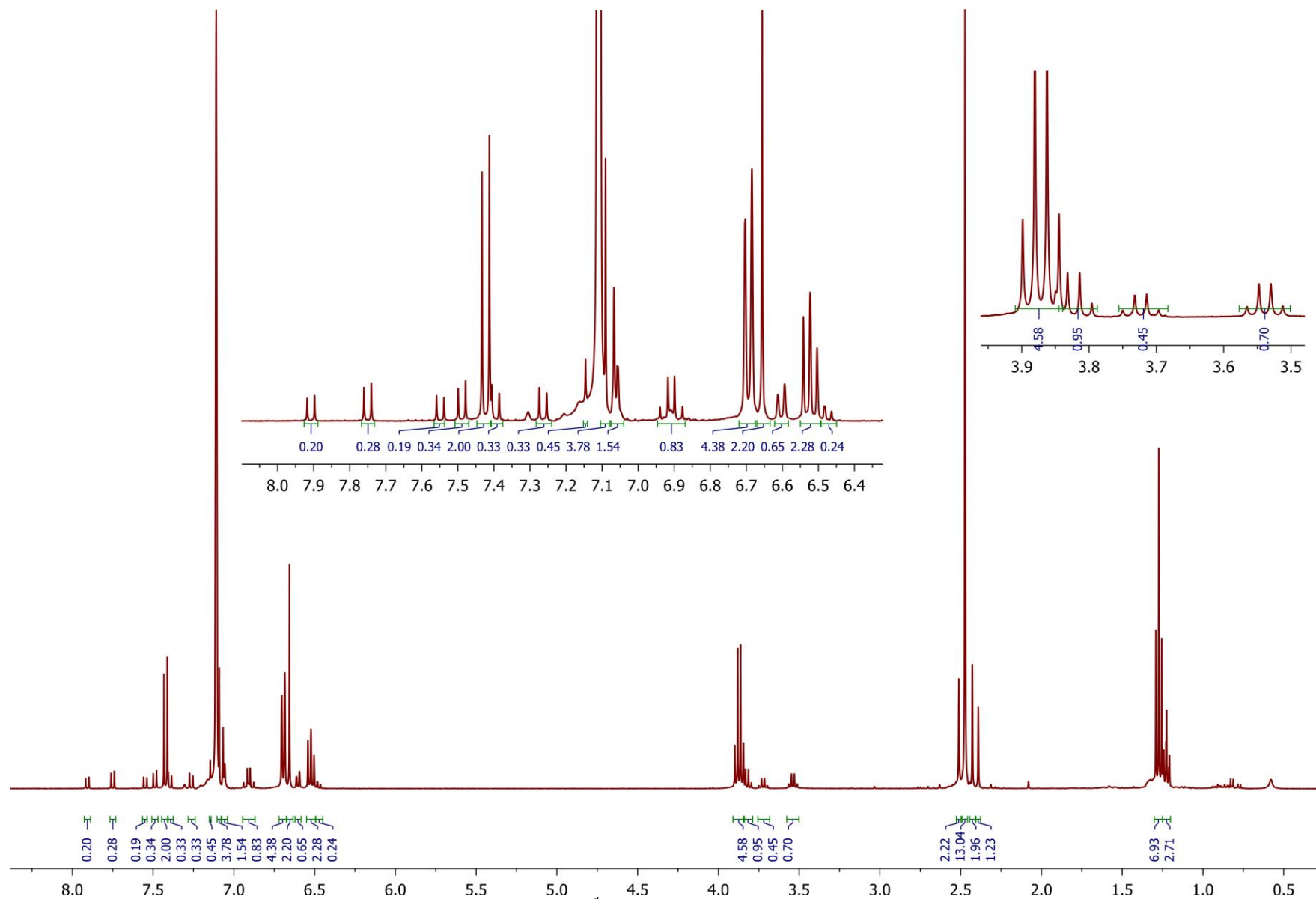


Figure S1. ¹H NMR spectrum in C₆D₆ at 25°C.

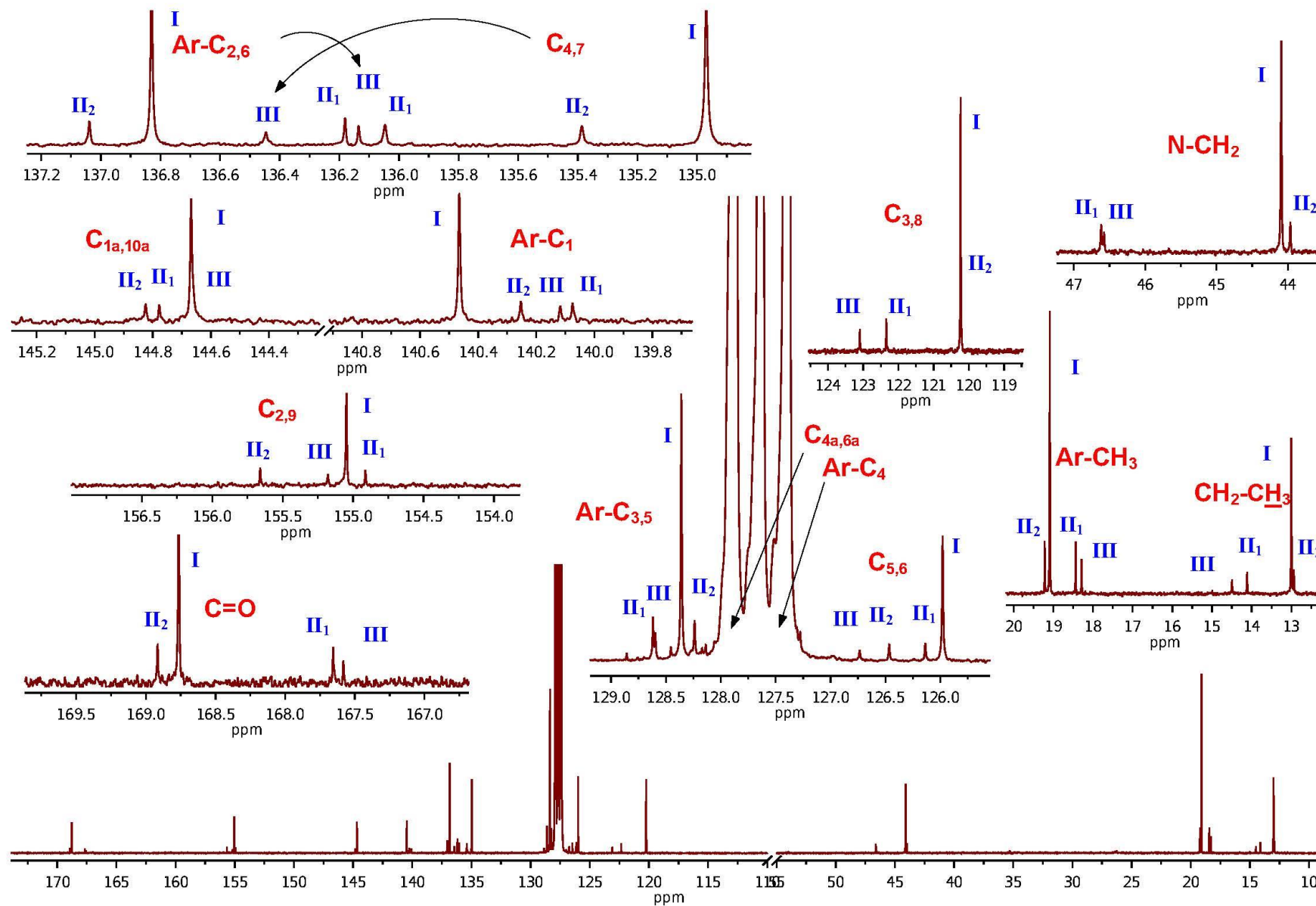


Figure S2. ^{13}C NMR spectrum in C_6D_6 at 25°C .

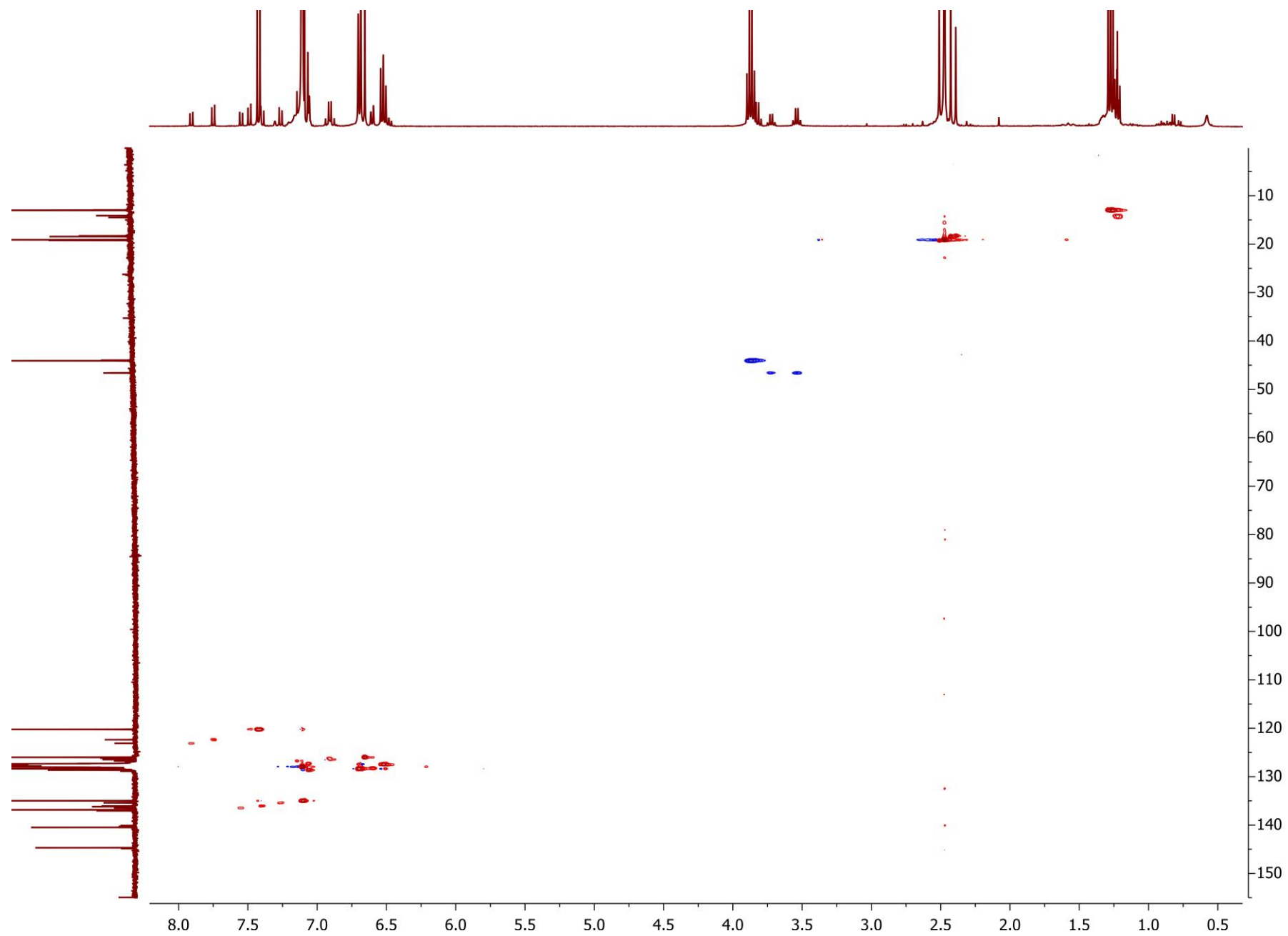


Figure S3. $^1\text{H}/^{13}\text{C}$ HSQC NMR spectrum in C_6D_6 at 25°C.

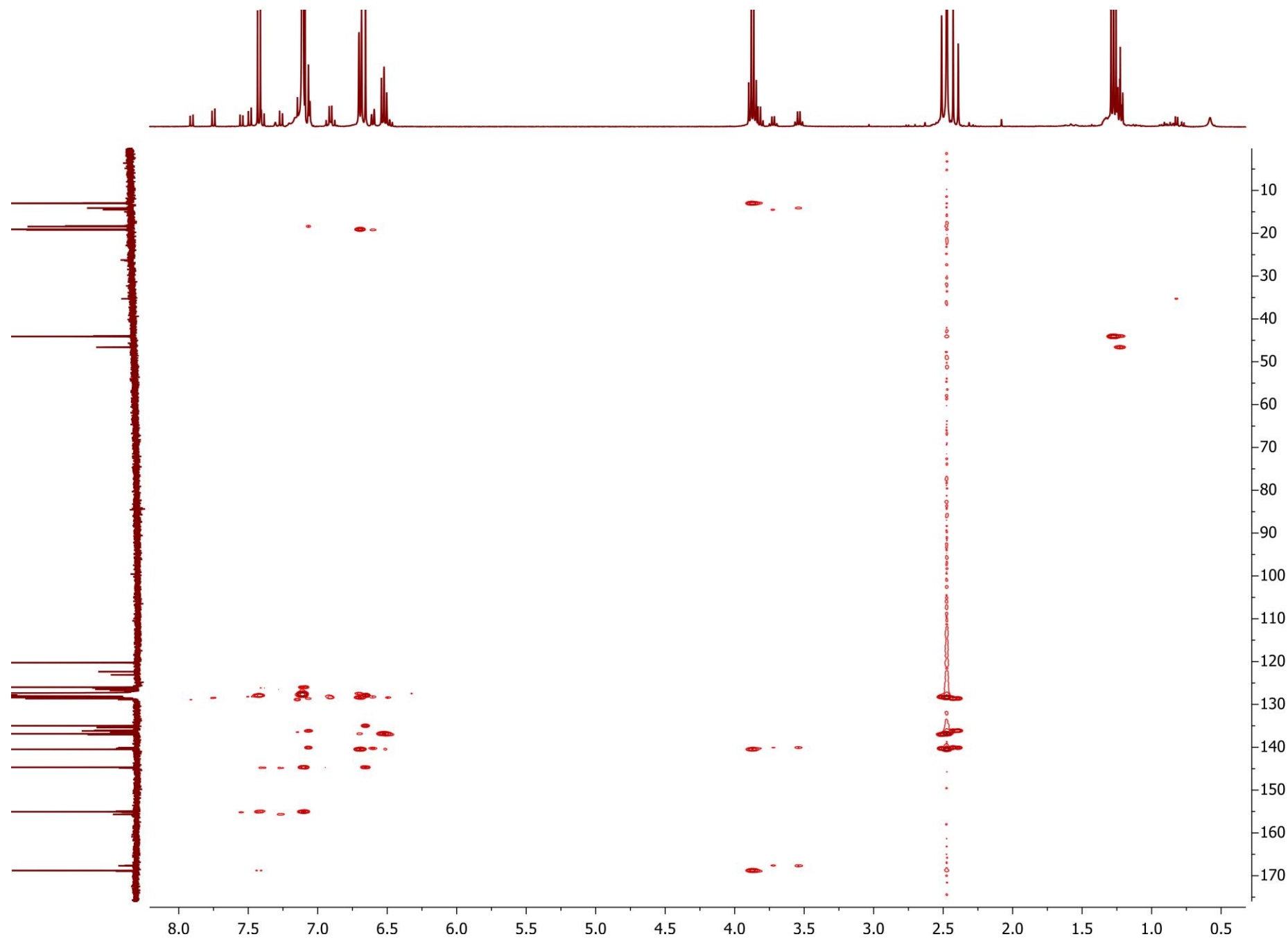


Figure S4. $^1\text{H}/^{13}\text{C}$ HMBC NMR spectrum in C_6D_6 at 25°C .

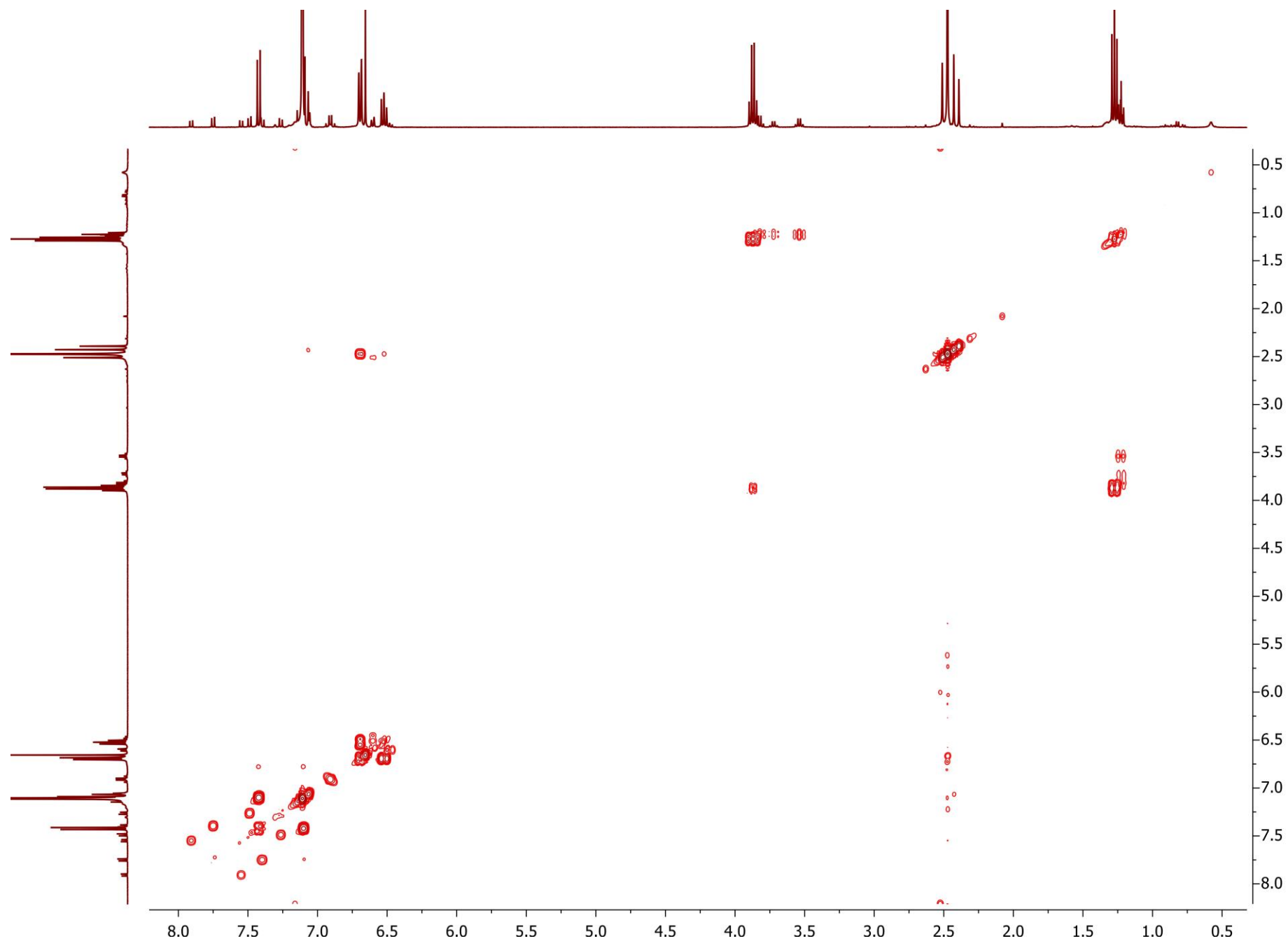


Figure S5. $^1\text{H}/^1\text{H}$ COSY NMR spectrum in C_6D_6 at 25°C .

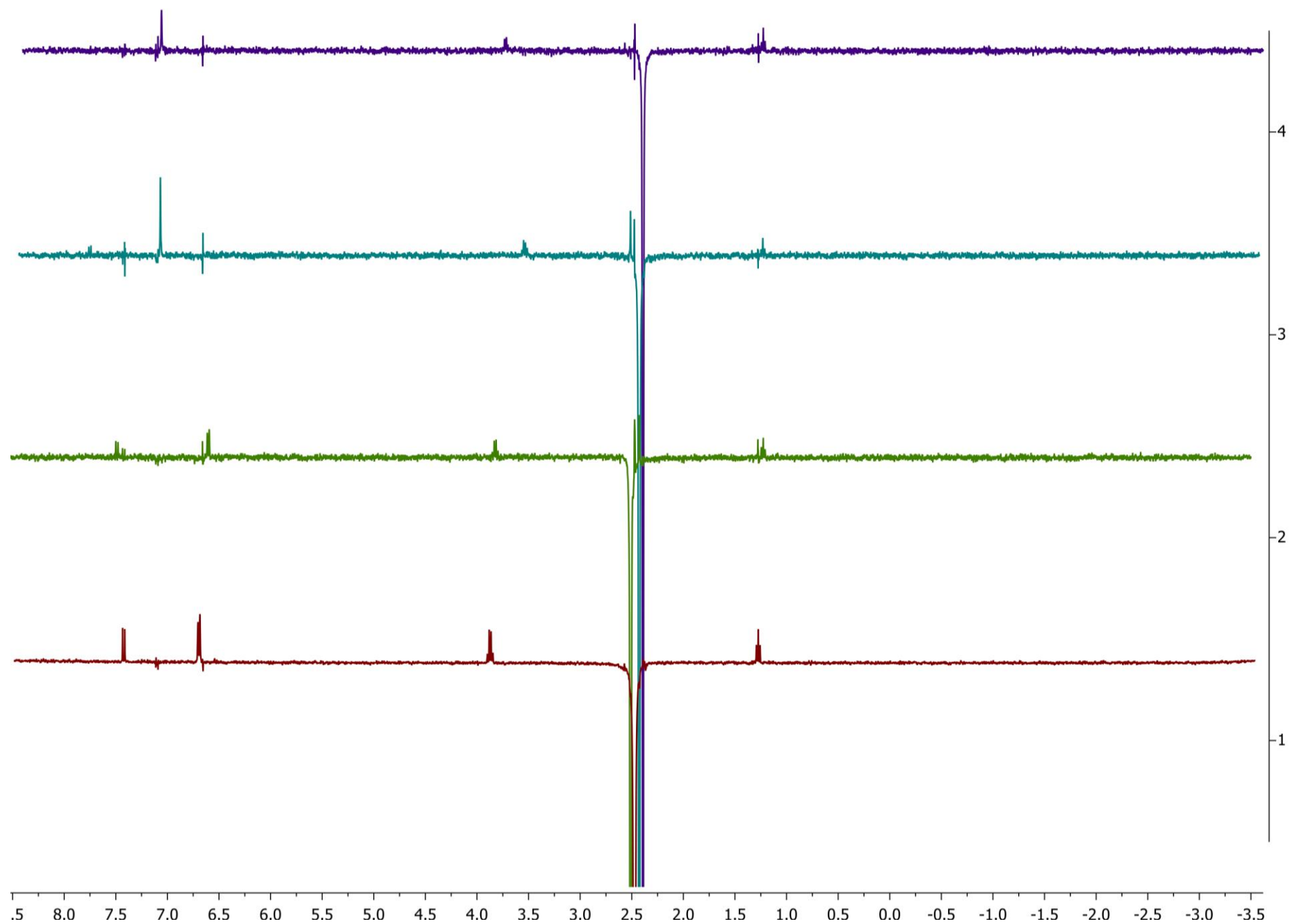


Figure S6. ^1H NOESY NMR spectrum in C_6D_6 at 25°C .

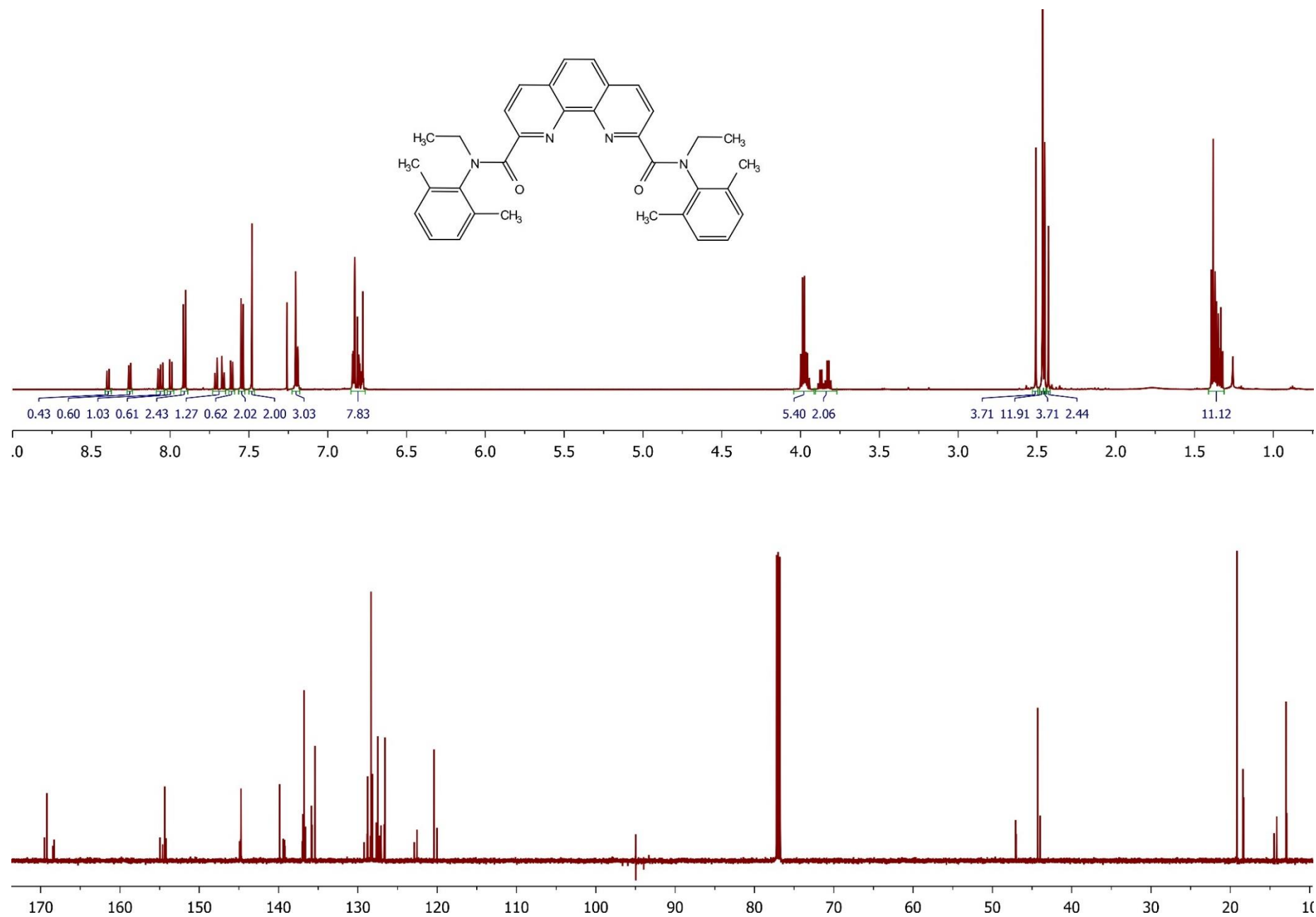


Figure S7. ^1H and ^{13}C NMR spectra in CDCl_3 at 25°C .

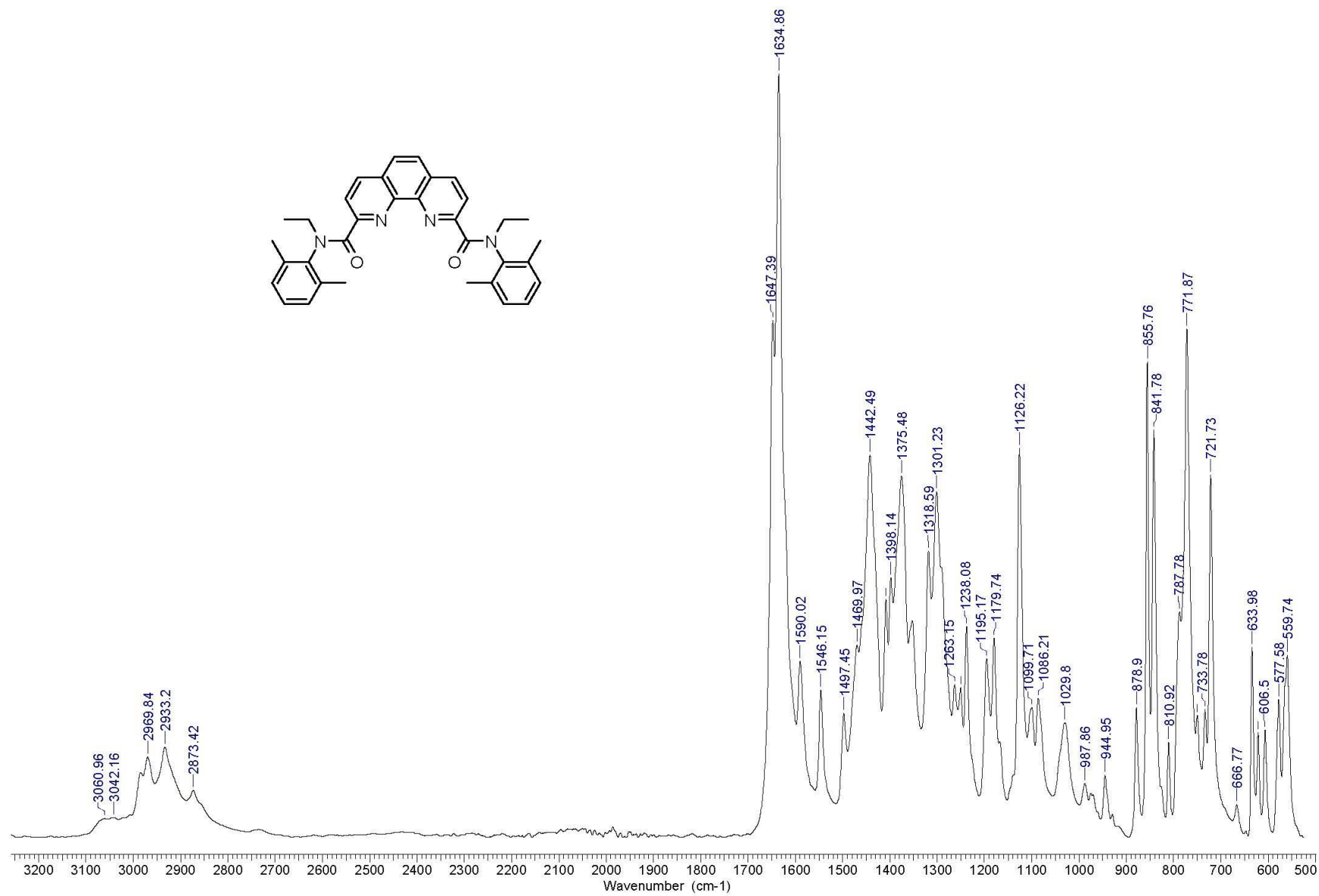


Figure S8. Solid-state IR spectrum at 25°C

N²,N⁹-bis(2,6-diethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide (L2)

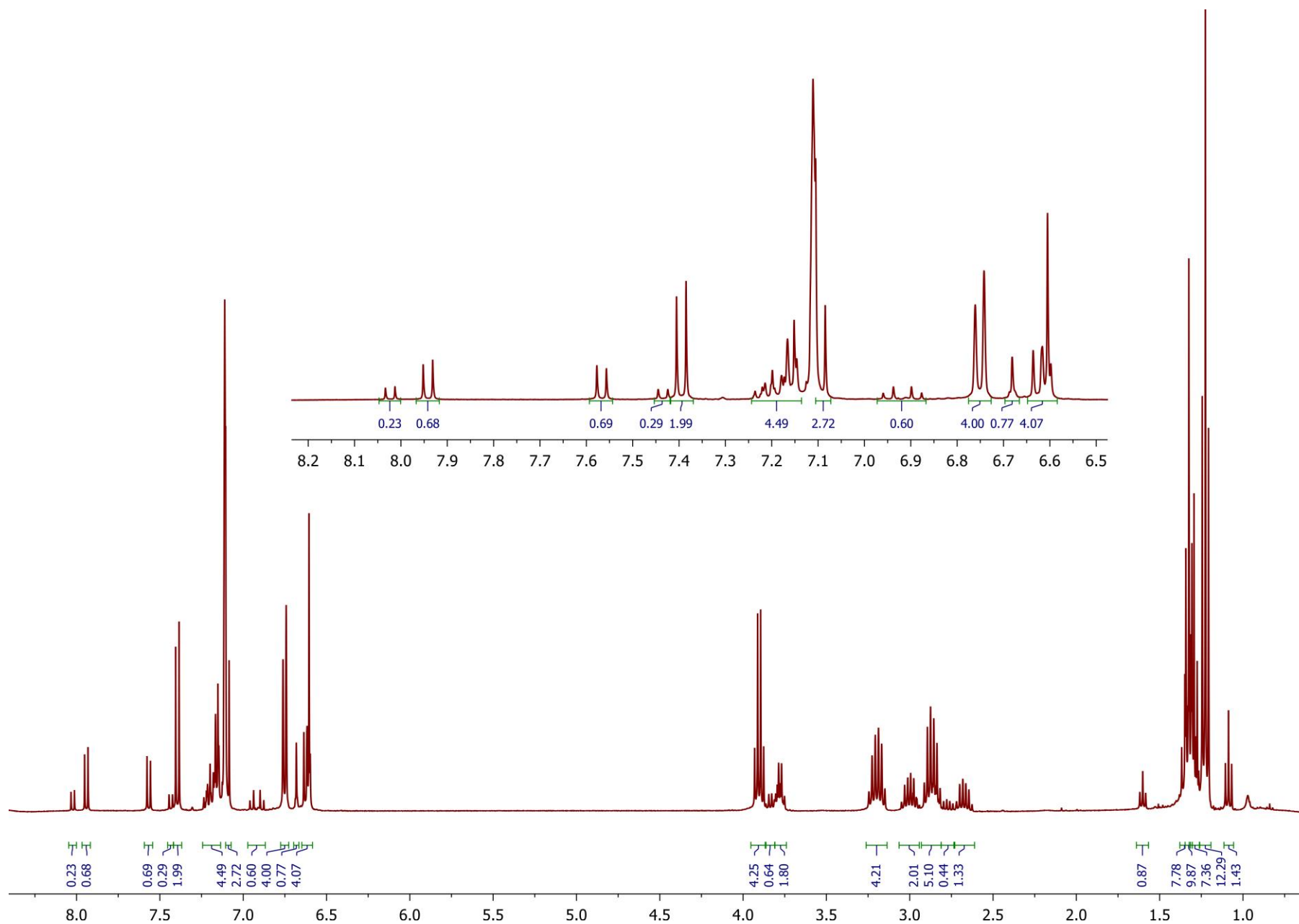


Figure S9. ¹H NMR spectrum in C₆D₆ at 25°C.

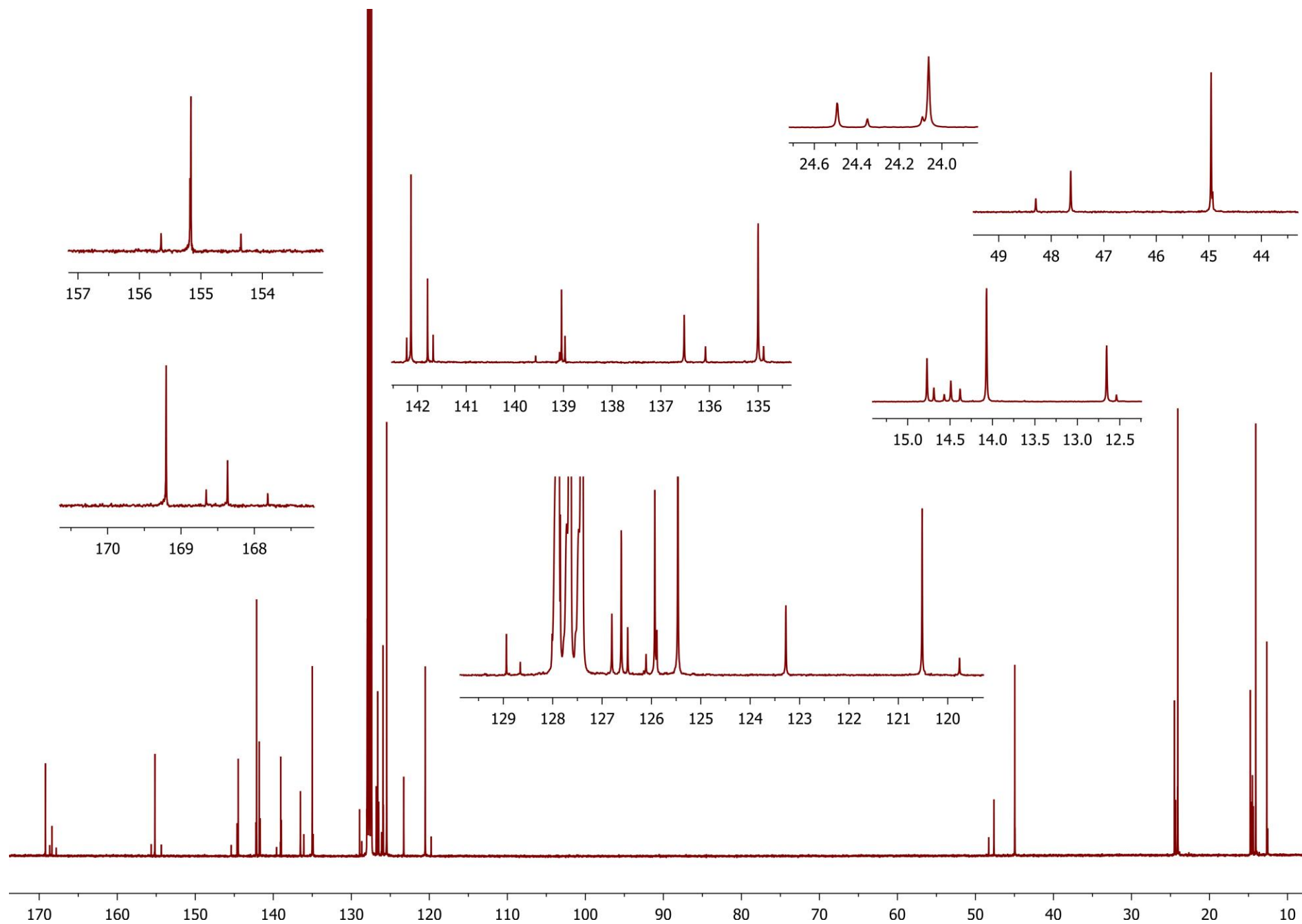


Figure S10. ^{13}C NMR spectrum in C_6D_6 at 25°C .

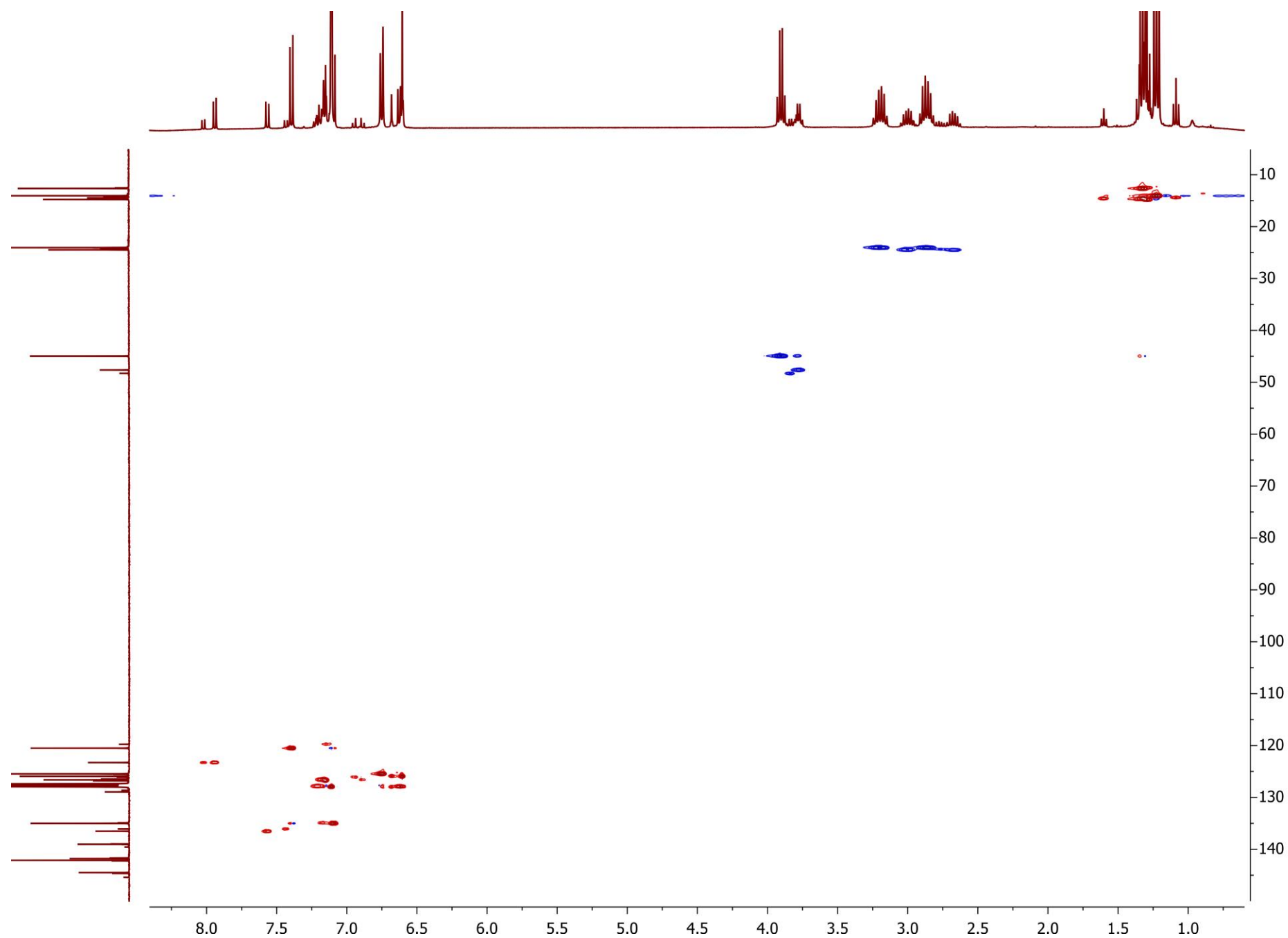


Figure S11. $^1\text{H}/^{13}\text{C}$ HSQC NMR spectrum in C_6D_6 at 25°C .

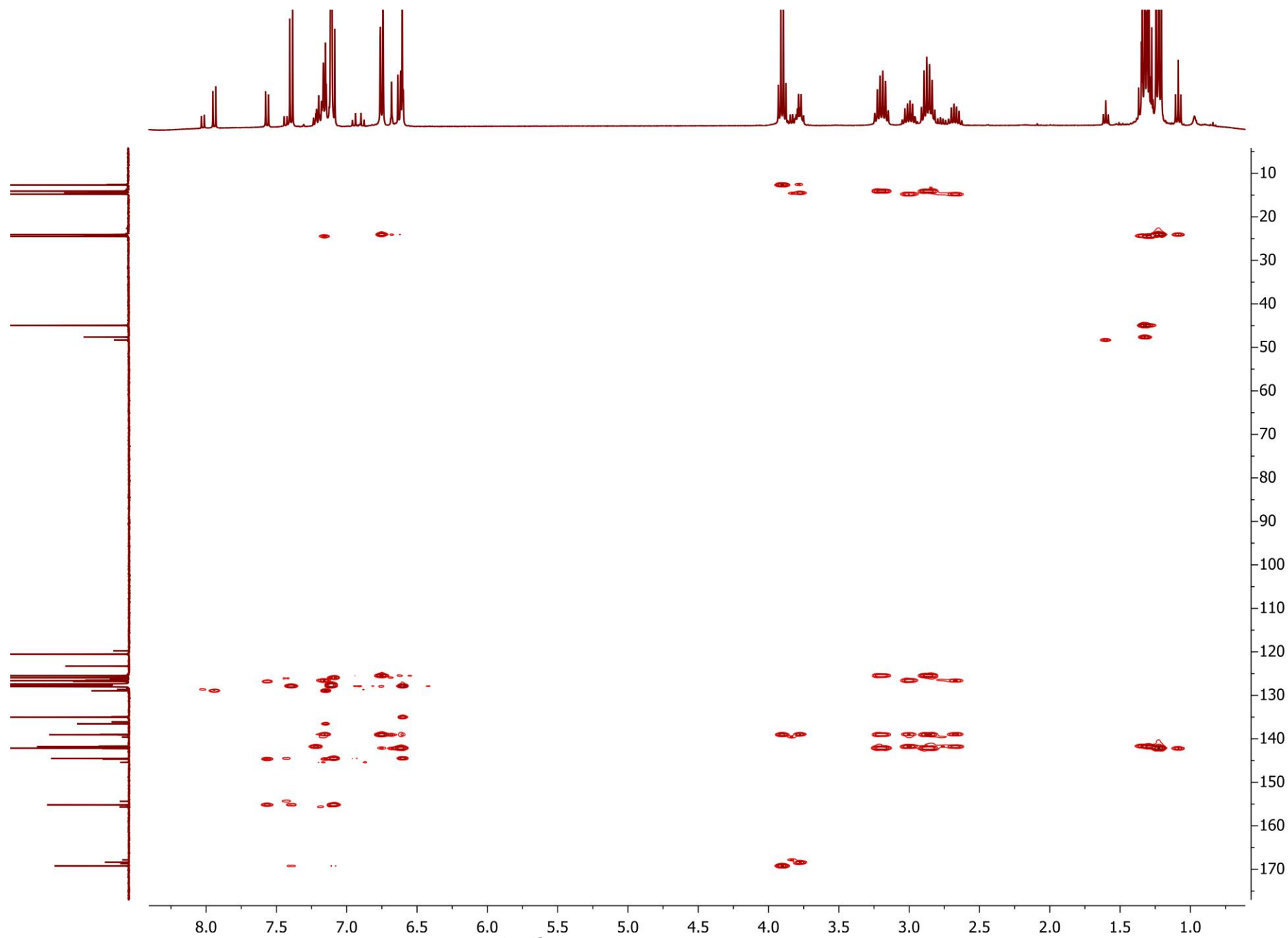
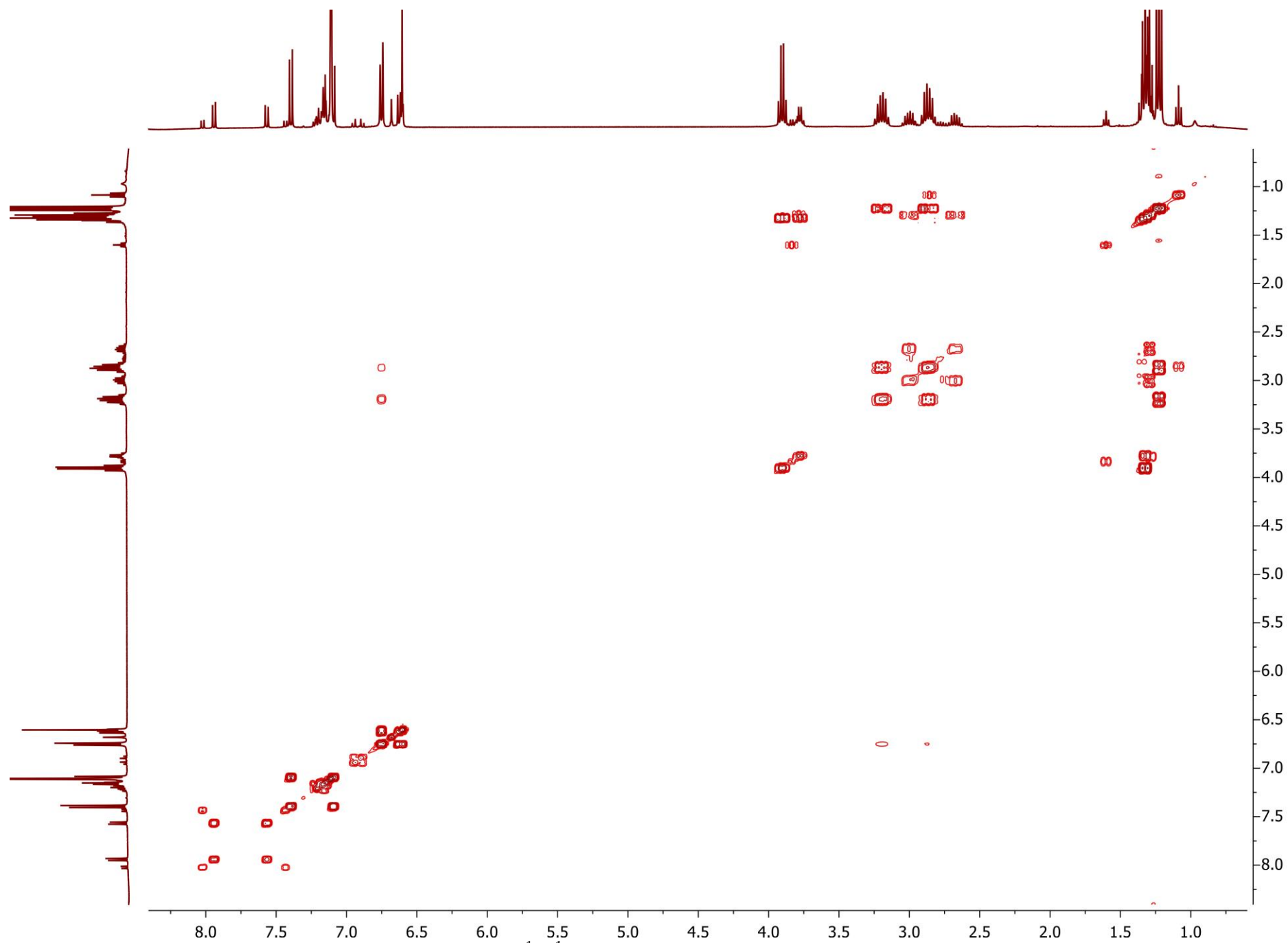


Figure S12. $^1\text{H}/^{13}\text{C}$ HMBC NMR spectrum in C_6D_6 at 25°C .



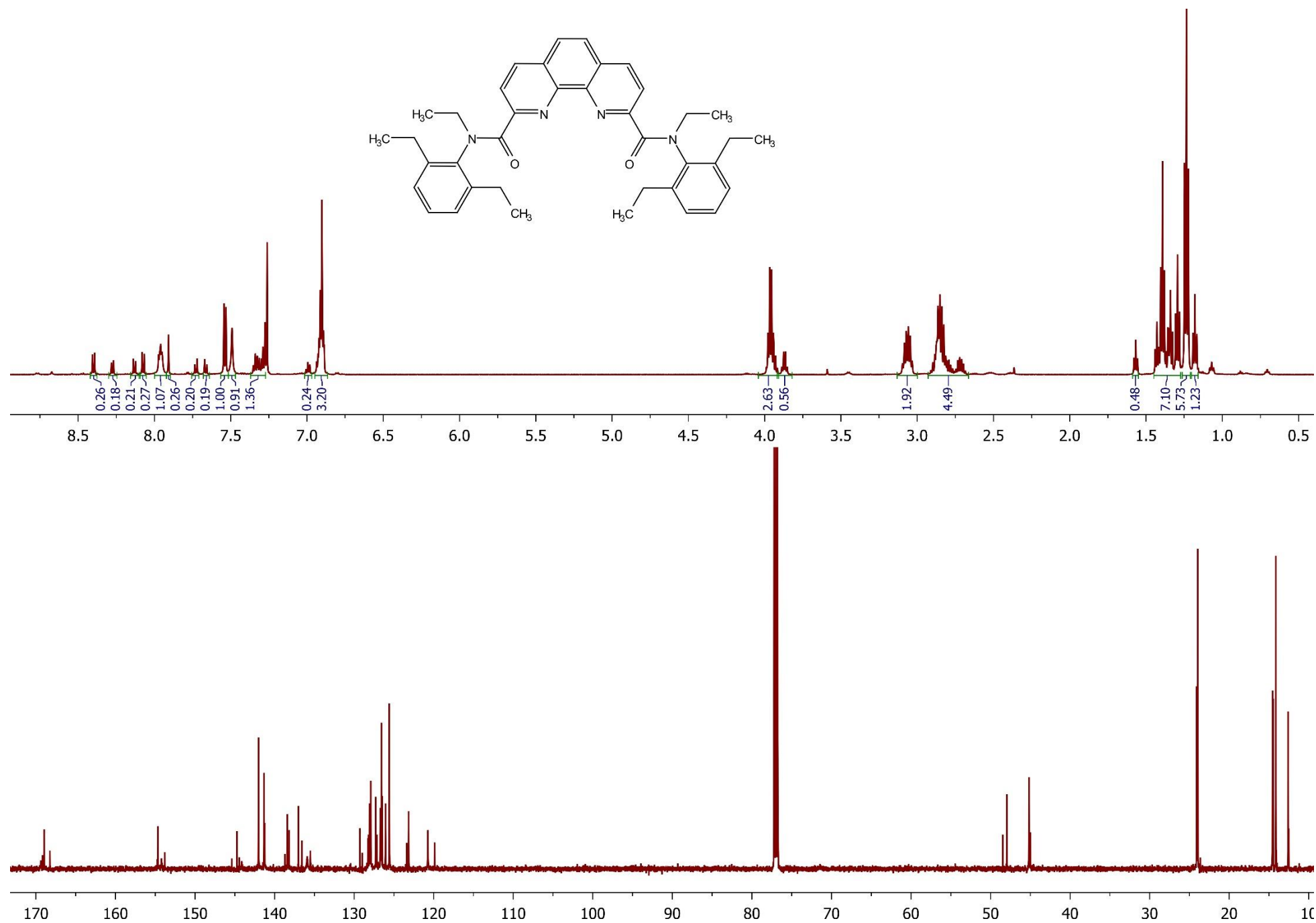


Figure S14. ^1H and ^{13}C NMR spectra in CDCl_3 at 25°C .

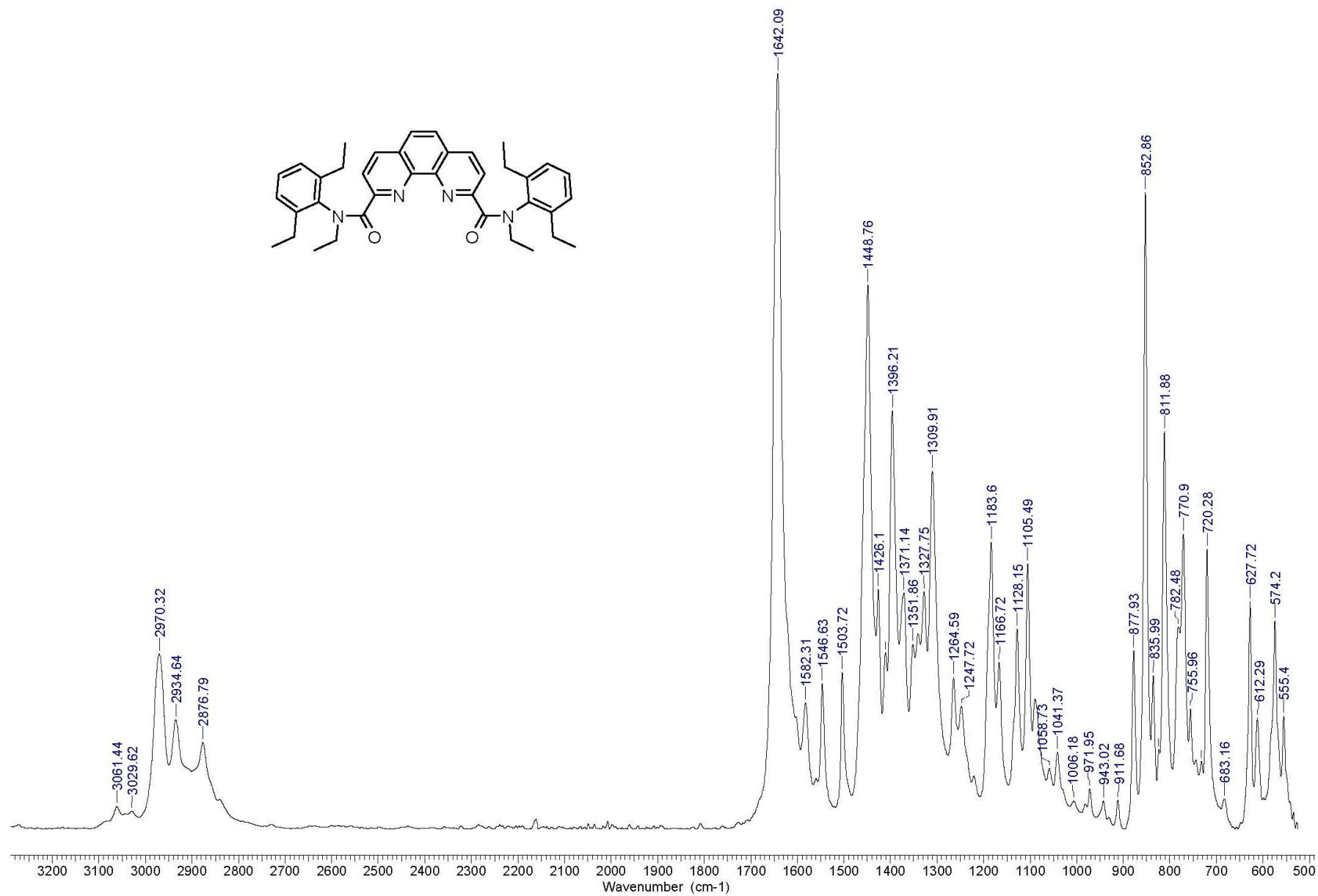


Figure S15. Solid-state IR spectrum at 25°C

N²,N⁹-bis(2,6-diisopropylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide (L3)

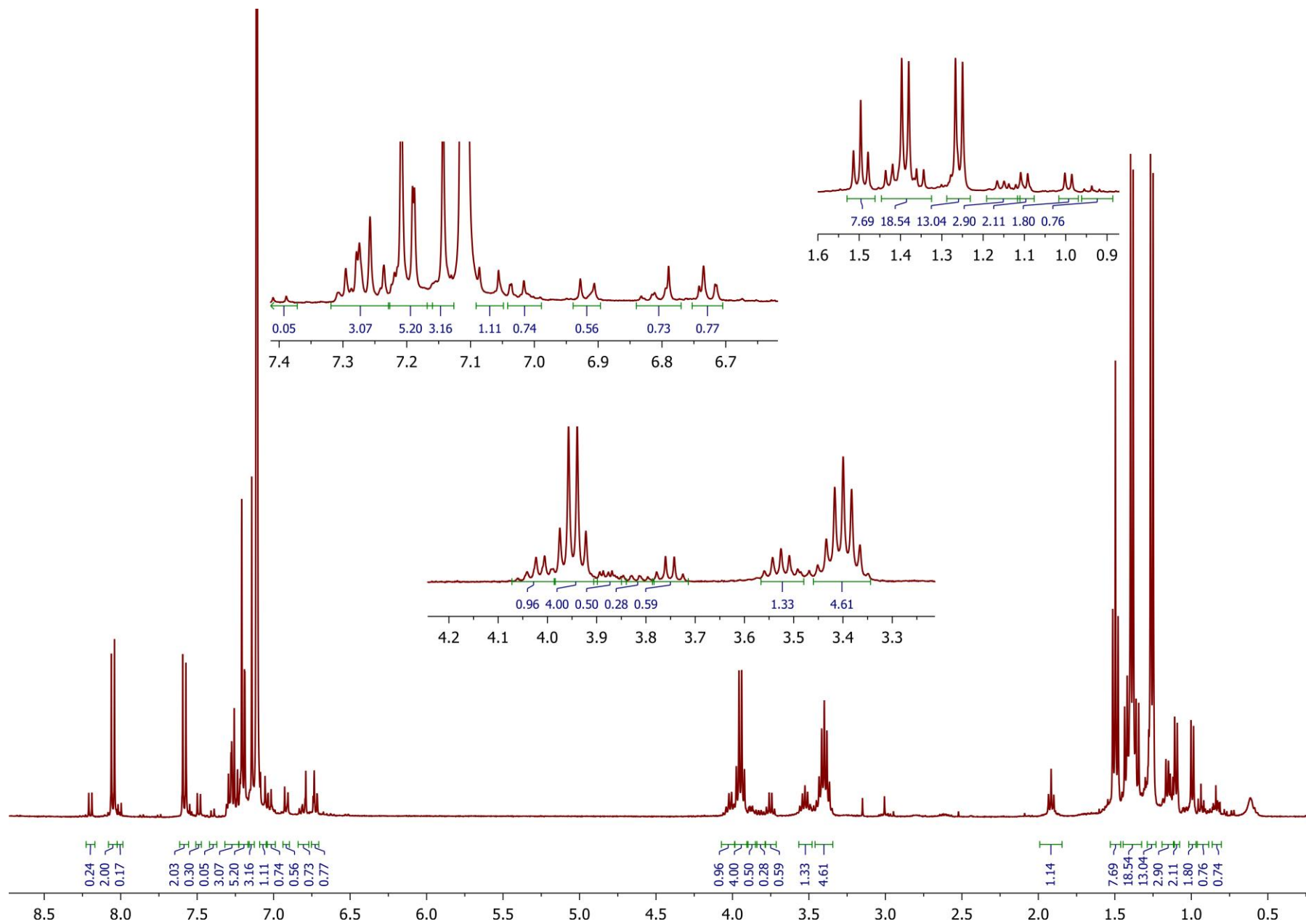


Figure S16. ¹H NMR spectrum in C₆D₆ at 25°C.

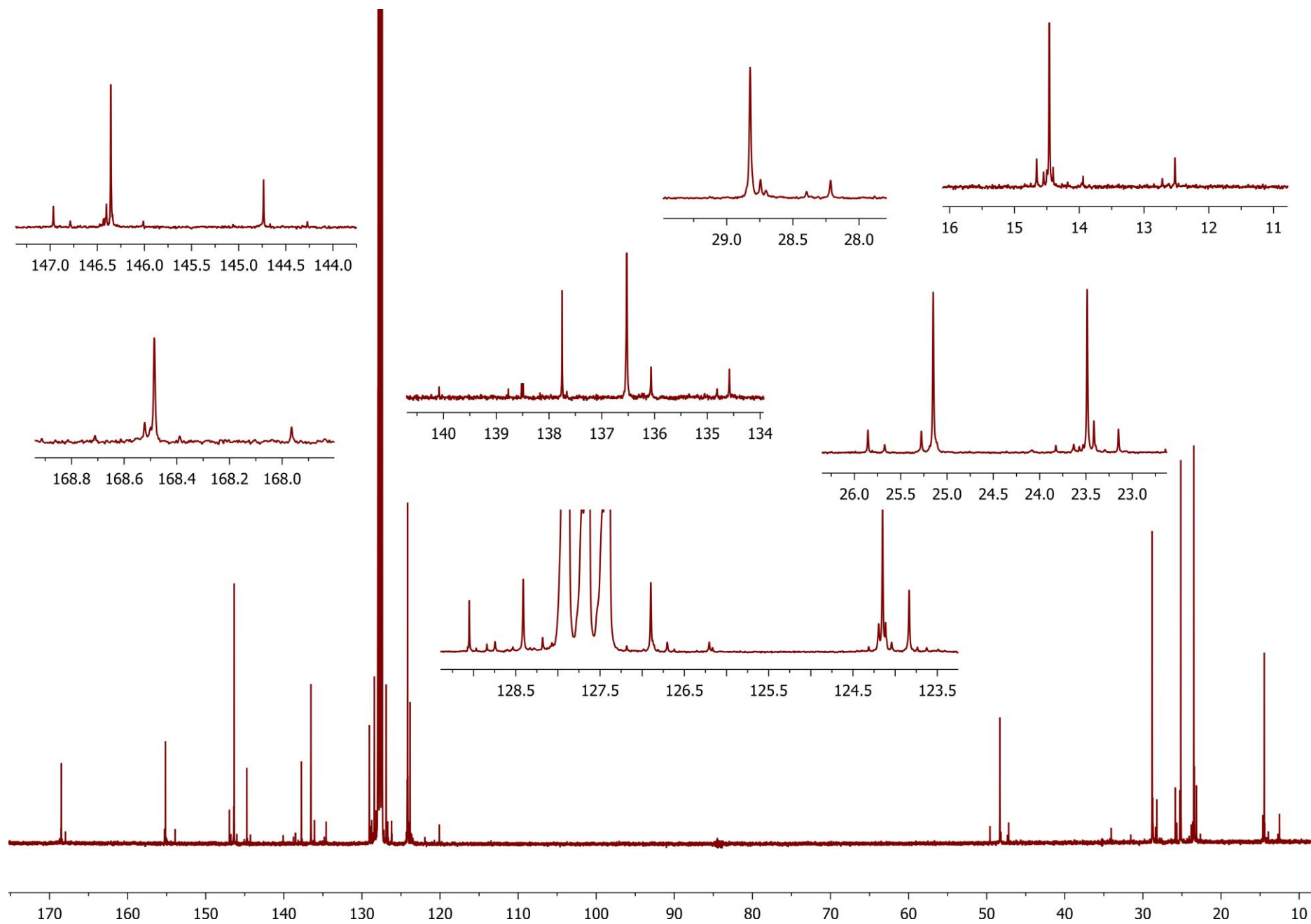


Figure S17. ^{13}C NMR spectrum in C_6D_6 at 25°C .

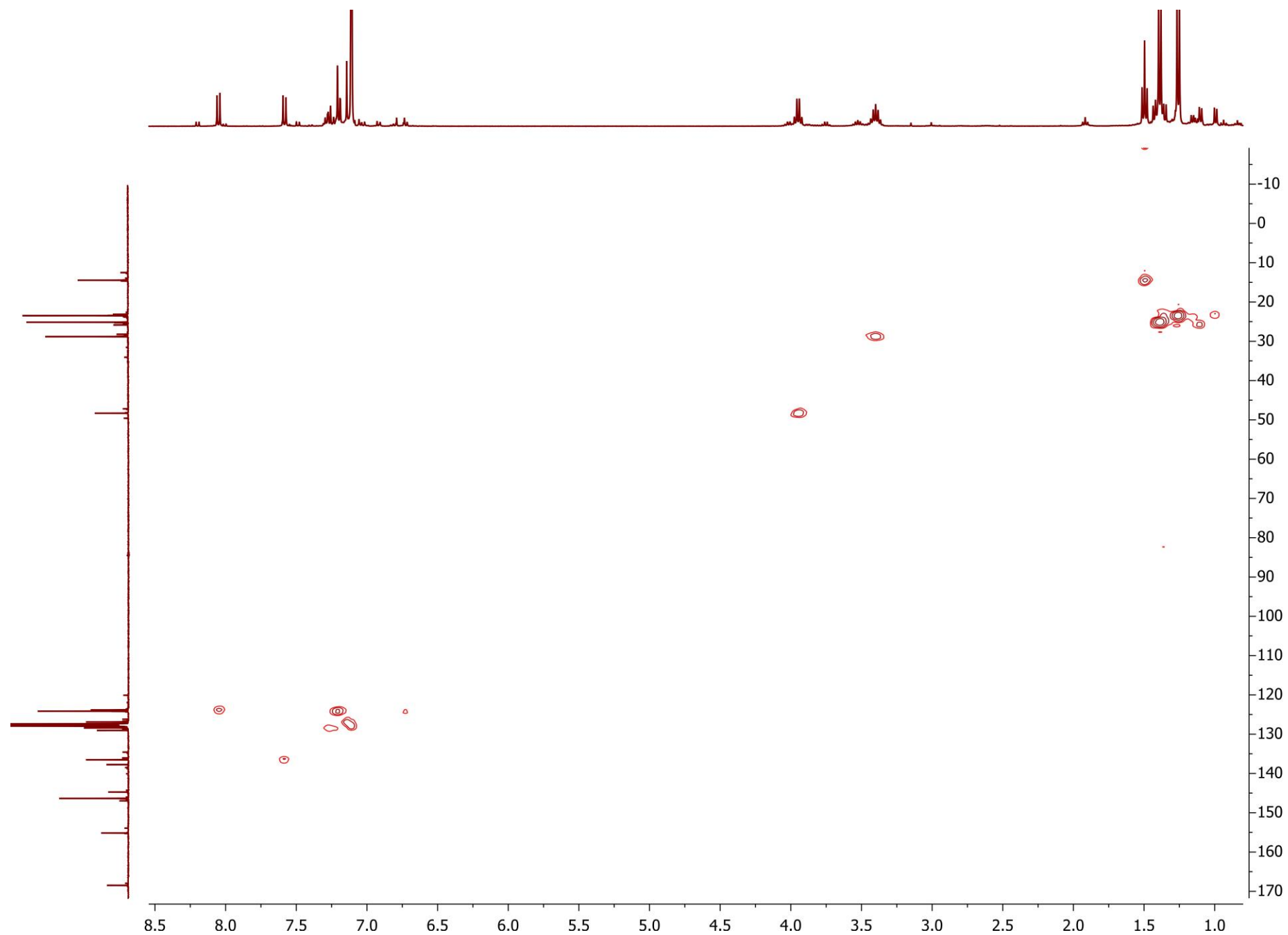


Figure S18. $^1\text{H}/^{13}\text{C}$ ASAPHSQC NMR spectrum in C_6D_6 at 25°C .

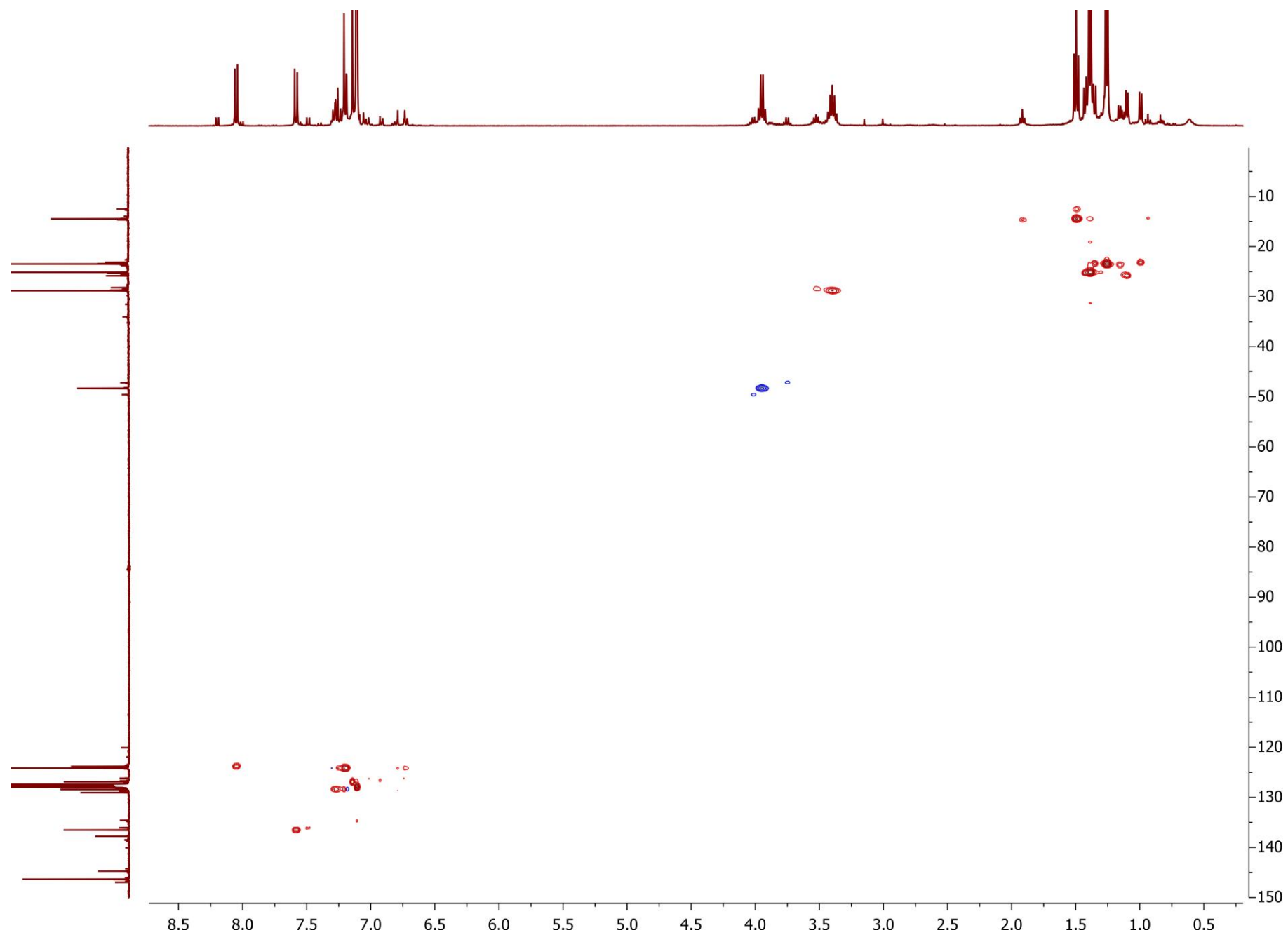


Figure S19. $^1\text{H}/^{13}\text{C}$ HSQC NMR spectrum in C_6D_6 at 25°C .

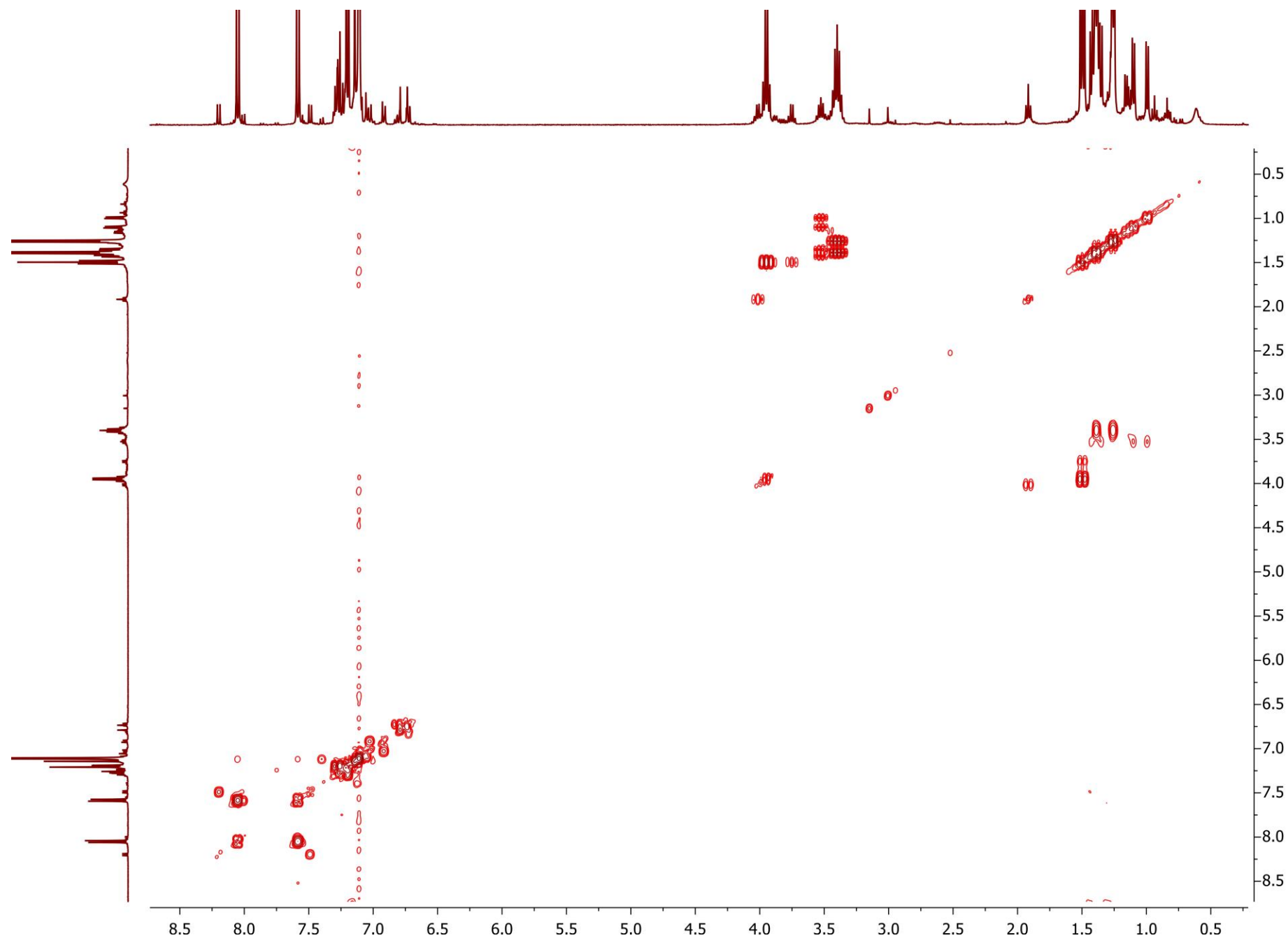


Figure S20. $^1\text{H}/^1\text{H}$ COSY NMR spectrum in C_6D_6 at 25°C .

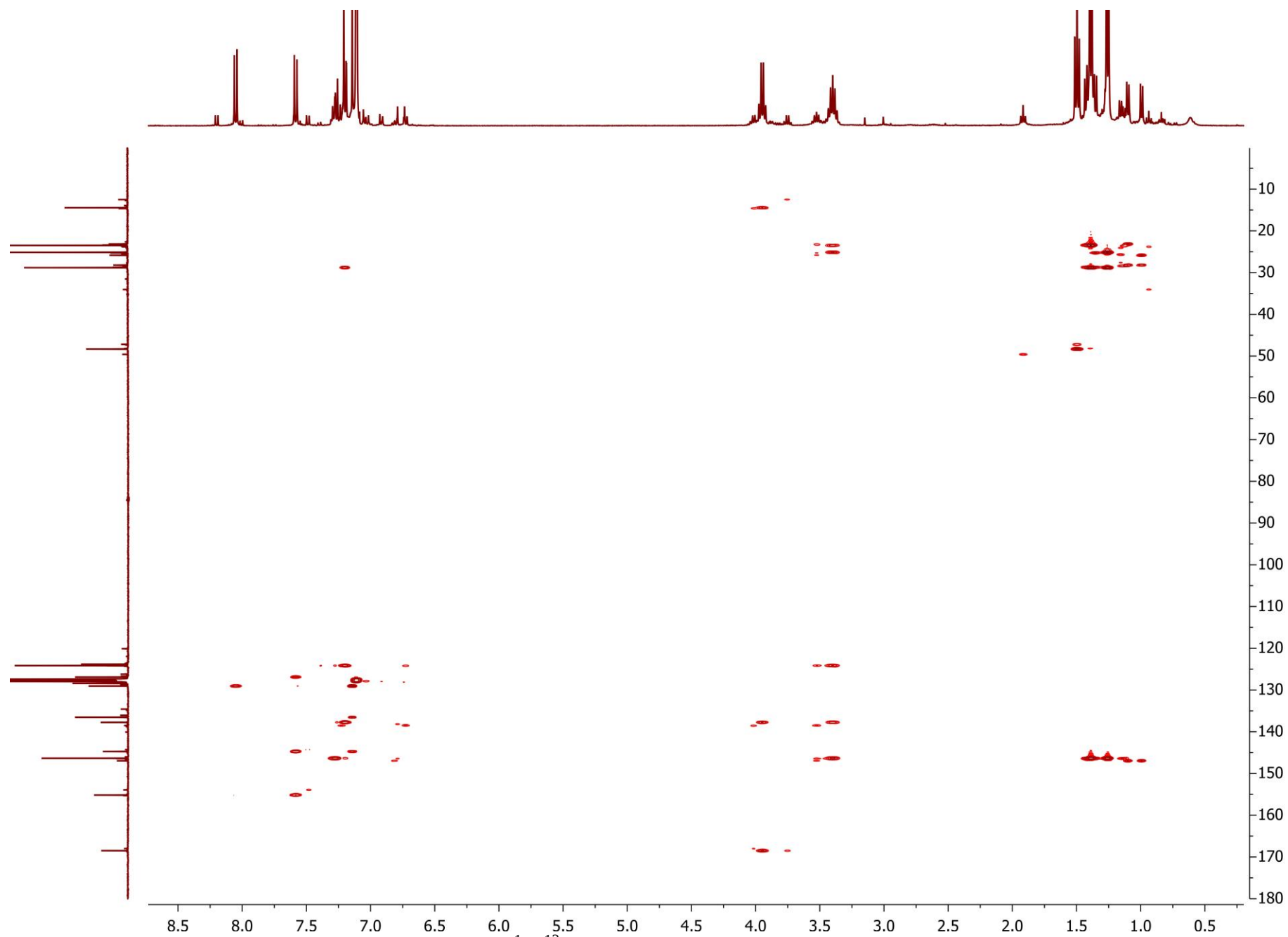


Figure S21. $^1\text{H}/^{13}\text{C}$ HMBC NMR spectrum in C_6D_6 at 25°C.

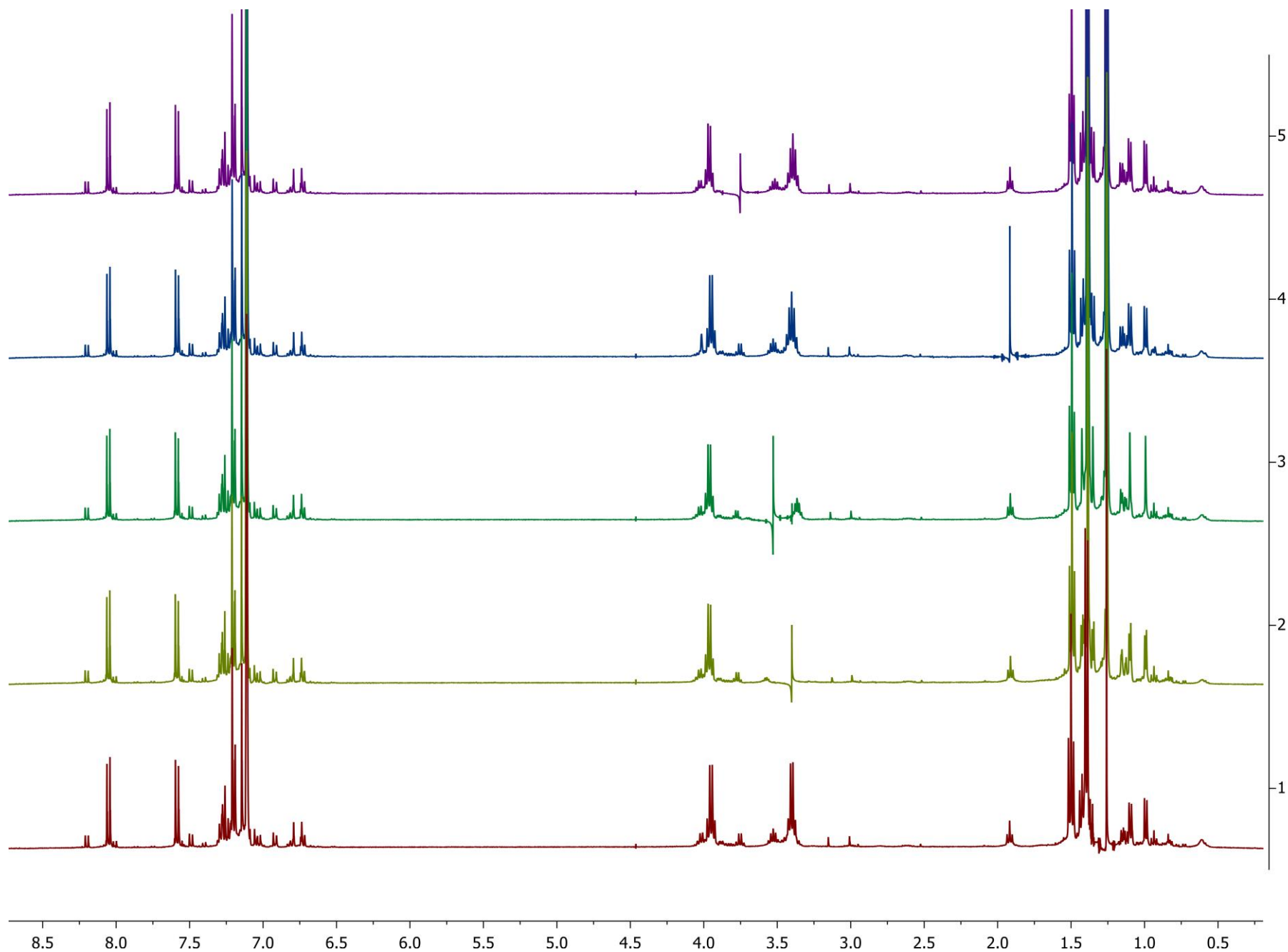


Figure S22. ^1H HOMODEC NMR spectrum in C_6D_6 at 25°C.

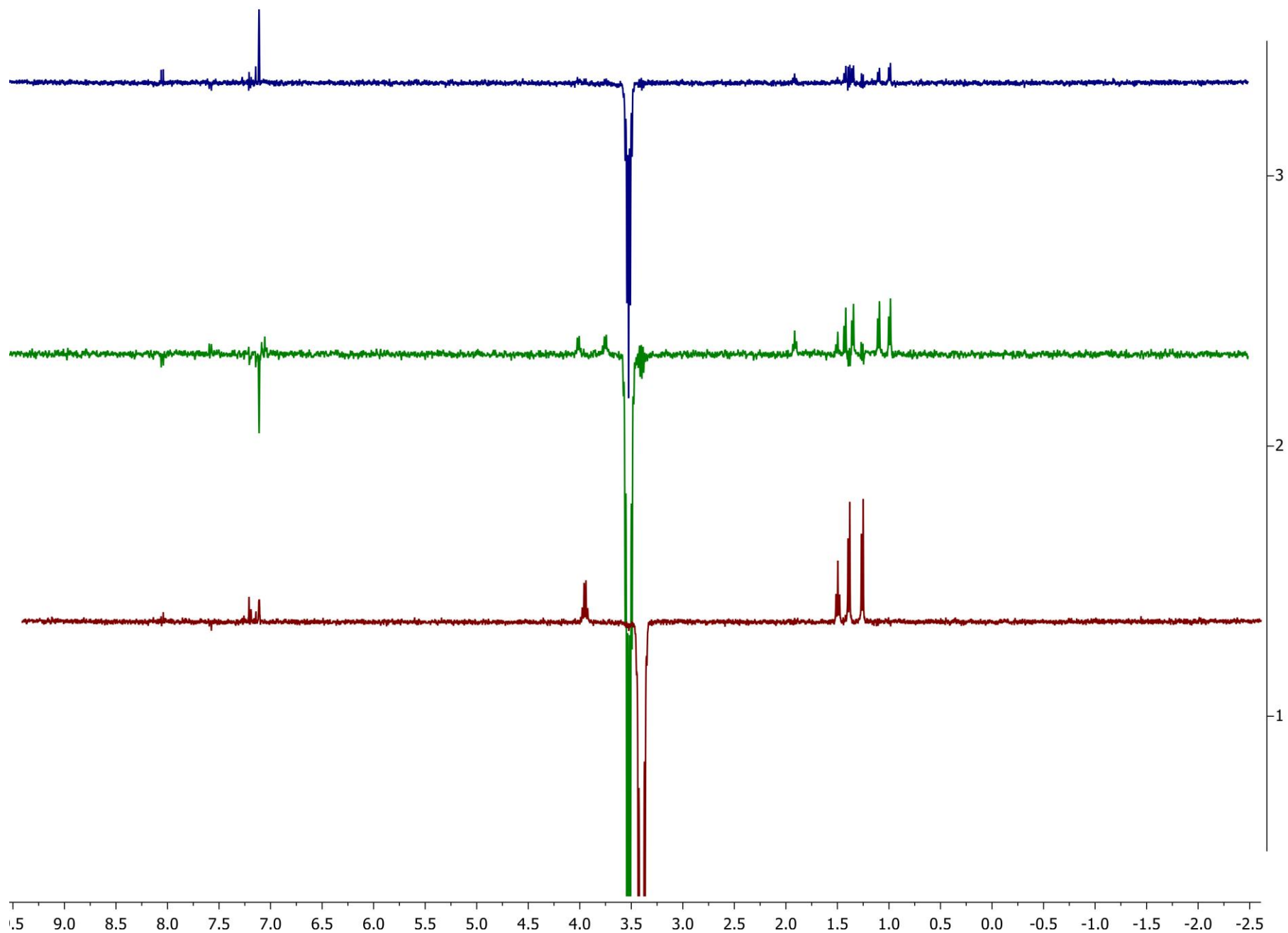


Figure S23. ^1H NOESY NMR spectrum in C_6D_6 at 25°C .

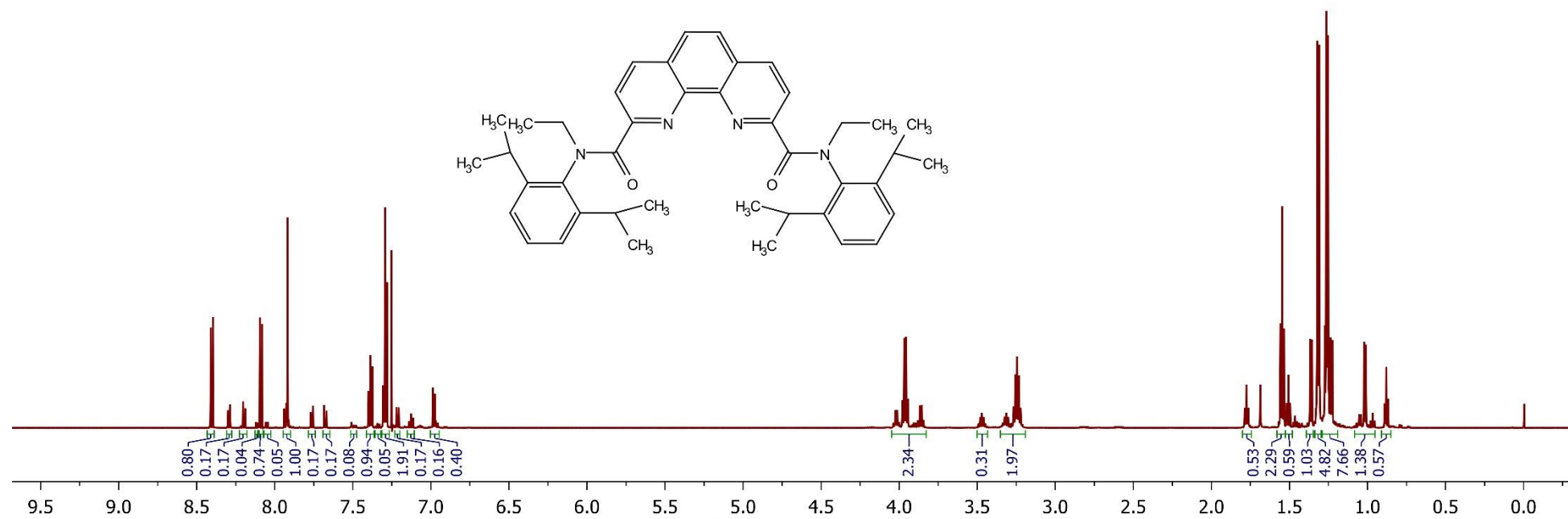


Figure S24. ^1H NMR spectrum in CDCl_3 at 25°C .

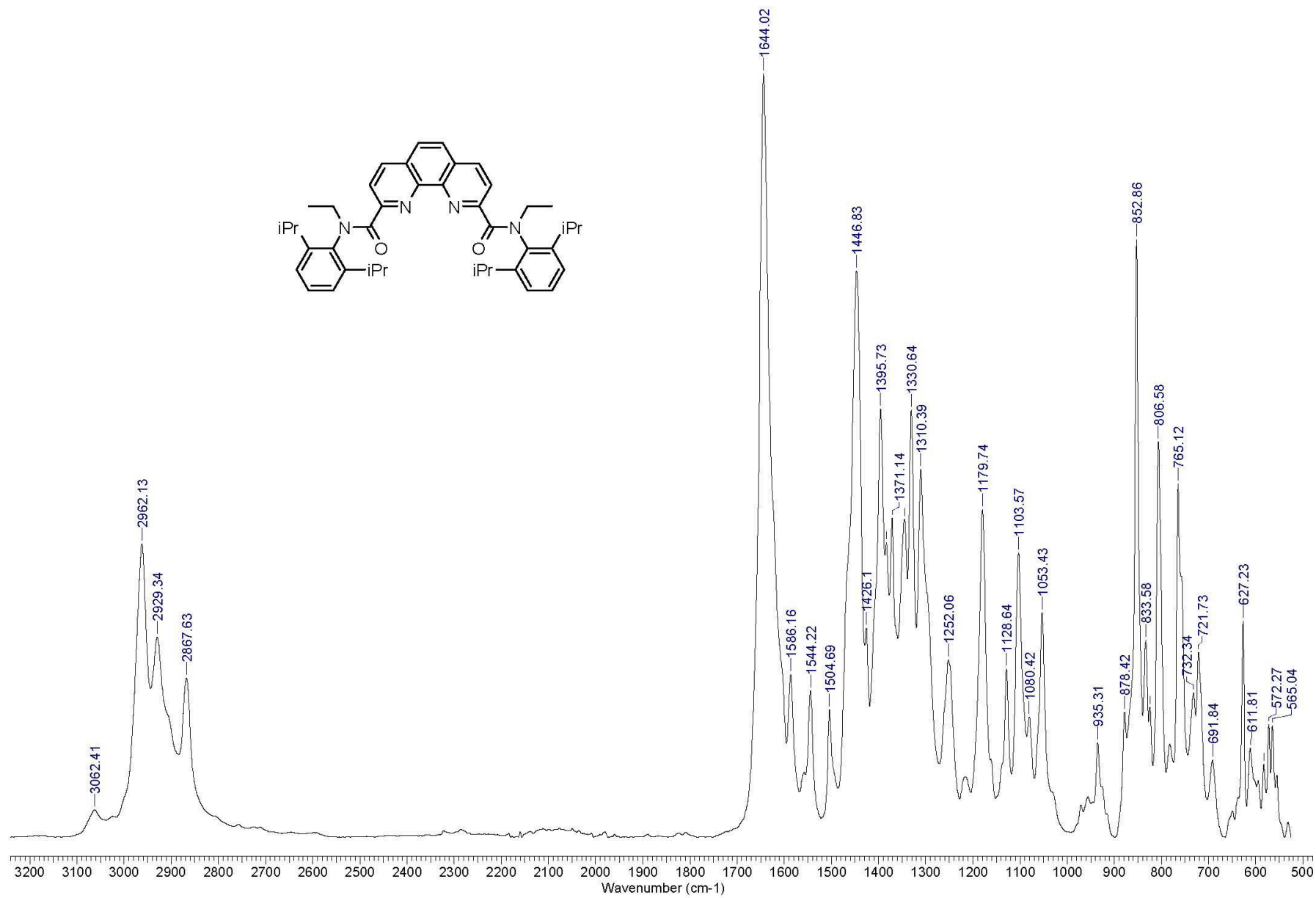


Figure S25. Solid-state IR spectrum at 25°C

N²,N⁹-bis(2,6-dimethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide lanthanum trinitrate L1•La(NO₃)₃

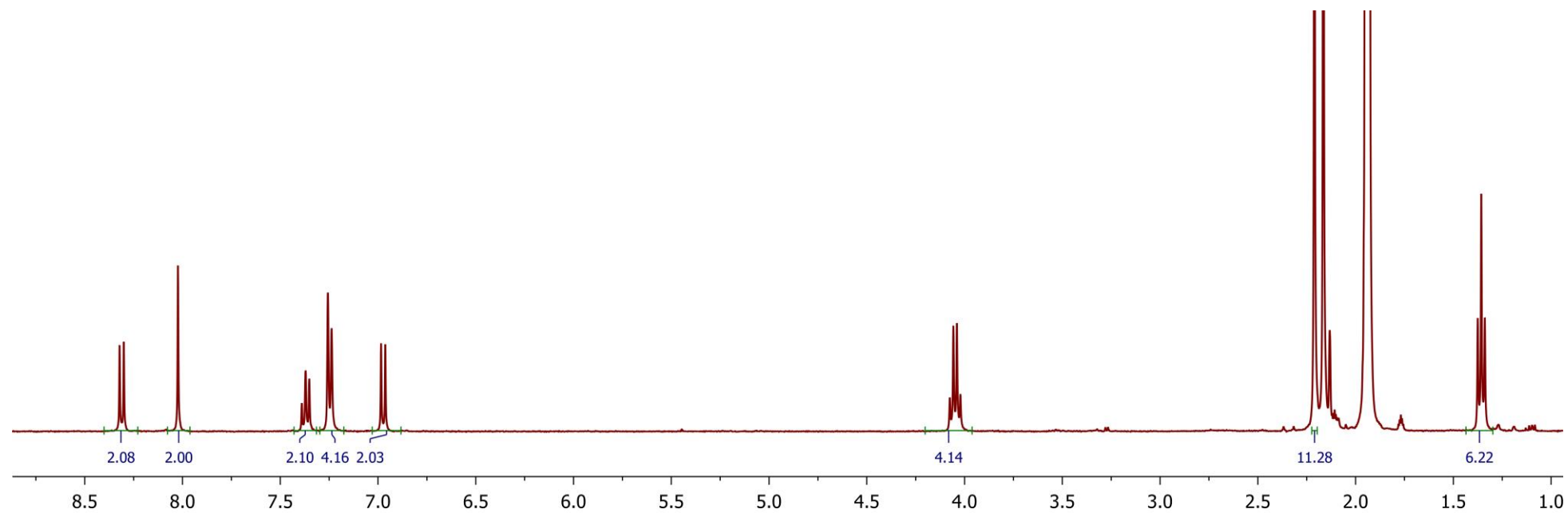


Figure S26. ¹H NMR spectrum in CD₃CN at 25°C.

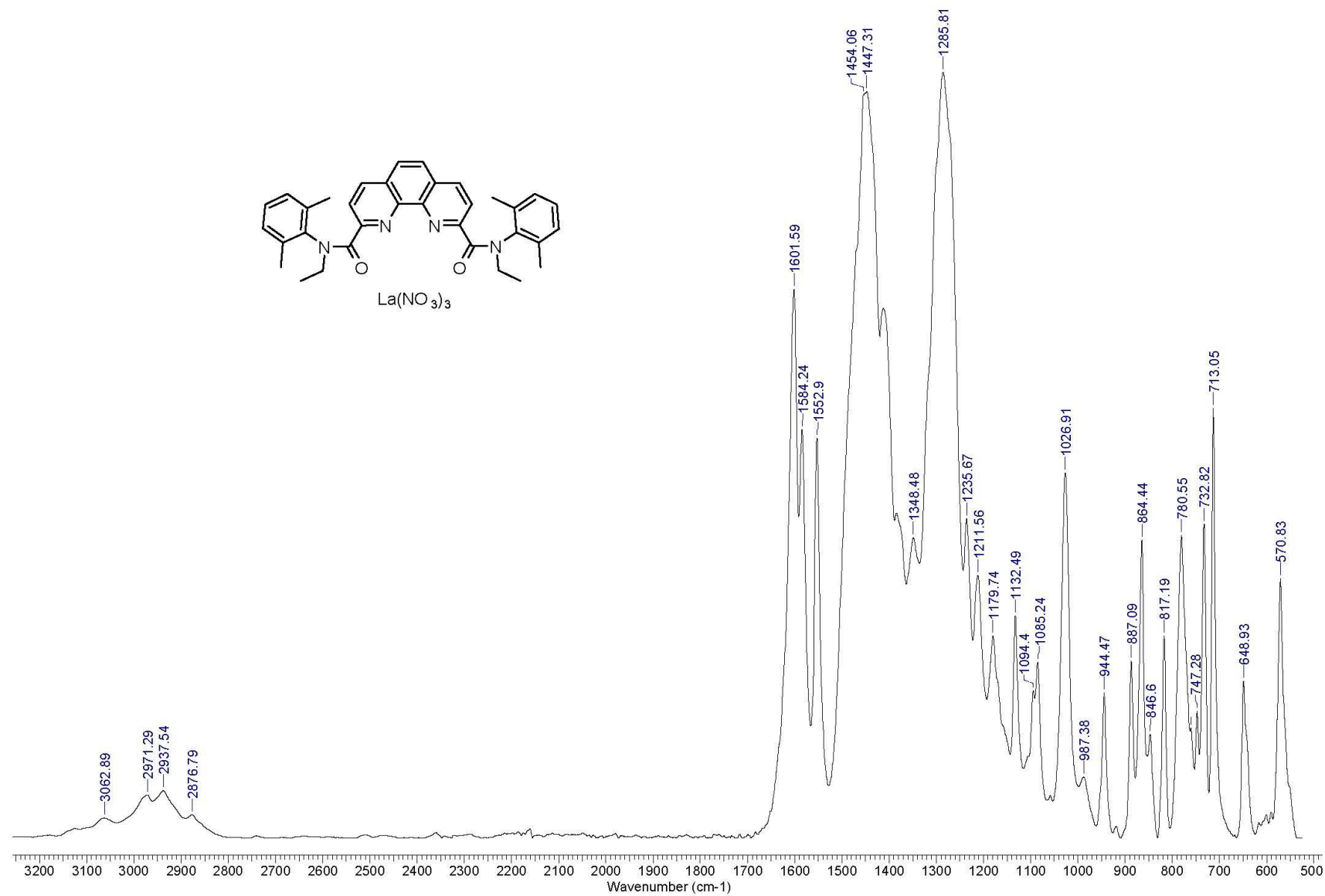


Figure S27. Solid-state IR spectrum at 25°C

N²,N⁹-bis(2,6-dimethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide lutetium trinitrate L1•Lu(NO₃)₃

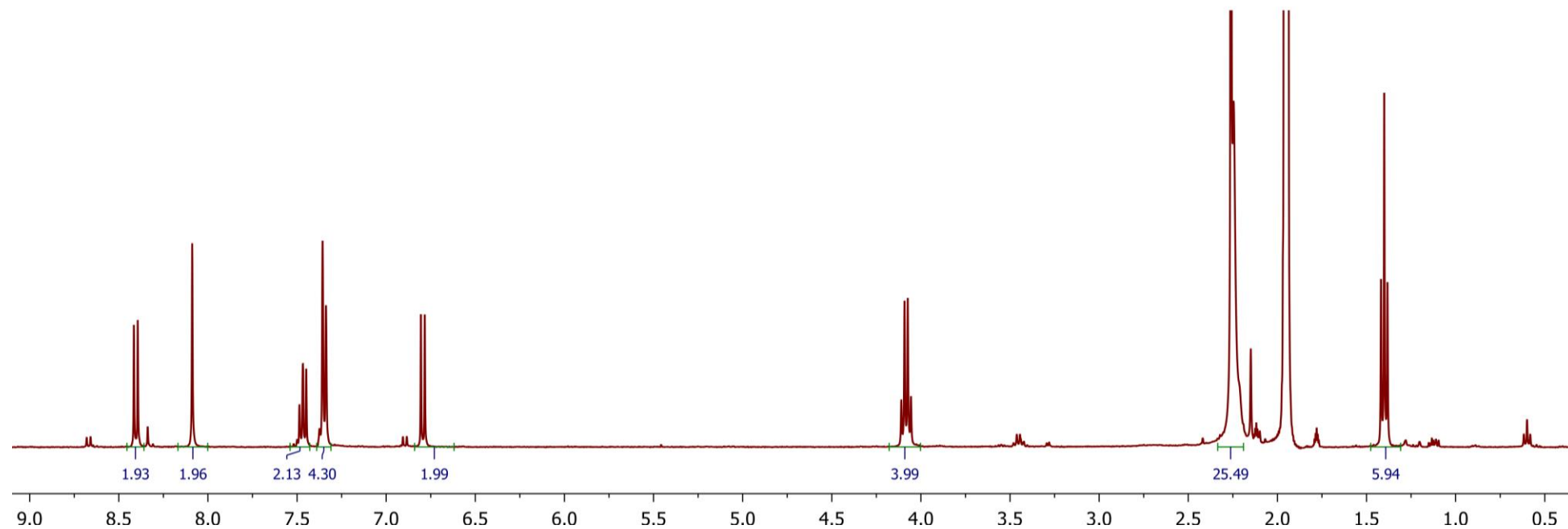


Figure S28. ¹H NMR spectrum in CD₃CN at 25°C.

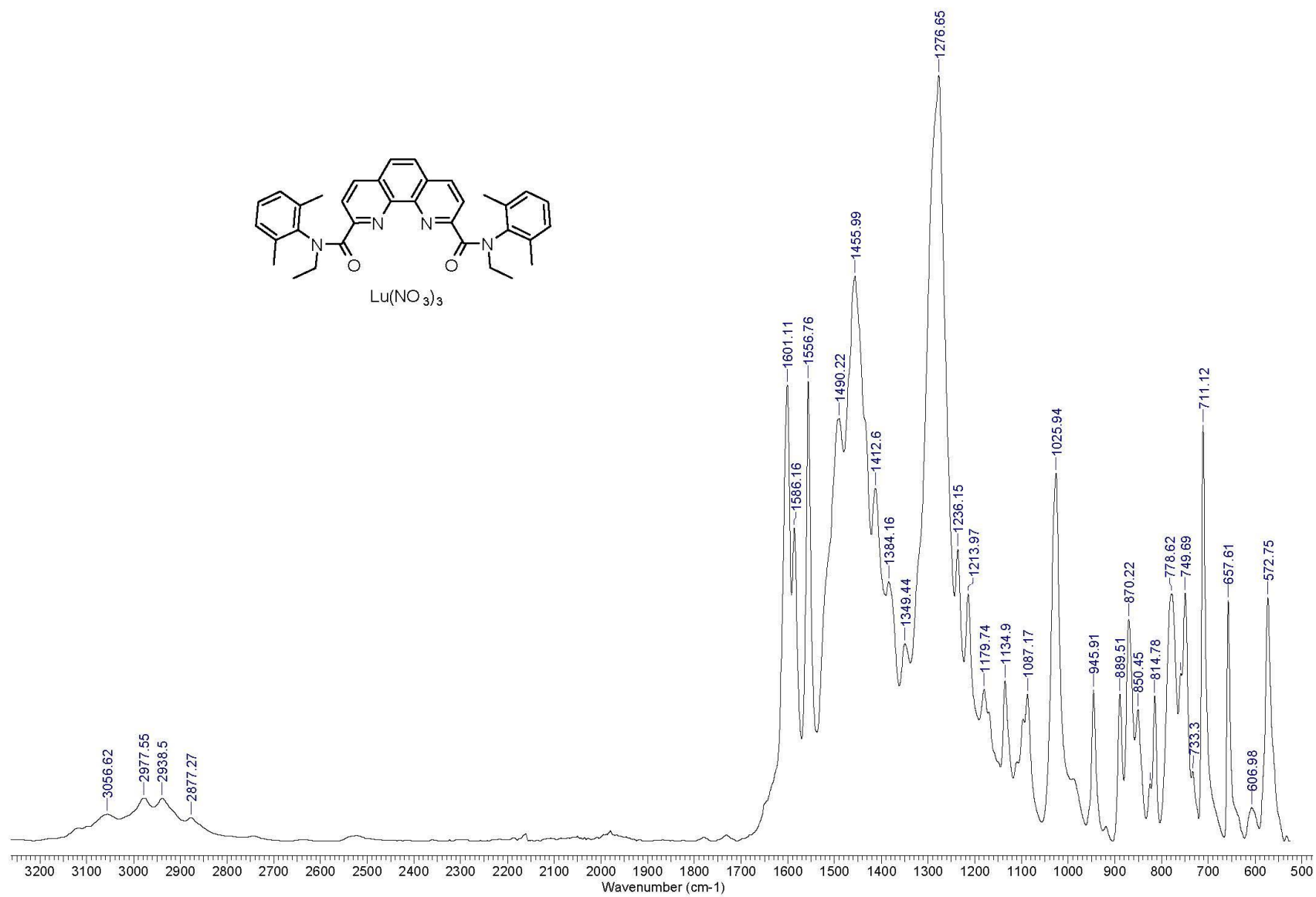


Figure S29. Solid-state IR spectrum at 25°C

N²,N⁹-bis(2,6-diethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide lanthanum trinitrate L2•La(NO₃)₃.

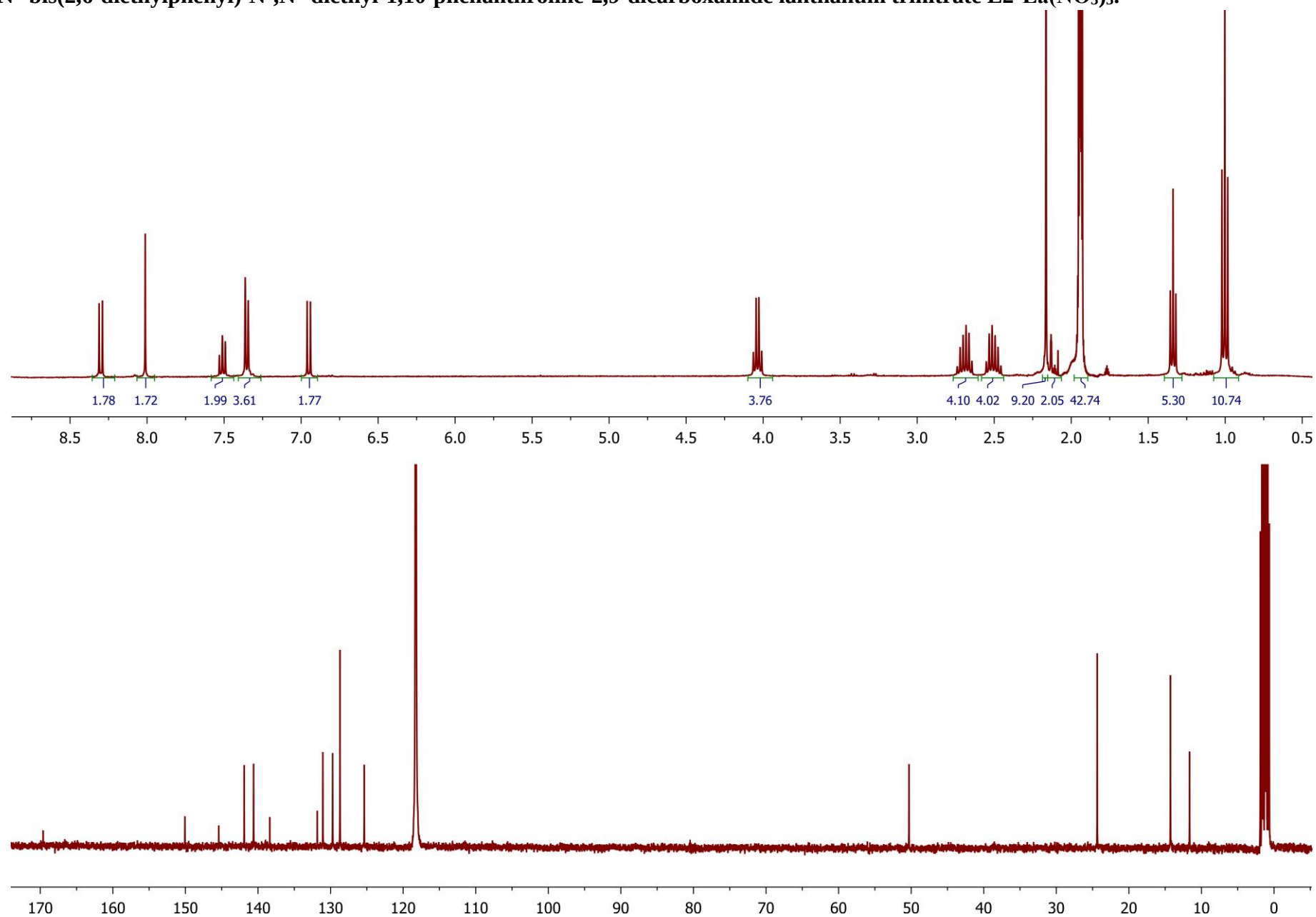


Figure S30. ¹H and ¹³C NMR spectra in CD₃CN at 25°C.

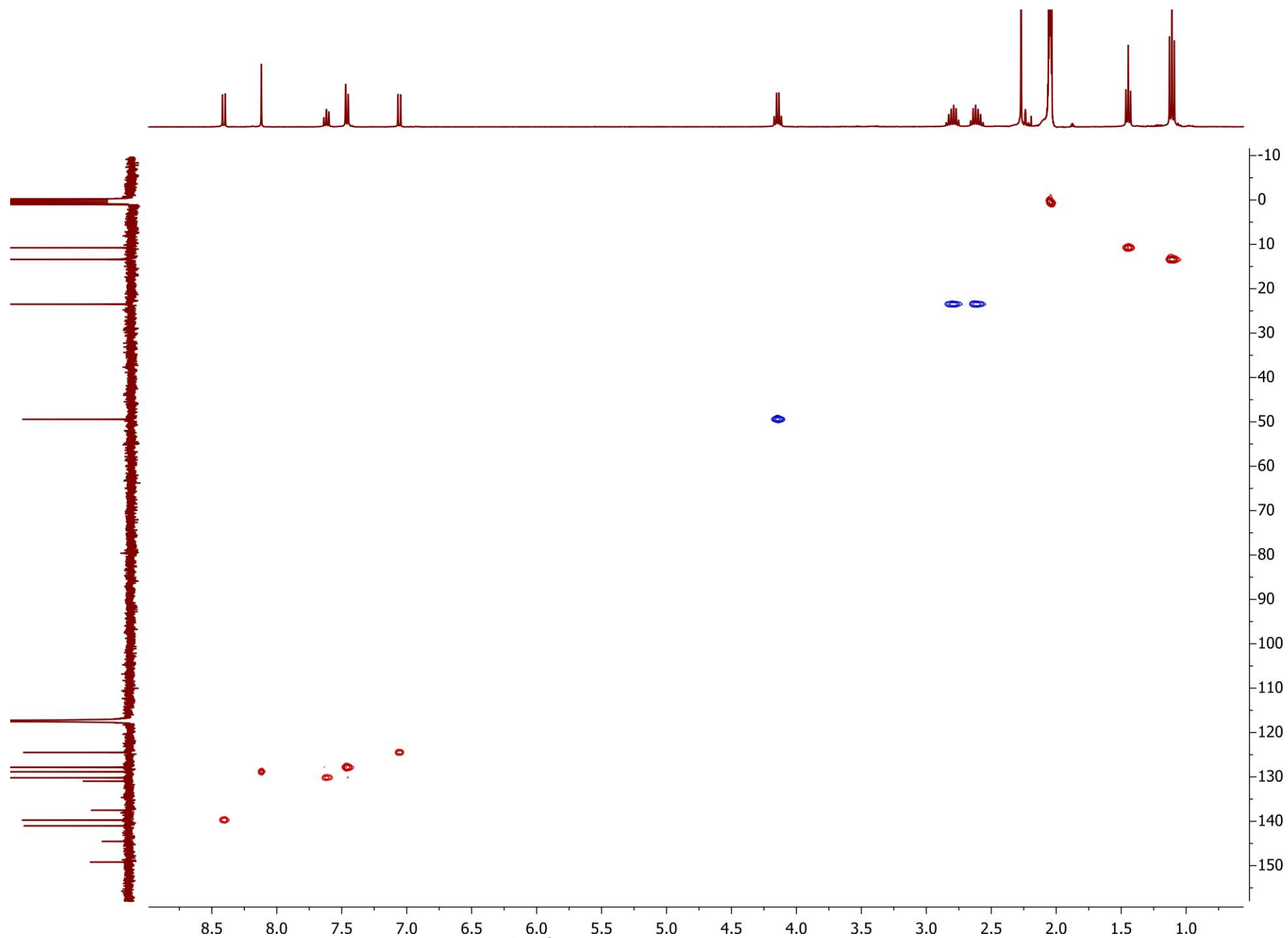


Figure S31. $^1\text{H}/^{13}\text{C}$ HSQC NMR spectrum in CD_3CN at 25°C .

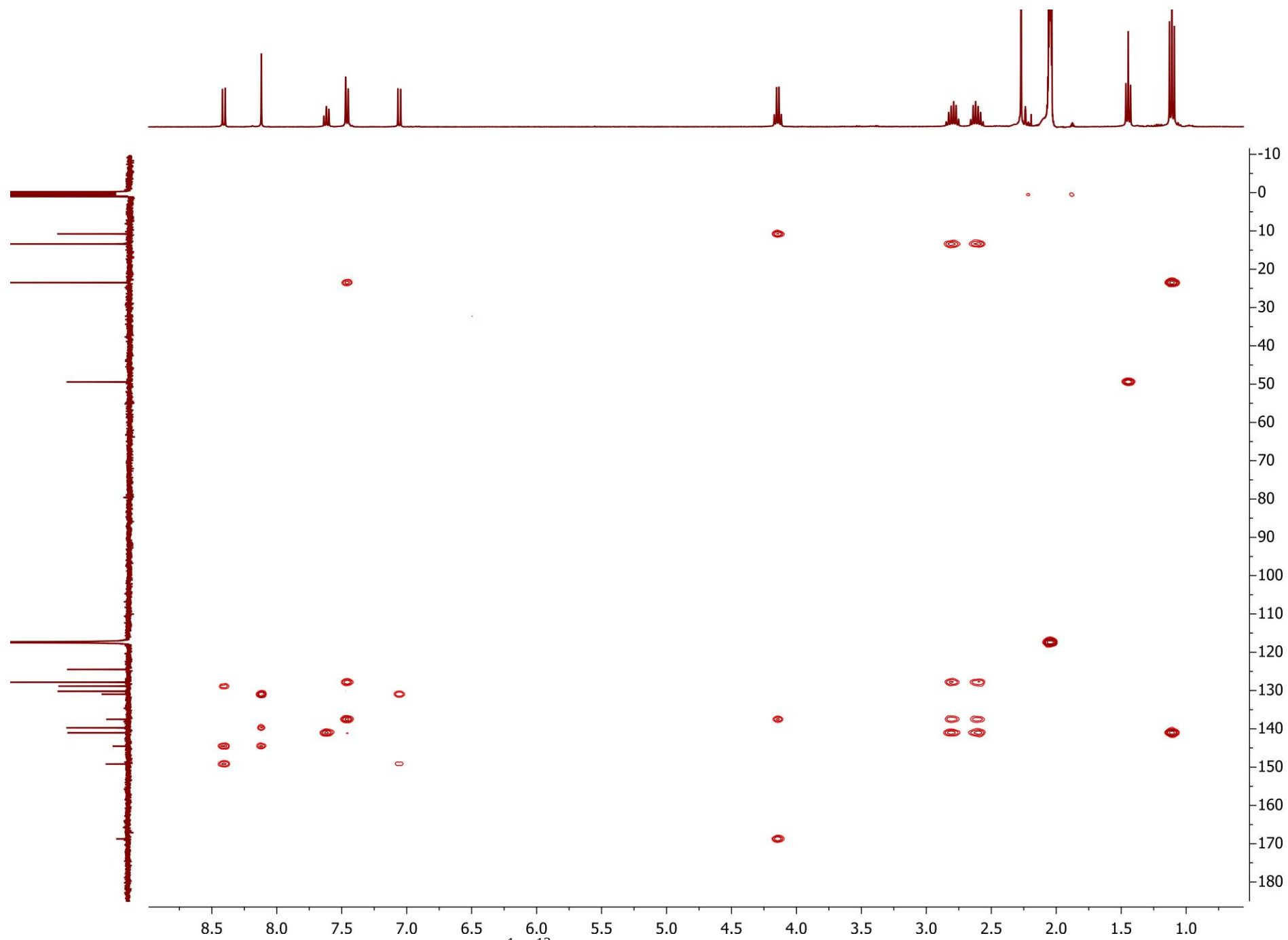


Figure S32. $^1\text{H}/^{13}\text{C}$ HMBC NMR spectrum in CD_3CN at 25°C.

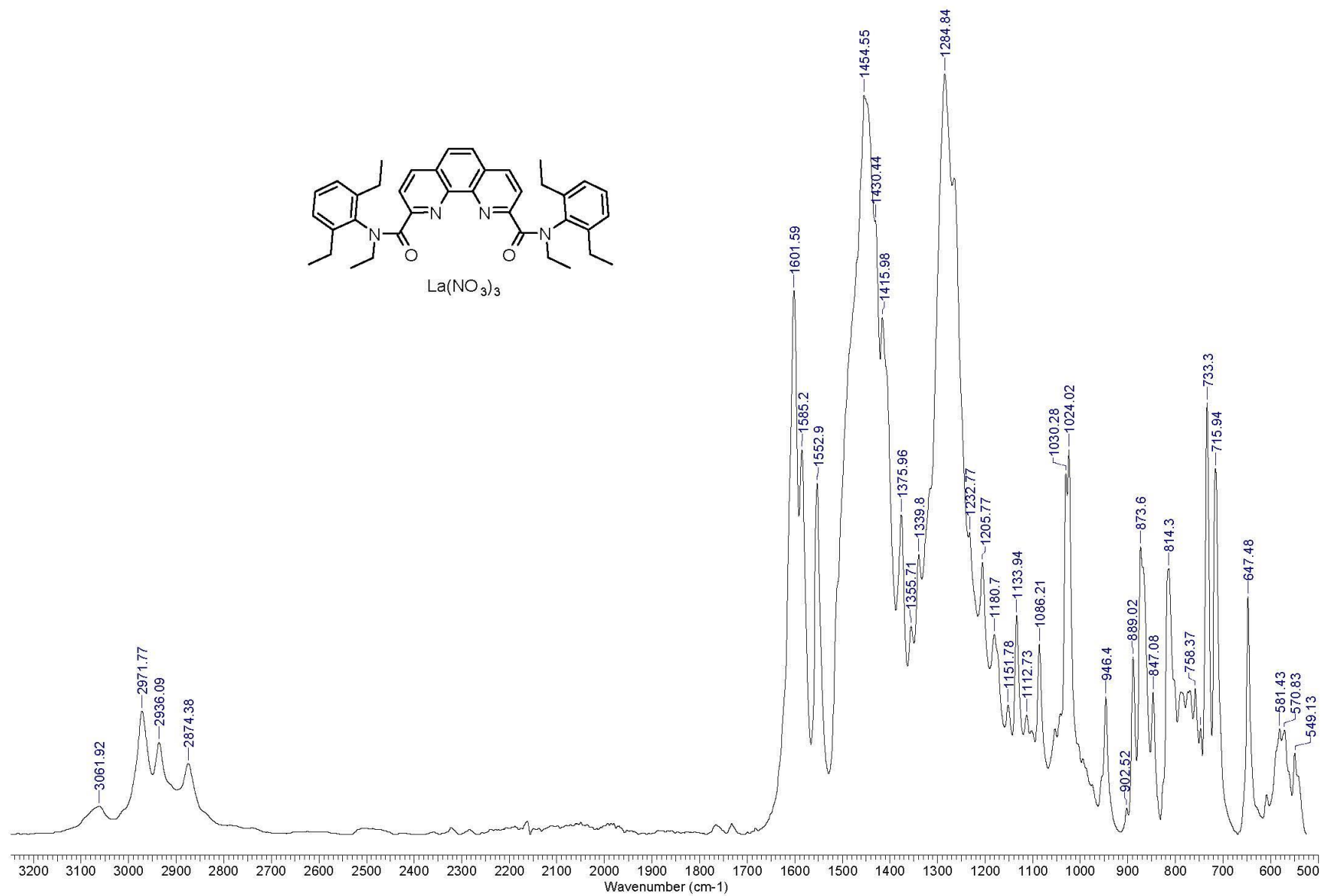


Figure S33. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,6-diethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide lutetium trinitrate $L2 \cdot Lu(NO_3)_3$

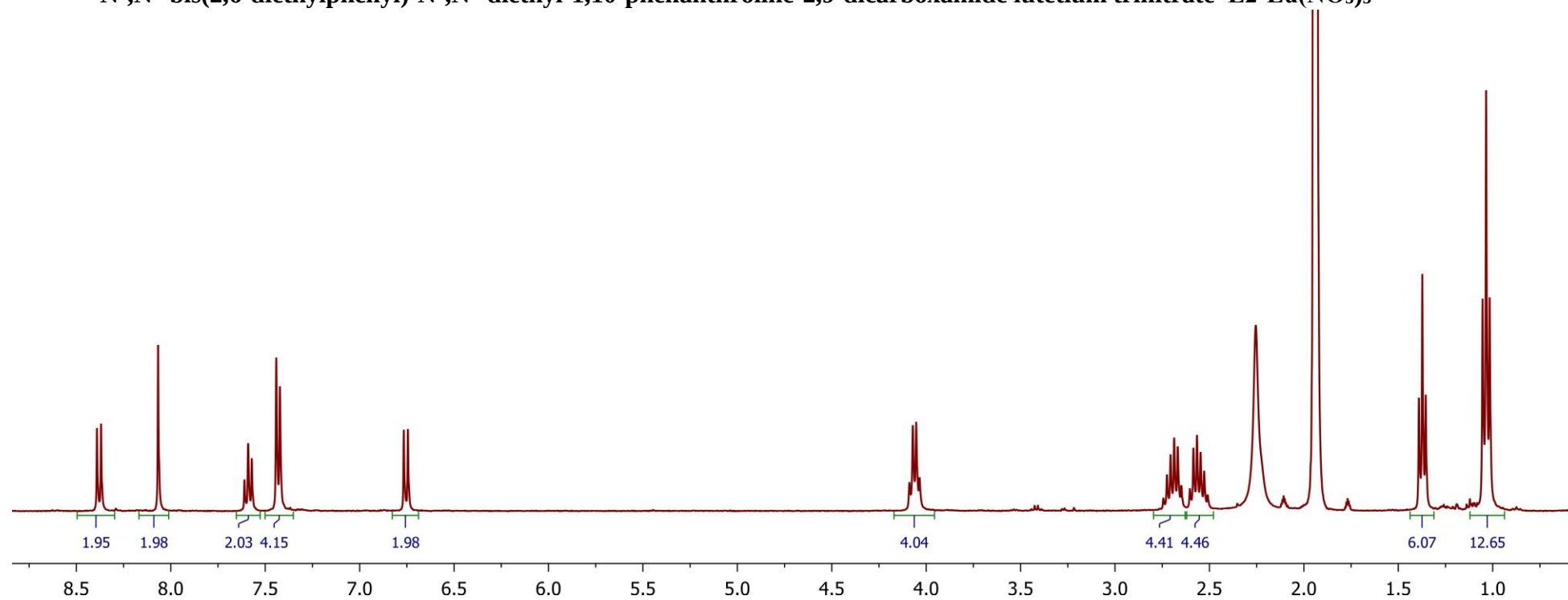


Figure S34. 1H NMR spectrum in CD_3CN at $25^\circ C$.

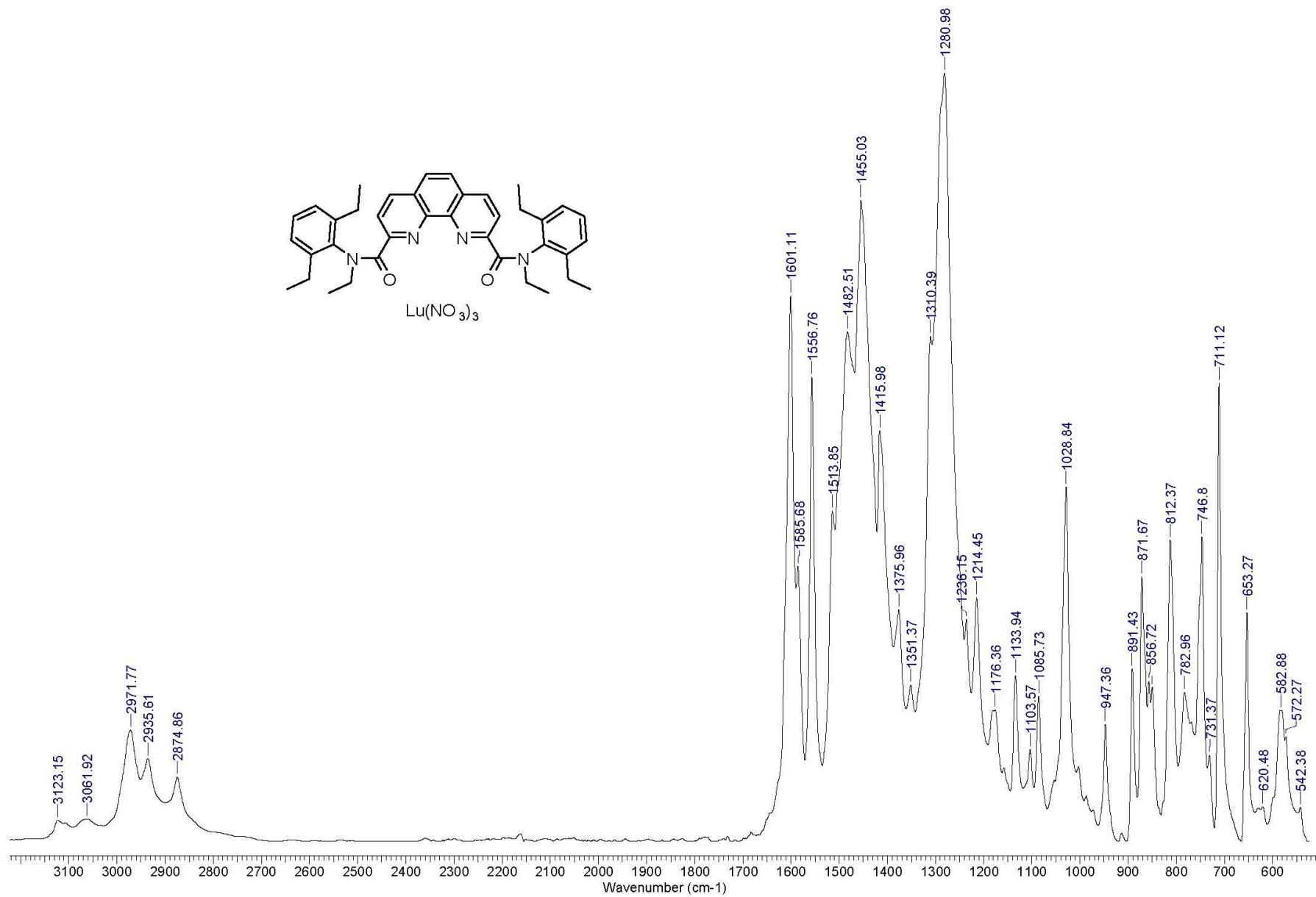


Figure S35. Solid-state IR spectrum at 25°C.

N²,N⁹-bis(2,6-diisopropylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide lanthanum trinitrate L3•La(NO₃)₃

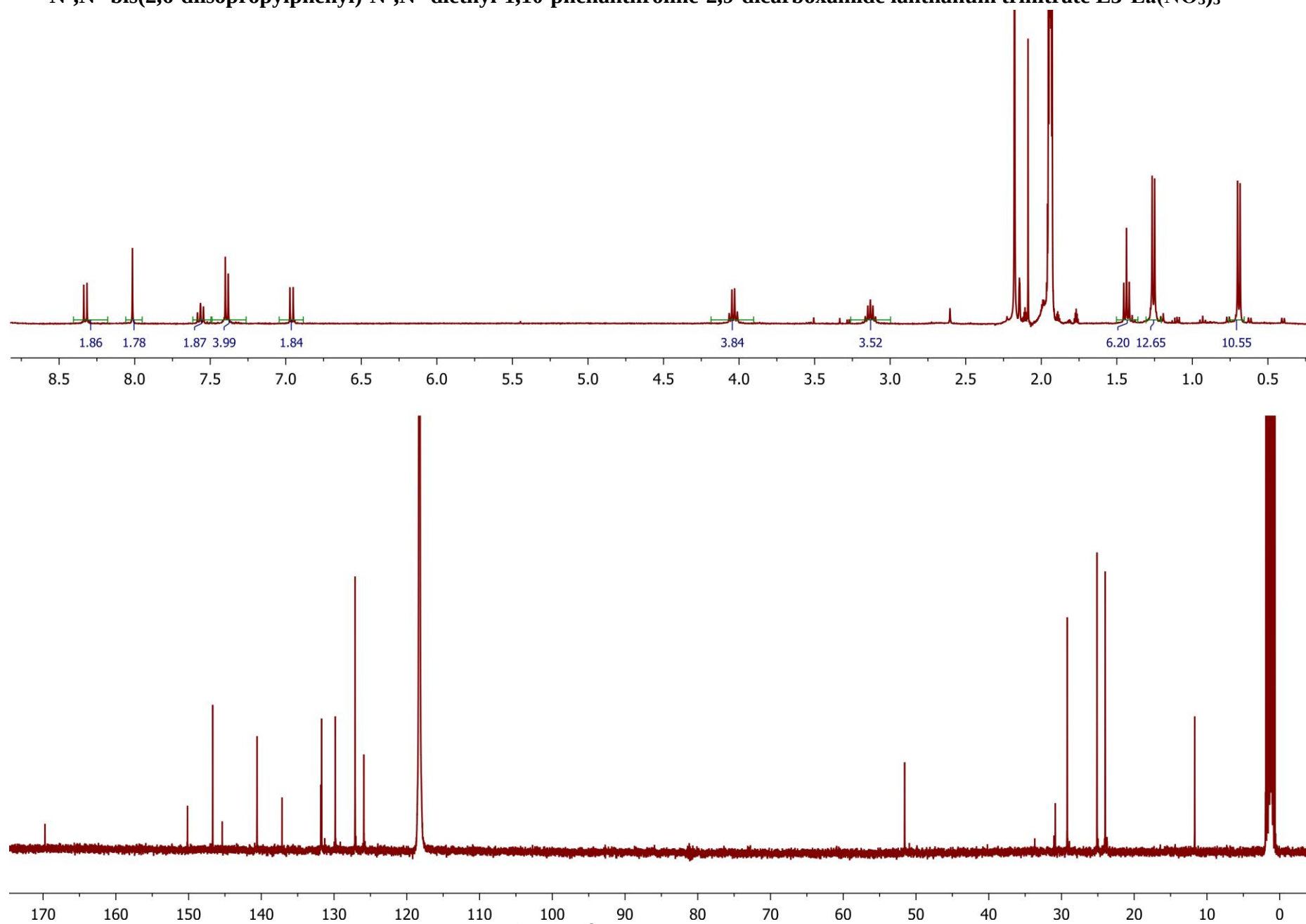


Figure S36. ¹H and ¹³C NMR spectra in CD₃CN at 25°C.

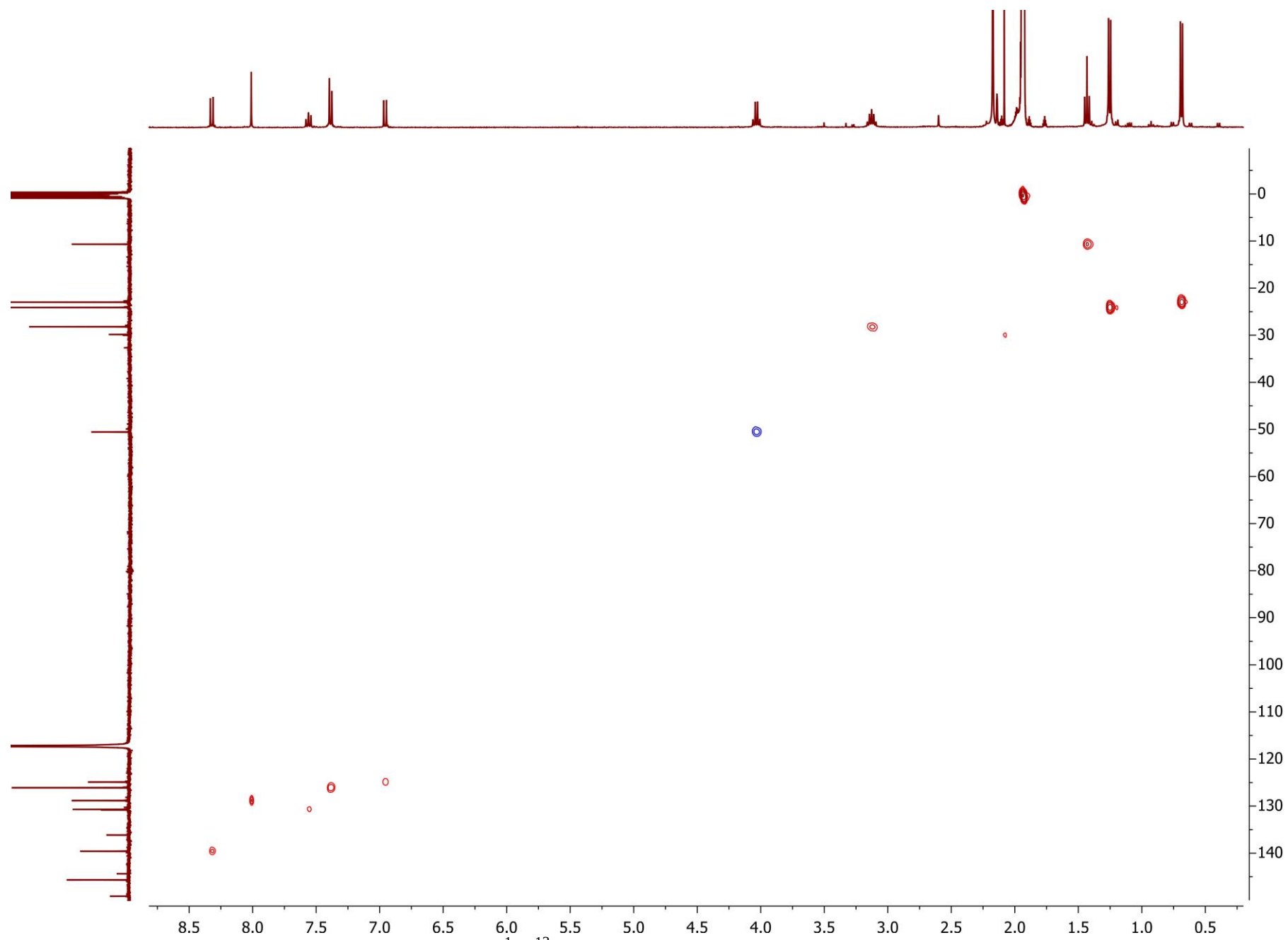


Figure S37. $^1\text{H}/^{13}\text{C}$ HSQC NMR spectrum in CD_3CN at 25°C .

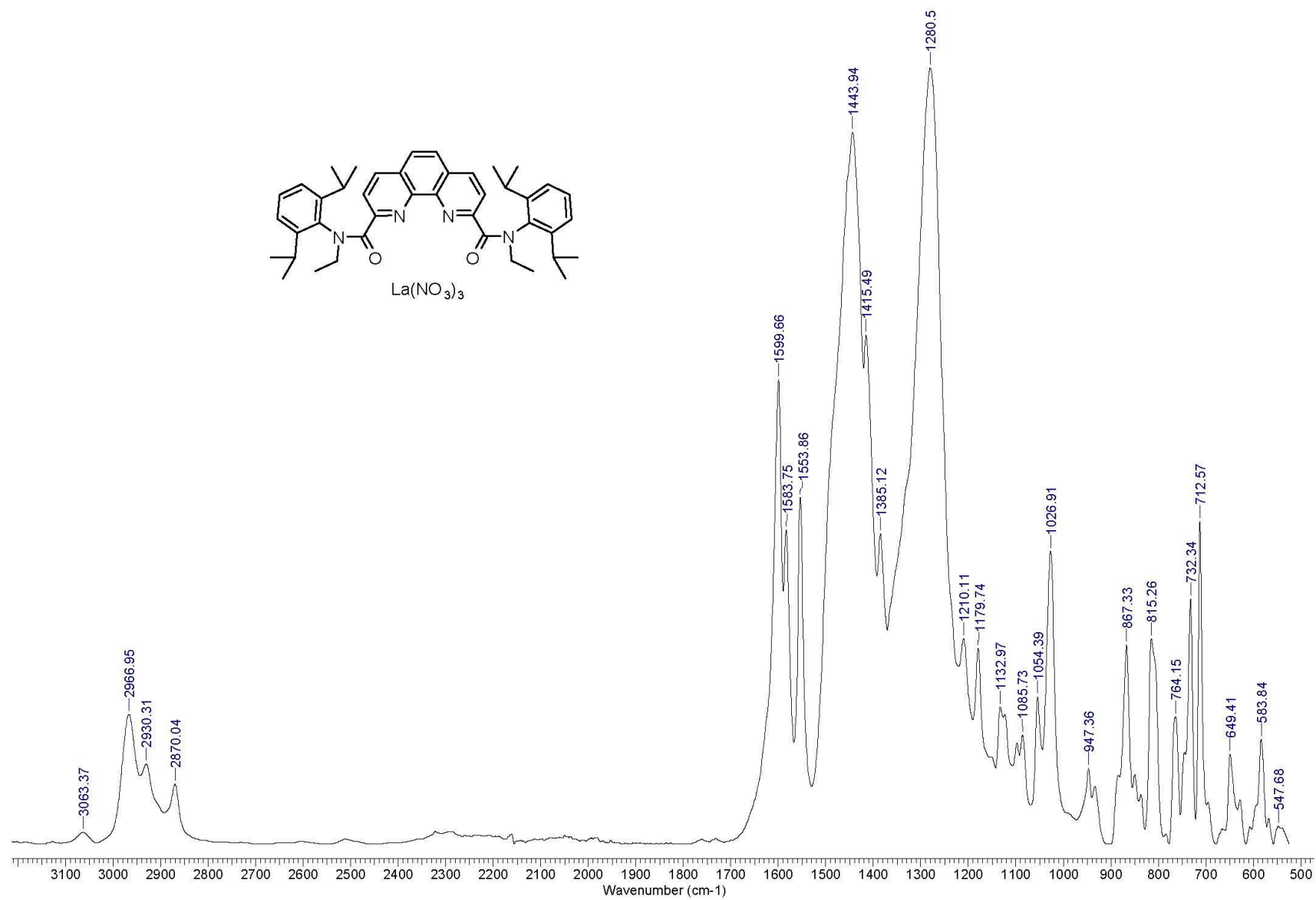


Figure S38. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,6-diisopropylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide lutetium trinitrate $L3 \cdot Lu(NO_3)_3$

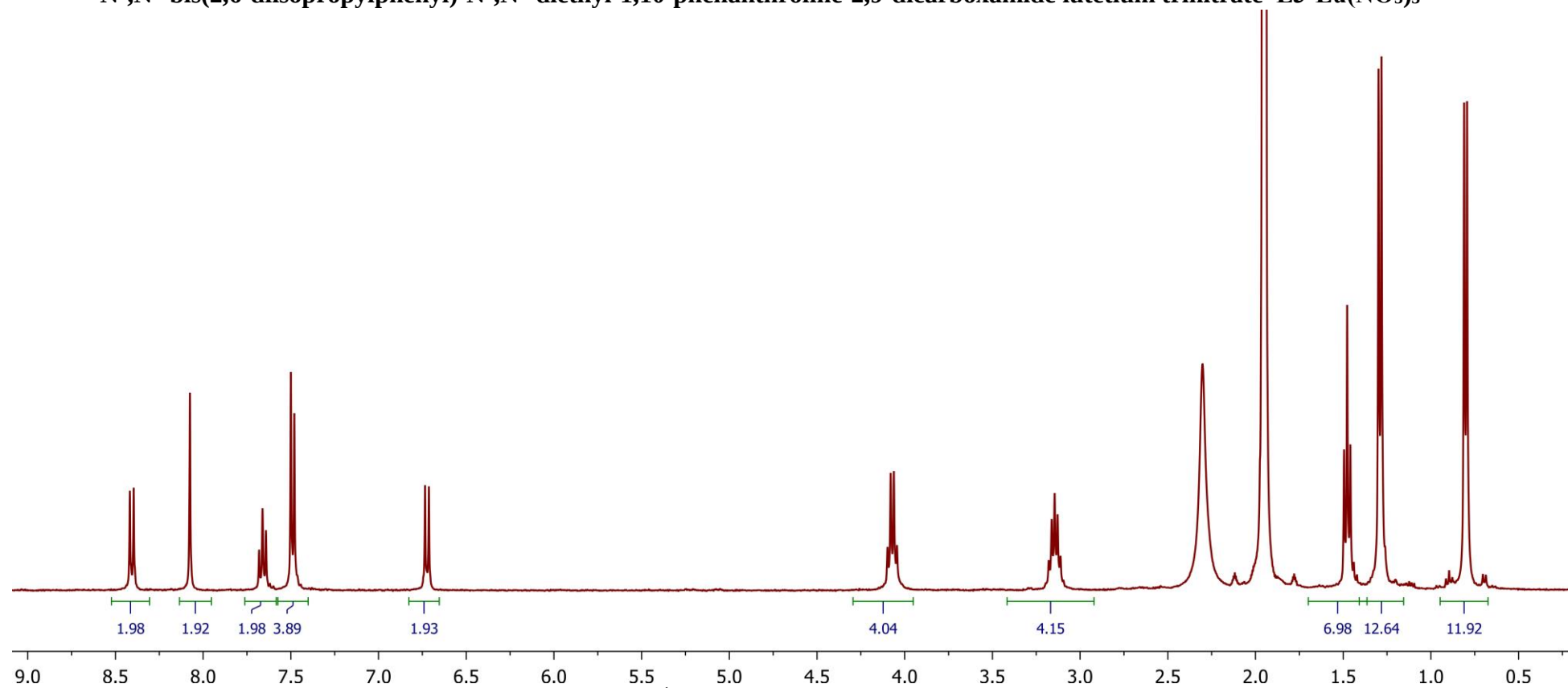


Figure S39. 1H NMR spectrum in CD_3CN at $25^\circ C$.

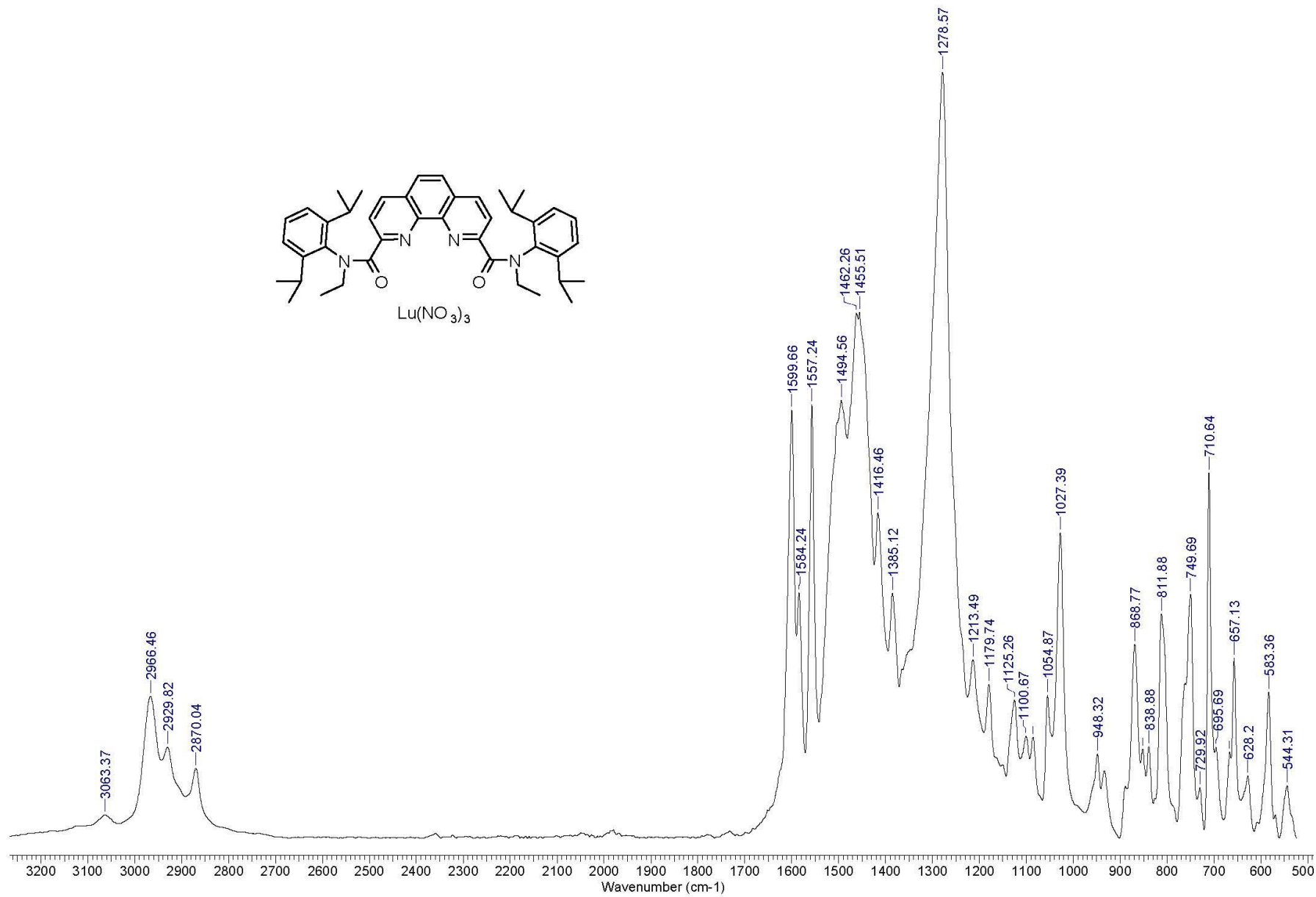


Figure S40. Solid-state IR spectrum at 25°C

3. NMR titration

N^2,N^9 -bis(2,6-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide (L1) with lanthanum trinitrate

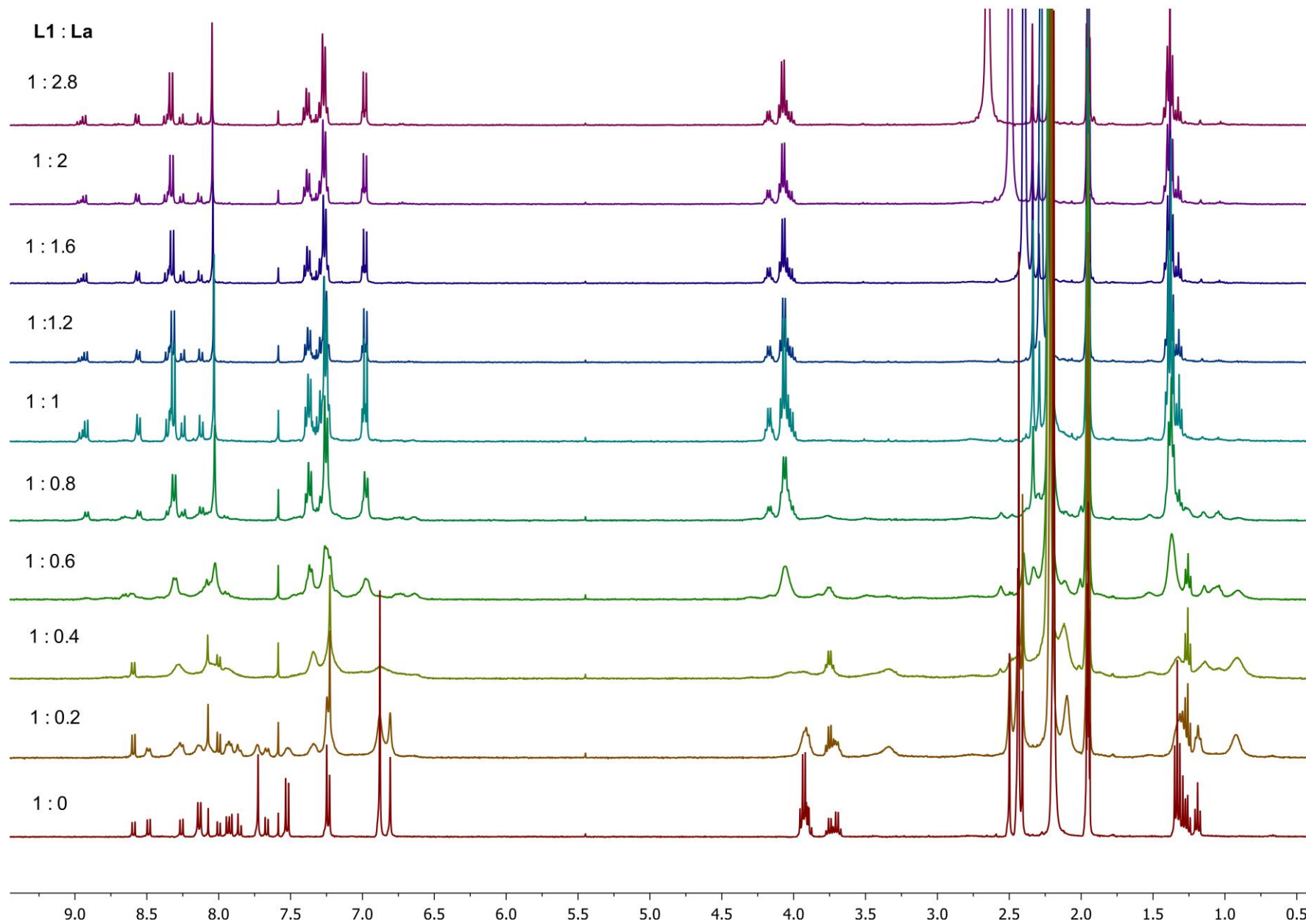


Figure S41. NMR titration of **L1** with $\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ in CD_3CN

N²,N⁹-bis(2,6-dimethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide (L1) with lutetium trinitrate

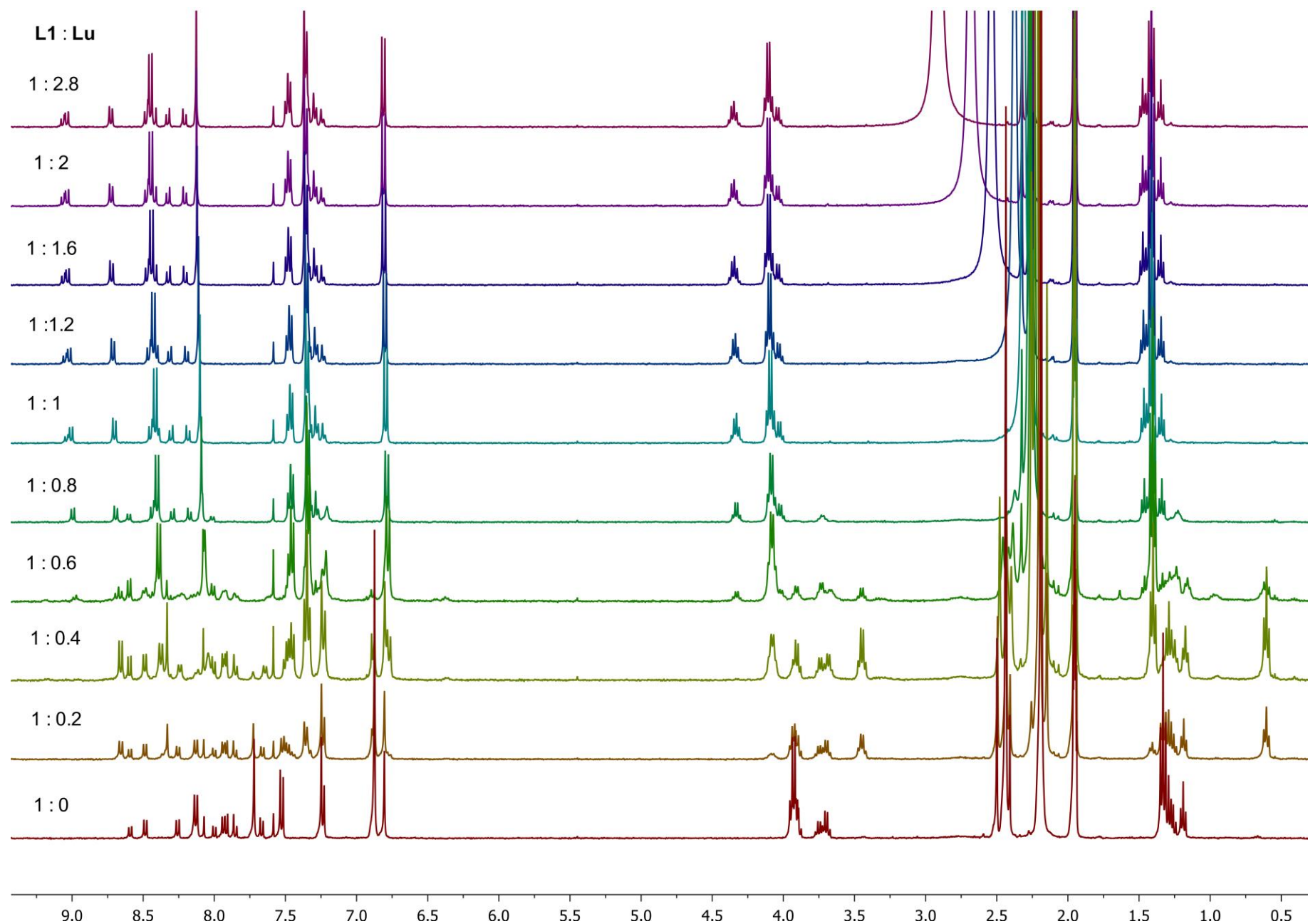


Figure S42. NMR titration of **L1** with Lu(NO₃)₃•5H₂O in CD₃CN

N²,N⁹-bis(2,6-diethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide (L2) with lanthanum trinitrate

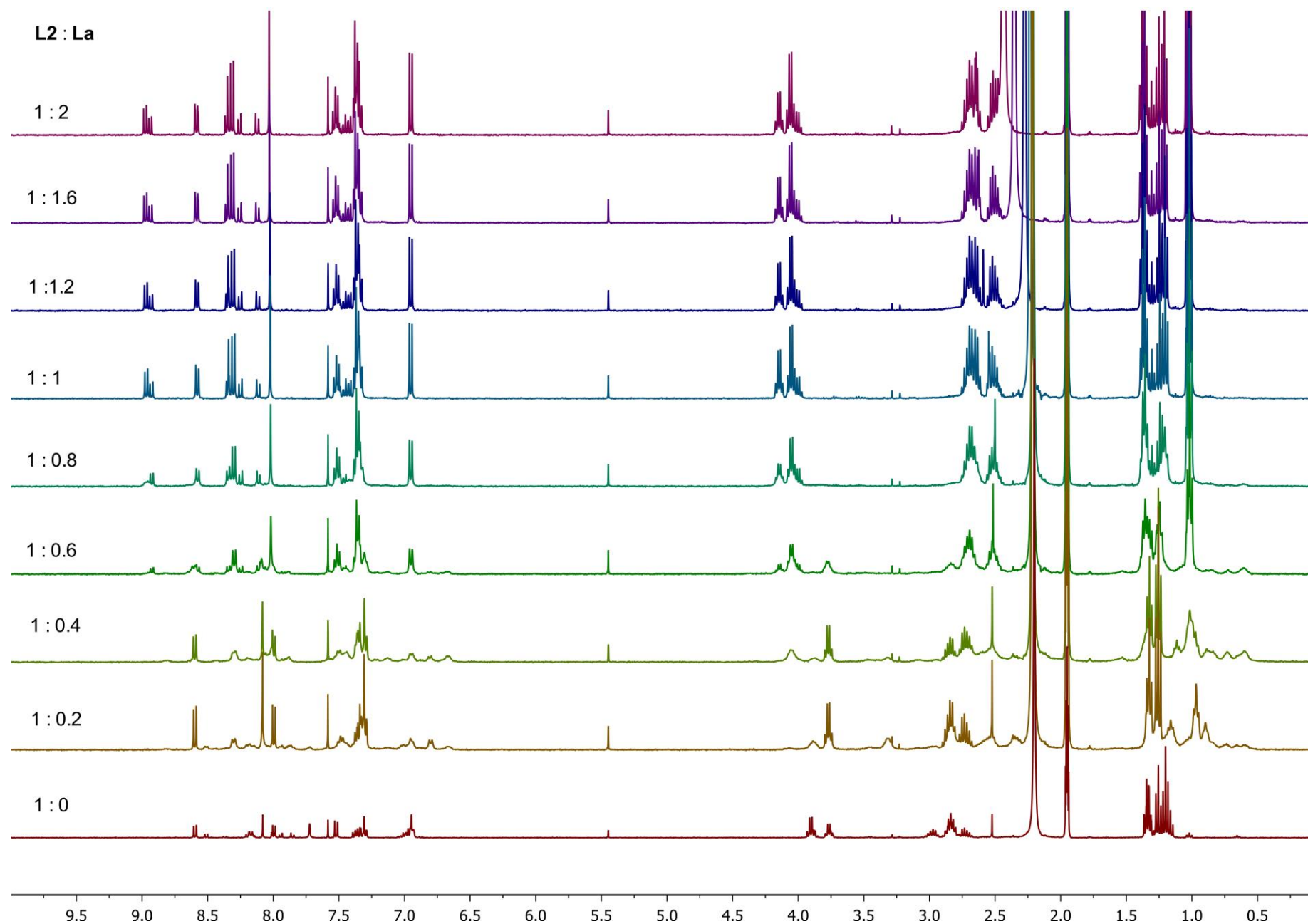


Figure S43. NMR titration of L2 with La(NO₃)₃·6H₂O in CD₃CN

N^2,N^9 -bis(2,6-diethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide (L2) with lutetium trinitrate

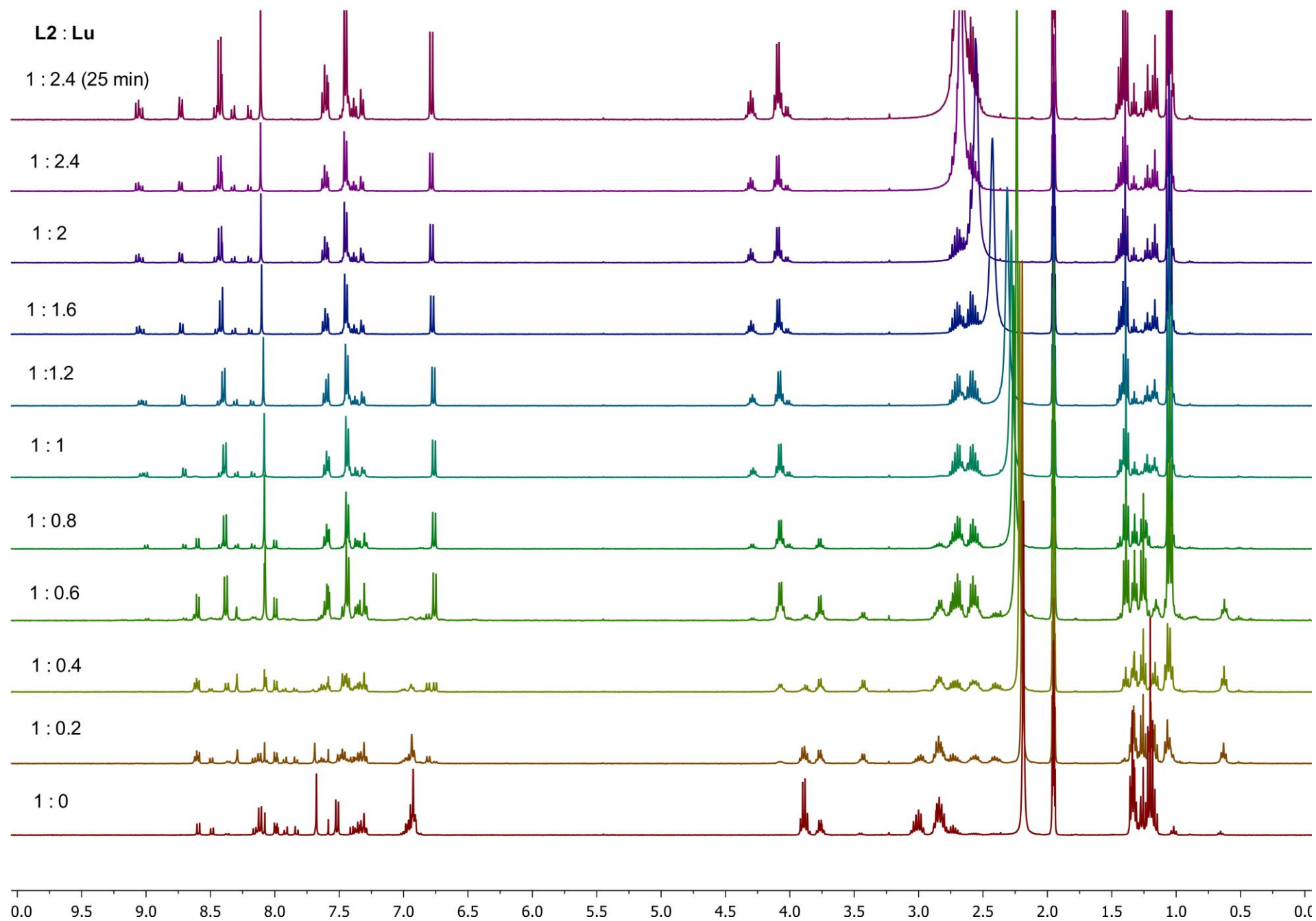


Figure S44. NMR titration of L2 with $\text{Lu}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$ in CD_3CN

N²,N⁹-bis(2,6-diisopropylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide (L3) with lanthanum trinitrate

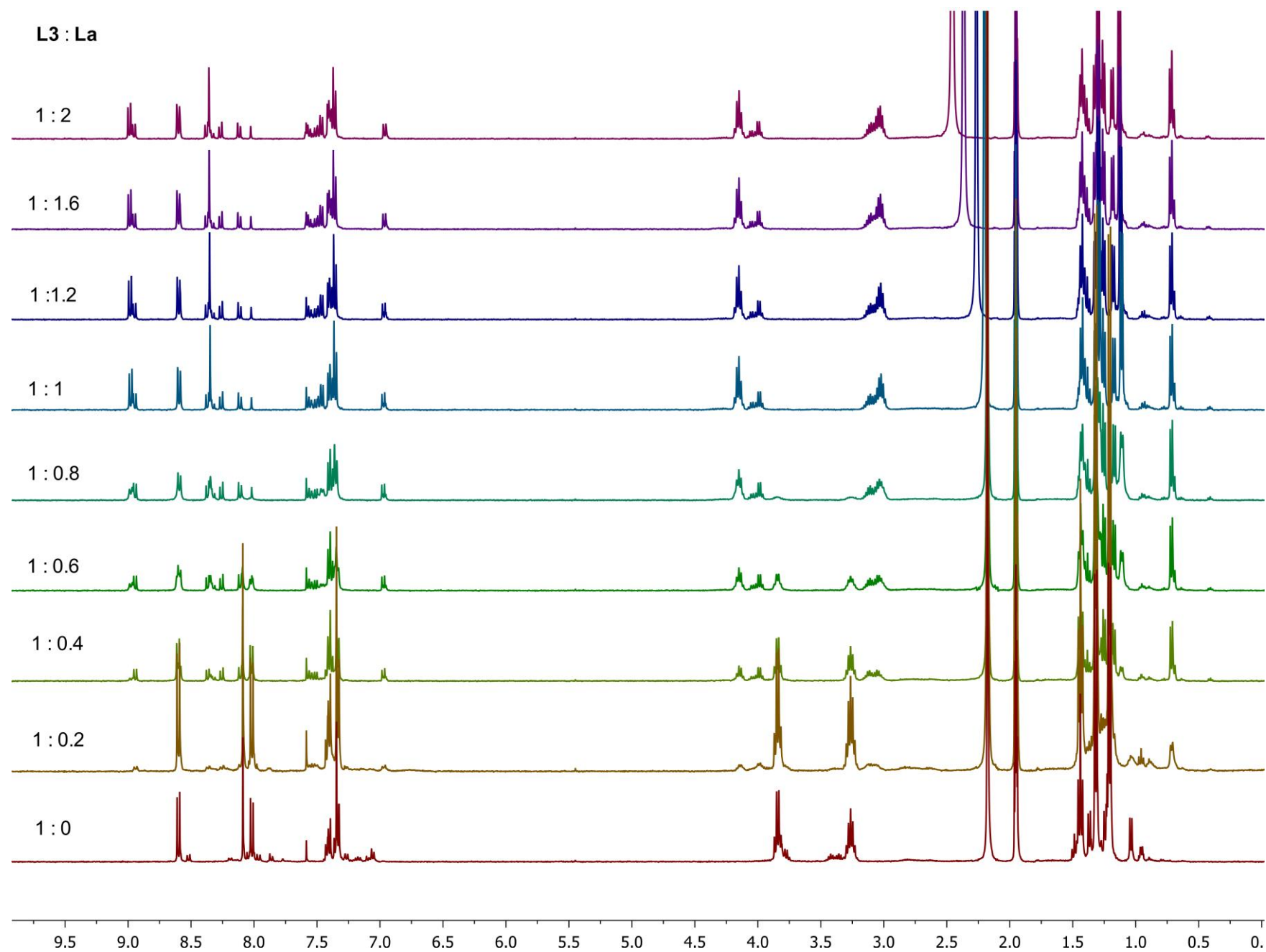


Figure S45. NMR titration of **L3** with $\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ in CD_3CN

N²,N⁹-bis(2,6-diisopropylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide (L3) with lutetium trinitrate

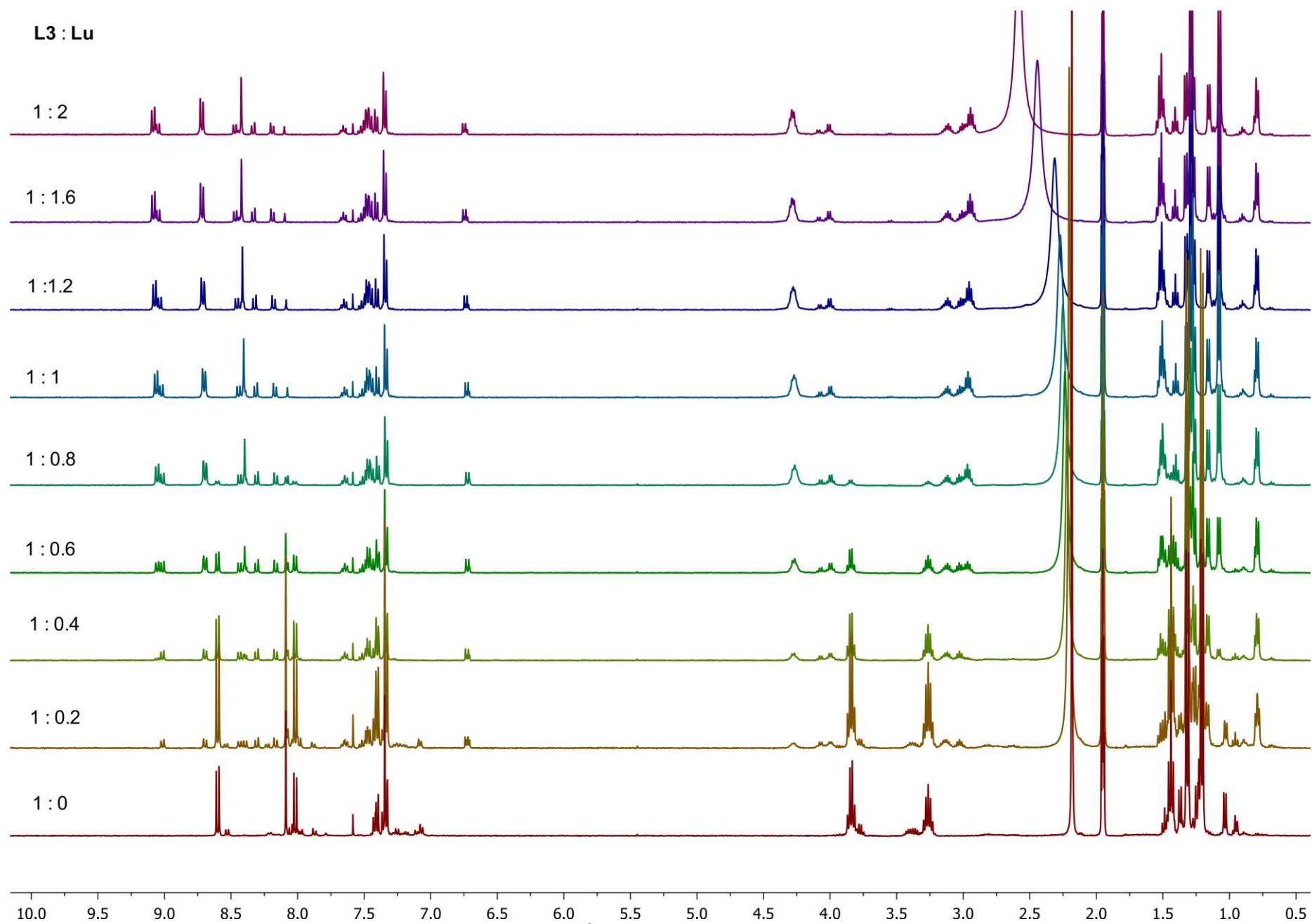


Figure S46. NMR titration of L3 with Lu(NO₃)₃•5H₂O in CD₃CN

4. X-ray analysis

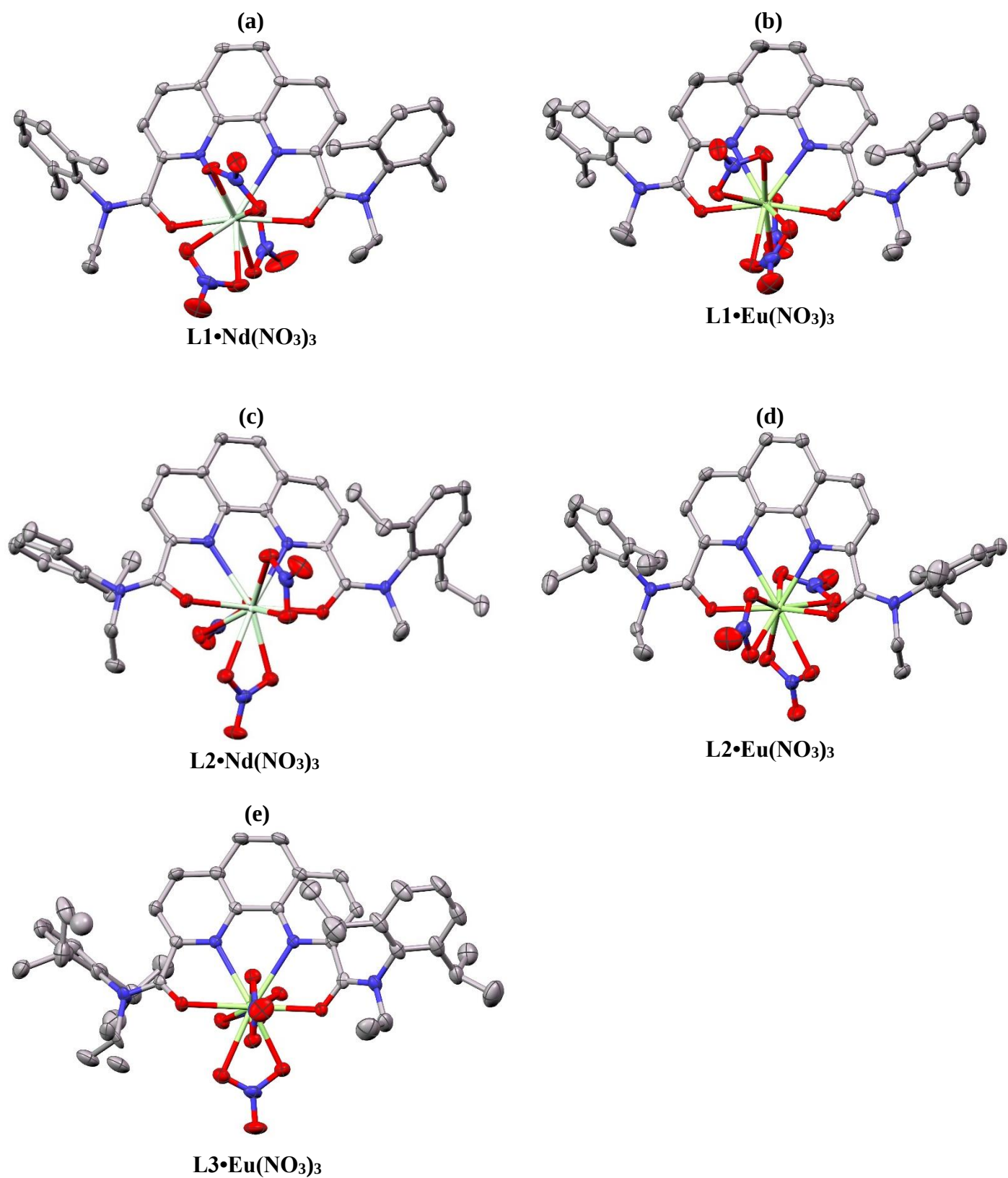


Figure S47. General views of (a) **L1•Nd(NO₃)₃**, (b) **L1•Eu(NO₃)₃**, (c) **L2•Nd(NO₃)₃**, (d) **L2•Eu(NO₃)₃** and (e) **L3•Eu(NO₃)₃**

Table S1. Crystal data and structure refinement parameters for diamides and complexes

	L1	L2	L1•Nd(NO₃)₃	L1•Eu(NO₃)₃	L2•Nd(NO₃)₃	L2•Eu(NO₃)₃	L3•Eu(NO₃)₃
CCDC	2391958	2393474	2394080	2394081	2394083	2394082	2394084
Empirical formula	C ₃₄ H ₃₄ N ₄ O ₂	C ₃₈ H ₄₂ N ₄ O ₂	C ₄₁ H ₄₂ N ₇ NdO ₁₁	C _{34.9} H _{34.9} Cl _{2.7} EuN ₇ O ₁₁	C ₄₂ H ₄₈ N ₉ NdO ₁₁	C _{42.5} H ₄₇ Cl ₃ EuN ₇ O ₁₁	C ₄₄ H ₅₃ EuN ₈ O ₁₁
Formula weight	530.65	586.75	953.05	976.07	999.13	1090.18	1021.90
T, K	295	120	150	150	150	150	150
Crystal system	monoclinic	Triclinic	monoclinic	monoclinic	triclinic	monoclinic	monoclinic
Space group	I2/c	P $\bar{1}$	P2 ₁ /n	P2 ₁ /n	P-1	P2 ₁ /n	P2 ₁ /n
Z	8	4	4	4	2	4	4
a, Å	14.8268(3)	8.974(2)	13.6420(9)	13.2958(7)	11.5385(7)	16.7236(10)	13.5781(7)
b, Å	14.1752(3)	14.552(4)	16.8587(10)	16.6797(10)	11.8765(7)	11.2923(6)	20.0588(13)
c, Å	27.6844(14)	24.460(6)	17.9926(13)	17.8009(9)	16.3609(10)	25.2063(14)	17.1370(9)
α, °	90.0	94.213(8)	90	90	91.291(2)	90	90
β, °	96.316(3)	92.420(8)	97.498(3)	98.562(2)	94.487(2)	102.531(2)	97.189(2)
γ, °	90.0	95.485(8)	90	90	95.961(2)	90	90
V, Å³	5783.2(3)	3167.2(14)	4102.7(5)	3903.7(4)	2222.0(2)	4646.8(5)	4630.7(5)
D_{calc} (g cm⁻³)	1.219	1.231	1.543	1.661	1.494	1.558	1.466
Linear absorption, μ (cm⁻¹)	0.606	0.77	0.1335	0.1860	0.1237	0.1588	0.1421
F(000)	2256	1256	1940.0	1961.0	1022.0	2212.0	2096.0
2θ_{max}, °	132	58	55	52	50	52	55
Reflections measured	20234	31633	44883	38169	22995		
Independent reflections	5072	16184	9410	7669	7738	9120	10635
Observed reflections [I > 2σ(I)]	2412	8515	7574	6079	6448	7117	8643
Parameters	368	807	557	528	576	590	606
R1	0.0448	0.0940	0.0338	0.0370	0.0469	0.0413	0.0354
wR2	0.1256	0.2956	0.0673	0.0862	0.0773	0.0879	0.0663
GOF	0.813	1.016	1.035	1.044	1.129	1.046	1.054
$\Delta\rho_{\text{max}}/\Delta\rho_{\text{min}}$ (e Å⁻³)	0.15/-0.14	0.389/-0.365	1.03/-0.61	0.81/-0.98	1.32/-1.68	1.21/-0.93	0.96/-0.64

Table S2. Some geometric parameters of coordination sites of complexes **L•Ln(NO₃)₃**

	L1•Nd(NO₃)₃	L1•Eu(NO₃)₃	L2•Nd(NO₃)₃	L2•Eu(NO₃)₃	L3•Eu(NO₃)₃
	Bond Length, Å				
R _{M-O(1)}	2.459(2)	2.422(3)	2.380(3)	2.439(2)	2.494(3)
R _{M-O(2)}	2.472(2)	2.421(3)	2.427(3)	2.401(2)	2.411(3)
R _{M-N(1)}	2.637(2)	2.570(5)	2.592(3)	2.625(2)	2.642(3)
R _{M-N(2)}	2.638(2)	2.581(3)	2.600(3)	2.601(2)	2.640(4)
R _{M-ONO2}	2.515(2)- 2.576(2)	2.461(4)- 2.545(4)	2.460(4)- 2.552(3)	2.457(2)- 2.550(2)	2.521(3)- 2.573(4)
Out-of-plane	0.180	0.002	0.500	0.375	0.154
	Torsions (°)				
N _{phen} -C-C=O	20.2(4), 18.4(4)	22.5(7), 17.1(7)	8.6(6), 26.3(6)	21.6(4), 17.3(4)	25.1(6), 18.8(6)
C-N _{amide} -C=O	173.9(3), 2.3(4)	172.2(5), 0.02(7)	172.7(4), 2.8(6)	167.7(3), 3.2(4)	170.2(4), 0.04(6)
C-N _{amide} -C=O	165.9(3), 5.5(4)	166.9(5), 3.6(7)	167.4(4), 3.5(6)	179.0(3), 8.8(7)	162.3(4), 5.2(6)

5. DFT calculations

All structures were optimized at the DFT level in the gas phase (tolerance on gradient: 10^{-7} au). The generalized gradient approximation (GGA) functional PBE was used for the geometry optimization and frequency calculations of all structures. All stationary points on the potential energy surface (PES) were checked by vibrational analysis and none of them had imaginary frequencies. Full electron relativistic L1 basis set [3] of TZ quality including one polarization function was used for all the atoms to provide the most reliable result. All thermodynamic calculations are performed using the PBE/L1 theoretical level. The CREST 3.0 program was used to find the most stable conformations of the ligands [4].

The reaction (1) was used to calculate the energy of formation of complexes LM stoichiometry:

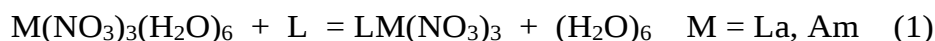


Table S3. The electronic energy (ΔE) change in the reaction (1) from different conformers, kcal/mol (the change in free energy (ΔG) is given in brackets, kcal/mol)

	Conformer	La(NO ₃) ₃	Am(NO ₃) ₃
L1	I	-14.9 (-10.4)	-18.3 (-12.2)
	II	-16.8 (-11.6)	-20.2 (-13.4)
	III	-16.9 (-12.0)	-20.2 (-13.9)
L2	I	-17.3 (-10.1)	-19.7 (-12.6)
	II	-19.5 (-12.8)	-21.9 (-15.2)
	III	-15.6 (-10.7)	-18.0 (-13.2)
L3	I	-20.1 (-15.0)	-23.4 (-17.3)
	II	-19.3 (-12.4)	-22.5 (-14.7)
	III	-17.0 (-9.9)	-20.2 (-12.2)

The reaction (2)-(4) were used to calculate the energy of formation of complex cations $[L_2M]^{3+}$, $[L_2M(NO_3)]^{2+}$ and $[L_2M(NO_3)_2]^+$:

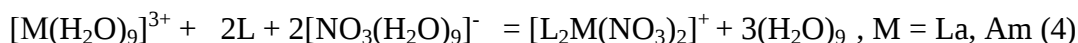
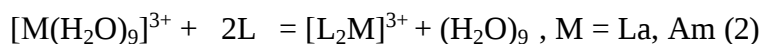


Table S4. The electronic energy (ΔE) change in the reactions (2)-(4) from different conformers, kcal/mol (the change in free energy (ΔG) is given in brackets, kcal/mol)

	Conformer	The composition of the complex cation	La(NO ₃) ₃	Am(NO ₃) ₃
L1	I	[L₂M]³⁺	-232.9 (-202.0)	-251.7 (-221.2)
	II		-236.7 (-204.4)	-255.5 (-223.6)
	III		-236.9 (-205.4)	-255.6 (-224.5)
	I	[L₂M(NO₃)]²⁺	-390.3 (-360.8)	-406.1 (-377.3)
	II		-394.1 (-363.2)	-409.8 (-379.7)
	III		-394.3 (-364.1)	-410.0 (-380.6)
	I	[L₂M(NO₃)₂]⁺	-488.1 (-459.1)	-496.1 (-468.1)
	II		-492.0 (-462.4)	-500.0 (-471.4)
	III		-491.9 (-461.5)	-499.9 (-470.5)
L2	I	[L₂M]³⁺	-238.1 (-204.3)	-256.9 (-223.1)
	II		-242.5 (-209.7)	-261.3 (-228.4)
	III		-234.8 (-205.6)	-253.6 (-224.3)
	I	[L₂M(NO₃)]²⁺	-394.0 (-361.0)	-409.6 (-377.6)
	II		-398.5 (-366.4)	-414.0 (-381.5)
	III		-390.7 (-362.3)	-406.2 (-377.4)
	I	[L₂M(NO₃)₂]⁺	-490.8 (-459.4)	-497.9 (-467.4)
	II		-495.3 (-464.8)	-502.4 (-472.7)
	III		-487.5 (-460.7)	-494.6 (-468.7)
L3	I	[L₂M]³⁺	-239.3 (-209.3)	-258.8 (-228.3)
	II		-237.6 (-204.0)	-257.2 (-223.1)
	III		-233.0 (-199.2)	-252.5 (-218.3)
	I	[L₂M(NO₃)]²⁺	-400.1 (-369.7)	-415.4 (-383.6)
	II		-398.5 (-364.5)	-413.8 (-378.4)
	III		-393.9 (-359.6)	-409.1 (-373.4)
	I	[L₂M(NO₃)₂]⁺	-489.6 (-460.6)	-496.6 (-467.8)
	II		-488.0 (-455.4)	-495.0 (-462.6)
	III		-483.4 (-450.6)	-490.4 (-457.8)

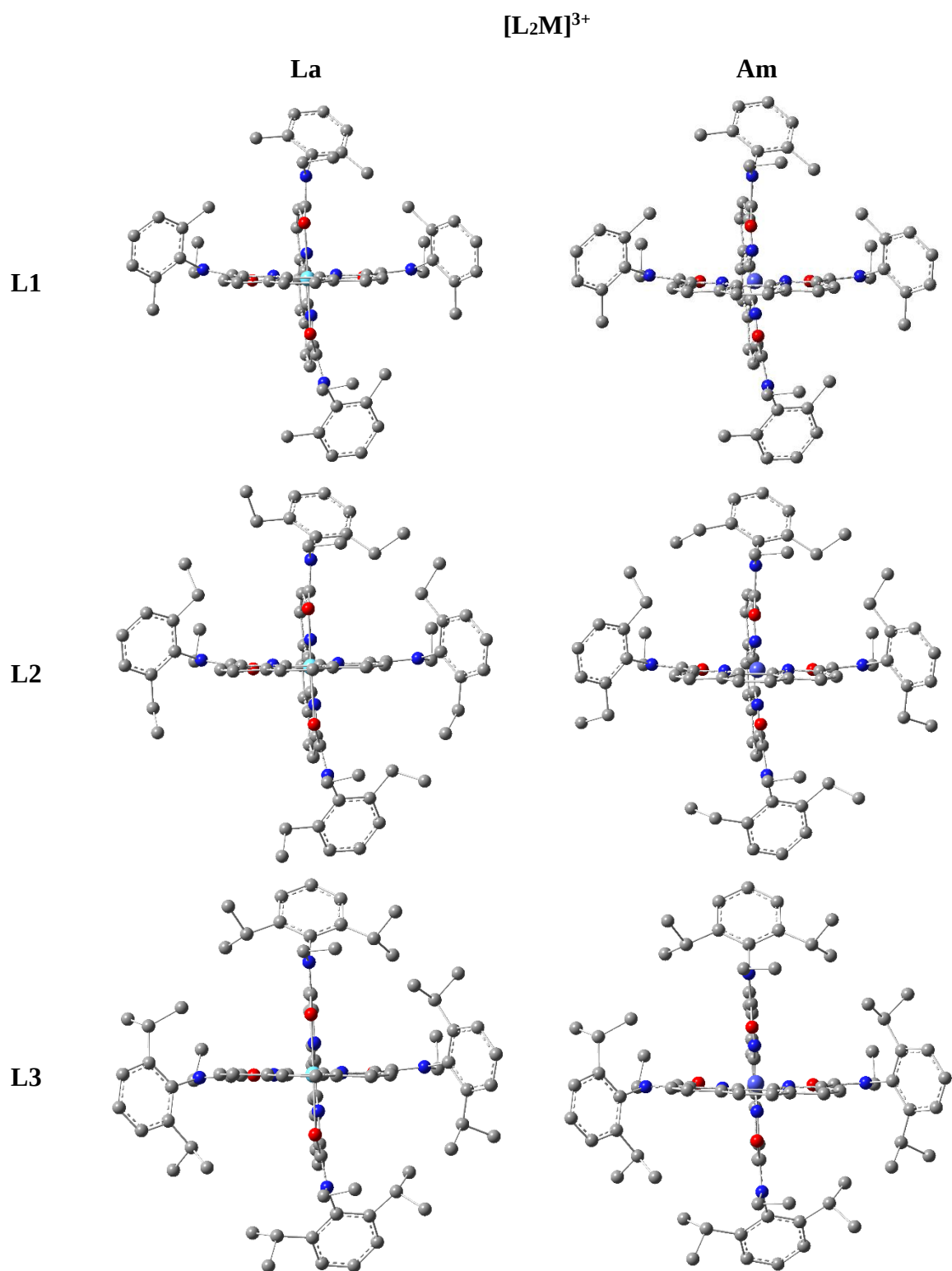


Figure S48. Structures of $[\text{L}_2\text{M}]^{3+}$ complex cations with lanthanum and americium

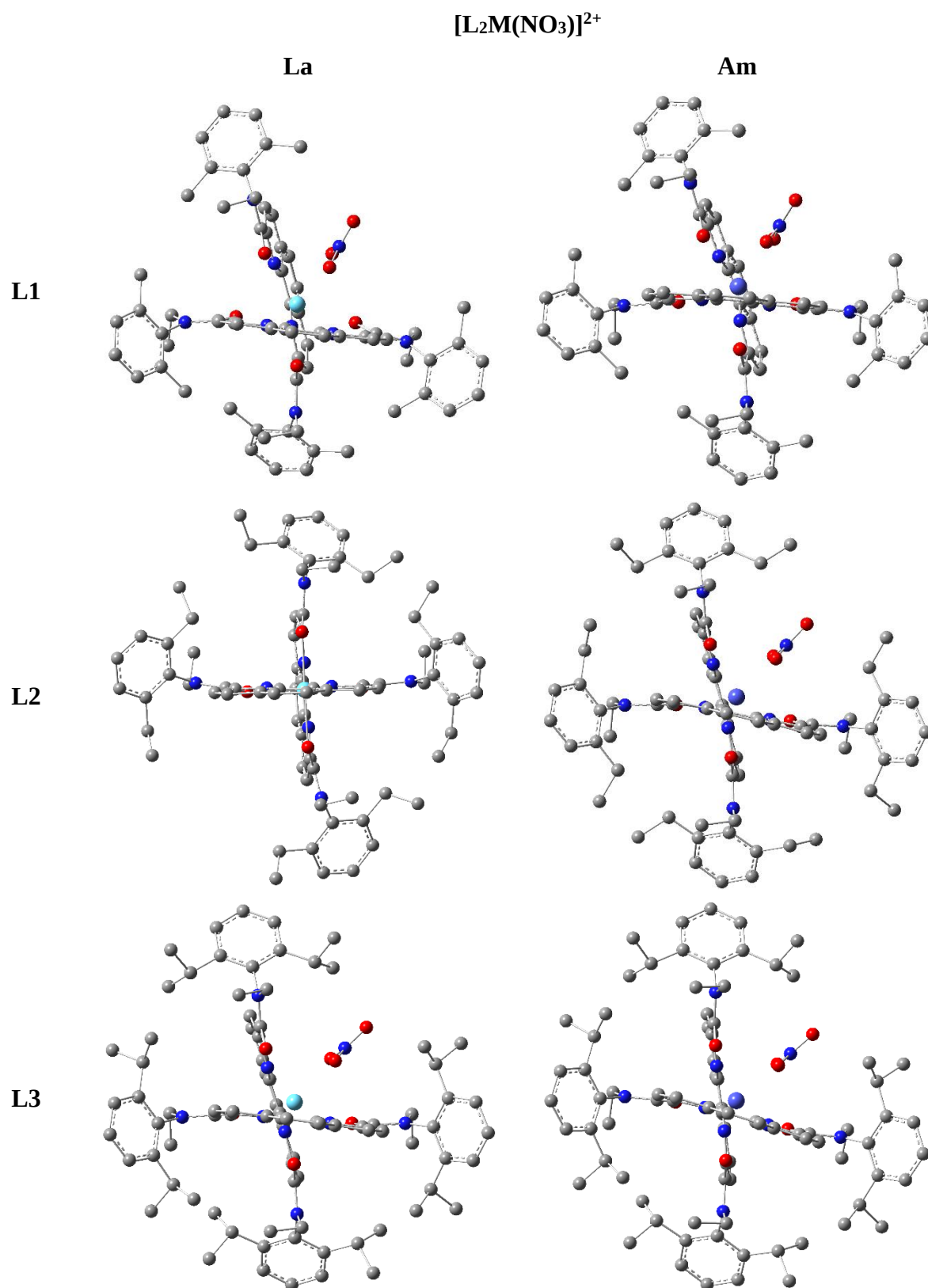


Figure S49. Structures of $[\text{L}_2\text{M}(\text{NO}_3)]^{2+}$ complex cations with lanthanum and americium

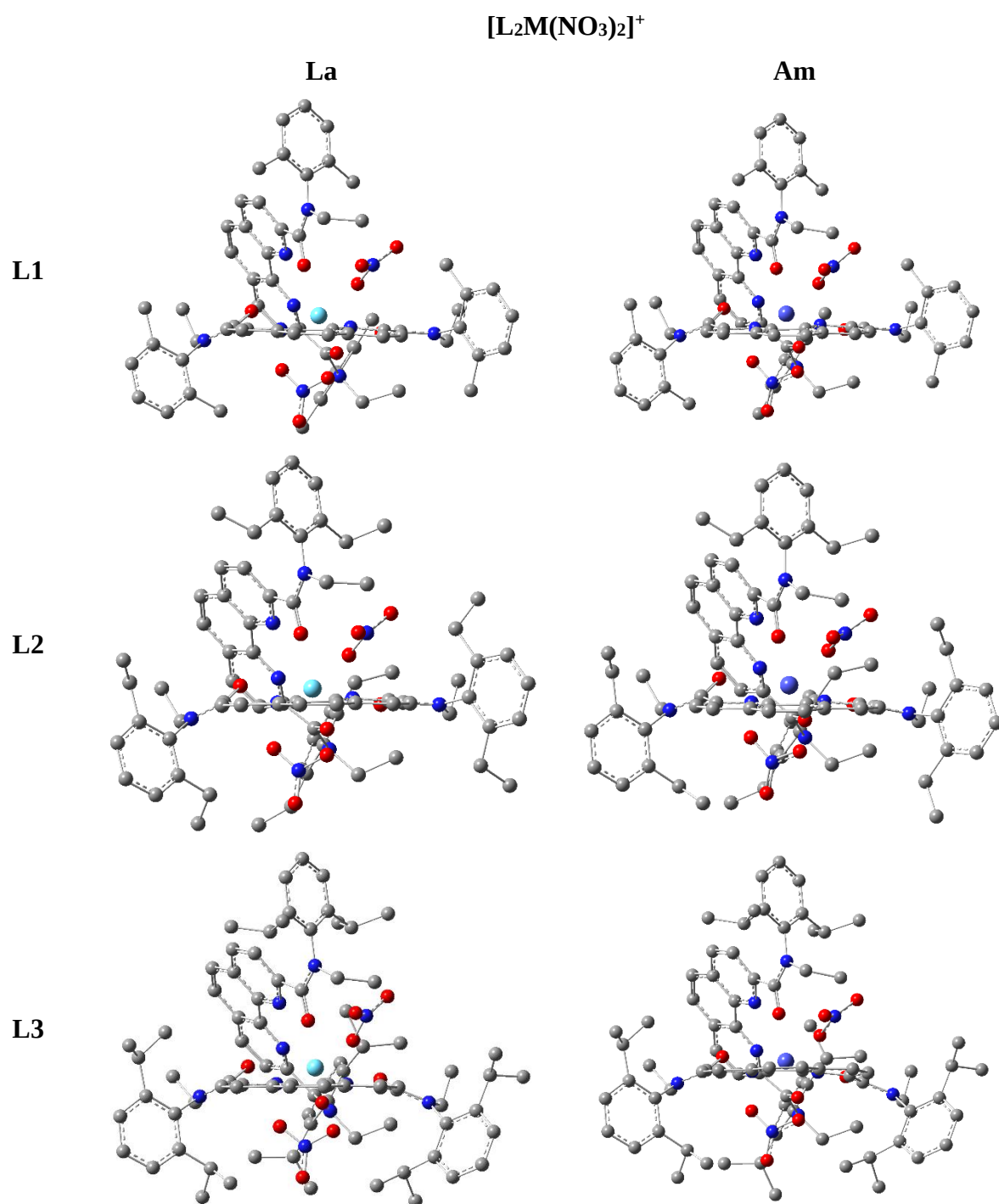
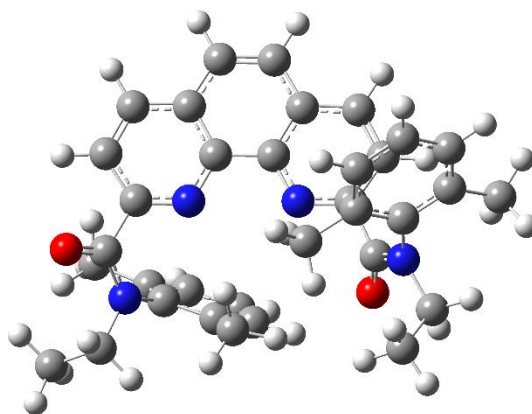


Figure S50. Structures of $[\text{L}_2\text{M}(\text{NO}_3)_2]^+$ complex cations with lanthanum and americium

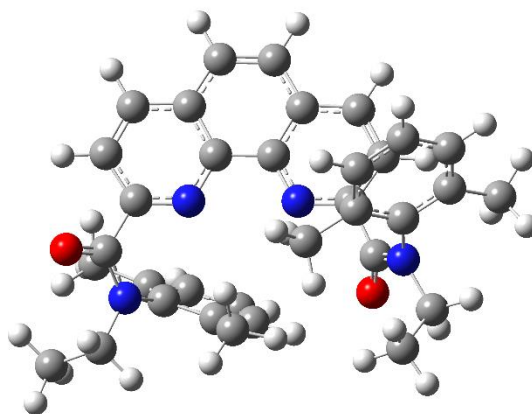
L1 (I)



O	-4.44131578	0.28807750	2.48682445
O	1.83517514	-1.70946086	-1.74646311
N	0.71807173	0.74741964	-0.48996566
N	-3.84565256	-0.96316507	0.65926187
N	-1.85263983	1.16437312	0.40972936
N	3.47923300	-1.24452970	-0.21596409
C	-1.12873374	2.22781829	-0.00005708
C	-3.41133290	-1.03534943	-0.71406979
C	-3.07430593	1.37489475	0.88064943
C	0.21783581	2.00189032	-0.51193758
C	-2.93219315	3.75042477	0.57224473
C	1.94006668	0.54228962	-0.96540701
C	-4.43684455	-2.16879884	1.27110418
H	-4.24188983	-2.10052859	2.35246058
H	-3.89321338	-3.03703080	0.86824360
C	-1.80005058	-1.78641758	-2.34964037
H	-0.83595649	-2.24815665	-2.57850921
C	-2.19761187	-1.69209802	-1.01191638
C	-4.20808483	-0.46942710	-1.73141916
C	0.95439930	3.11263833	-1.02306658
C	-3.64688719	2.66104149	1.02158018
H	-4.63324886	2.75658887	1.47943637
C	-3.86016654	0.18934021	1.40808764
C	2.39632546	-0.91138264	-1.00472630
C	-2.58560430	-1.24991846	-3.36942175
C	-0.85474198	4.64434427	-0.47696557
H	-1.27675992	5.65341100	-0.44662322
C	-1.63999896	3.56064892	0.02828987
C	-3.77449838	-0.59524503	-3.05943310
H	-4.38704537	-0.16411086	-3.85711979
C	0.39064940	4.42720480	-0.99352995
H	0.98292604	5.25832160	-1.38794993
C	-5.47209639	0.30110053	-1.43555039
H	-6.09284427	0.37844108	-2.34074439
H	-5.23988795	1.32861186	-1.10497831
H	-6.06980975	-0.16666248	-0.64136532
C	-5.93879226	-2.33074671	1.02737947

H	-6.16355539	-2.41953873	-0.04661218
H	-6.49174572	-1.47865488	1.44977200
H	-6.29217698	-3.24934232	1.52409310
C	2.24236794	2.85256990	-1.54306483
C	5.19840266	1.37790636	2.62656964
C	5.32862355	0.20695080	0.50098345
C	4.05316615	-0.34751636	0.75151106
C	3.34880233	-0.05414092	1.94306549
C	3.94366221	0.82115265	2.86237380
H	3.40575168	1.05831717	3.78465538
C	2.74107148	1.56699213	-1.51955047
H	3.73466654	1.34087054	-1.91142352
C	-1.29548403	-2.19439257	0.08288090
H	-0.35624550	-2.56846583	-0.34756665
H	-1.75722643	-3.00051401	0.67625989
H	-1.06208406	-1.35641736	0.75838907
C	1.99494117	-0.64399367	2.24407501
H	1.22364174	-0.26830860	1.54911386
H	1.68962149	-0.38535357	3.26832110
H	2.00280688	-1.74010458	2.15158501
C	5.88377792	1.06947547	1.45392296
H	6.86589909	1.51153825	1.26096862
C	6.09727538	-0.09064323	-0.76338616
H	6.76974081	-0.95639513	-0.63135347
H	6.72706081	0.76791477	-1.04160143
H	5.42783836	-0.32677331	-1.60366172
C	3.55667664	-3.56701639	0.76448261
H	2.46381053	-3.69221157	0.73674440
H	3.85371103	-3.20804332	1.76200178
H	4.01881452	-4.55540989	0.60827377
C	4.02220626	-2.61128497	-0.33487554
H	3.69019489	-2.97775584	-1.31836522
H	5.12136791	-2.54183923	-0.33474275
H	2.83269305	3.67722159	-1.95331100
H	-3.34571440	4.76164373	0.63165593
H	5.64342899	2.05592384	3.35939232
H	-2.26026452	-1.33021309	-4.41004390

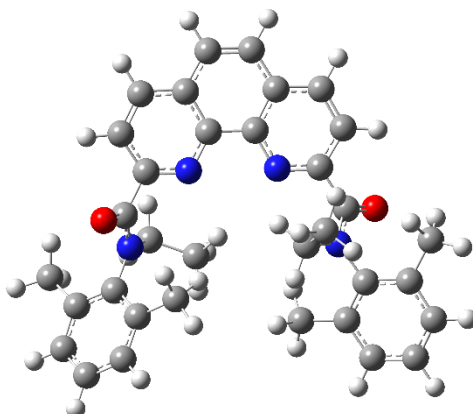
L1 (II)



O	3.46584139	-1.46418481	2.56027372
O	-3.59064948	1.31655340	-1.63899288
N	1.97027101	0.77612576	0.60485758
N	-0.53766482	1.72625992	-0.08448651
N	3.07652363	-2.01156952	0.36573650
N	-3.23334532	0.41316496	0.43815029
C	3.13905548	0.35156732	1.06911302
C	4.21299176	1.21318853	1.39172363
H	5.11977811	0.80273402	1.84053476
C	4.08218608	2.55584370	1.11068578
H	4.90190726	3.25540514	1.29937651
C	2.86448575	3.04189818	0.58003880
C	2.67325350	4.41918855	0.24693444
H	3.50895605	5.11140756	0.38647065
C	1.47705267	4.86134507	-0.24089236
H	1.33718691	5.91322901	-0.50711510
C	0.37146351	3.96705904	-0.39195105
C	-0.88983017	4.40045320	-0.86273612
H	-1.02271161	5.44609111	-1.15586248
C	-1.93049392	3.50274297	-0.94189454
H	-2.91262874	3.77973542	-1.32771218
C	-1.71759919	2.17471940	-0.49685663
C	0.50618390	2.58817841	-0.04946072
C	1.80700463	2.10073572	0.39225208
C	-2.91979934	1.24531902	-0.61266996
C	-2.48301857	0.35788537	1.71464233
H	-2.60348542	-0.66215857	2.10879801
H	-1.41873932	0.50404174	1.48603711
C	-2.96975674	1.36890241	2.75463351
H	-4.03207984	1.21402231	2.99934531
H	-2.83436978	2.40274282	2.39925393
H	-2.38579942	1.24943766	3.68179766
C	-4.44775420	-0.36620719	0.36121886
C	-5.70691157	0.27105876	0.41028128
C	-6.85665374	-0.52912247	0.40260860
H	-7.83573271	-0.04300400	0.44549803
C	-6.77123912	-1.91802615	0.33868467

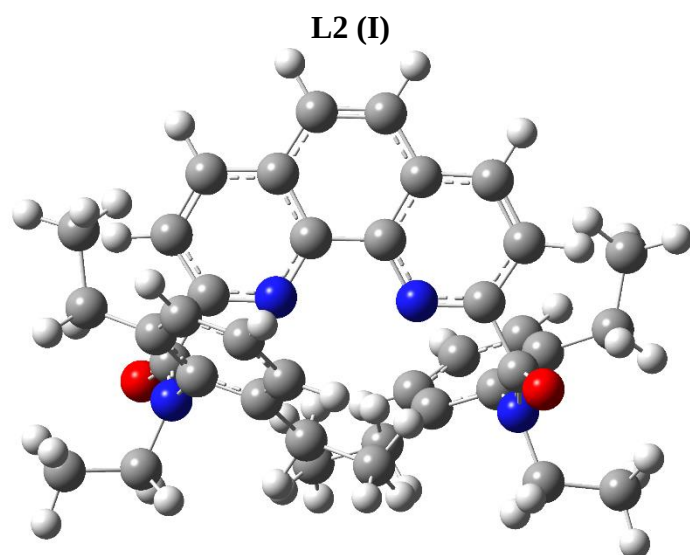
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L1 (III)



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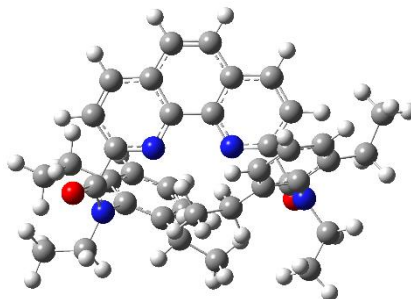


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L2 (II)

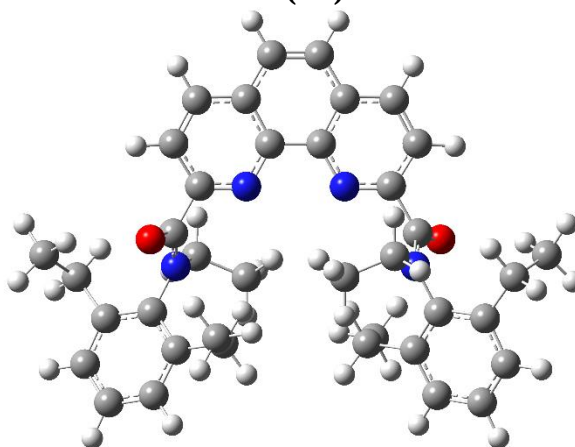


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L2 (III)

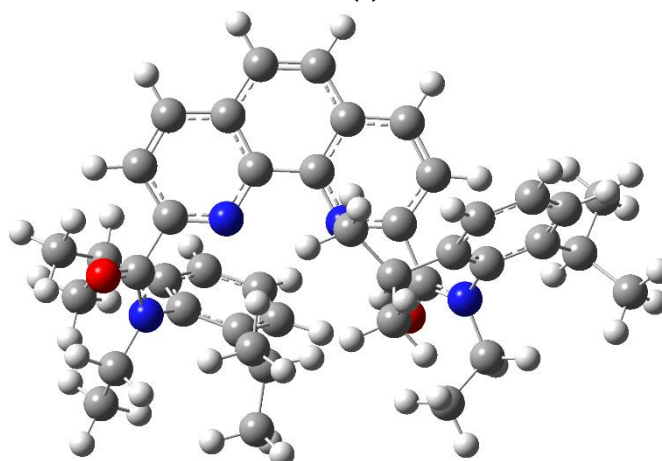


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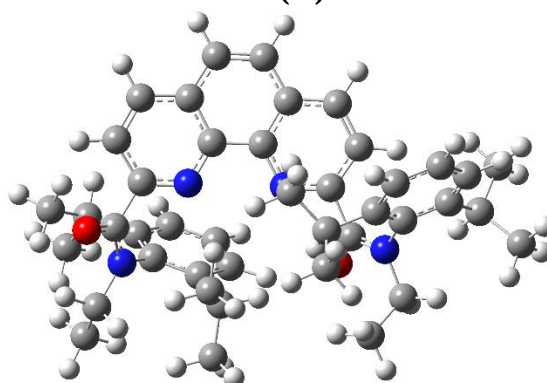


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L3(II)

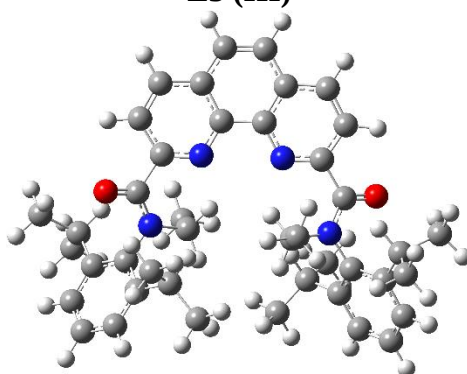


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L3 (III)

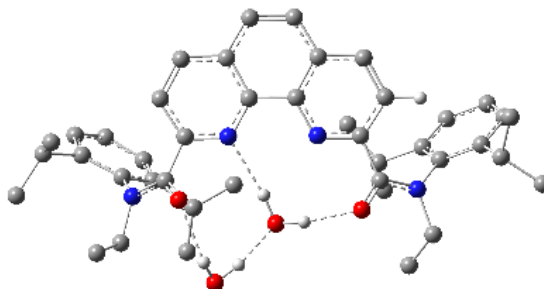


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H	5.31660333	-1.46328645	3.19449407
C	1.01461411	-2.86137473	-2.04342641
H	0.73382014	-3.22700376	-1.04267677
H	0.09841910	-2.53067635	-2.55972821
H	1.41958850	-3.71332110	-2.61340808
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H	-6.94099468	-1.78402612	-2.53999028
H	-6.59191481	-0.22944237	-3.32516986
H	-5.31563298	-1.47094629	-3.19525390
H	-1.51868237	-0.85828524	1.44956762
C	-2.42400204	-1.20461660	3.36284159
H	-1.53427932	-0.87828266	3.92696028

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L3*2H2O (I)

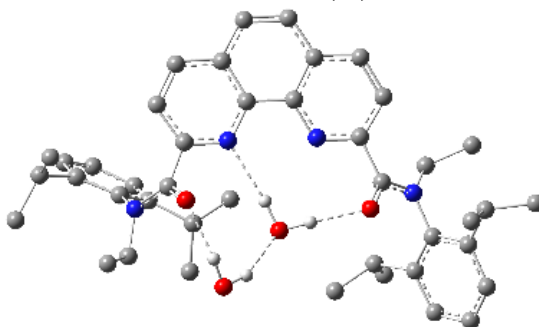


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N	-1.70137906	3.06382632	-2.69905376
N	0.38131613	0.27740633	-1.86454570
N	-0.24036528	-4.06167984	2.28636980
C	1.63763762	-0.19736037	-1.79722154
C	-0.80466926	4.19217062	-2.70880699
C	0.12401769	1.33657432	-2.62695837
C	1.90660405	-1.35562217	-0.94673592
C	2.40379381	1.47391343	-3.37372017
H	3.19431186	1.93199706	-3.97531986
C	1.13146567	-3.01448202	0.46283376
C	-3.15959620	3.34176445	-2.67712474
H	-3.64346838	2.58550692	-3.31384206
H	-3.29966331	4.33365107	-3.12948489
C	0.15230235	6.06436062	-3.90939331
H	0.25669315	6.65287352	-4.82519817
C	-0.68354249	4.94229078	-3.90793610
C	-0.10131302	4.56501150	-1.53807175
C	3.25132370	-1.82333350	-0.84461391
C	1.11209393	1.95964468	-3.42232394
H	0.86580616	2.81216550	-4.05399799
C	-1.34835243	1.73398364	-2.61998940
C	-0.11272438	-3.75508094	0.95034009
C	0.85896397	6.43874407	-2.76893592
C	4.04273701	-0.13487887	-2.40897012
H	4.84601927	0.33658028	-2.98262000
C	2.71566129	0.38389954	-2.53353024
C	0.73139900	5.69192743	-1.60290074
H	1.28556252	5.99243212	-0.70965844
C	4.30036163	-1.19226778	-1.58592963
H	5.31674480	-1.58398902	-1.48352993
C	-3.77006936	3.30310082	-1.27549422
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C	2.35559106	-2.28635979	5.14722347
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H	3.14763737	-4.26415586	5.45098543
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H	1.50975943	7.31681061	-2.79013419
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C	-0.54305058	-1.24092952	2.85208665
H	-1.51333687	-1.74999796	2.82969502
C	1.62798607	-5.81767069	3.77392612
H	0.90339405	-6.34450437	4.40521070
C	3.02470176	-6.37386038	4.10774992
H	3.14619846	-6.52627710	5.18622854
H	3.19808641	-7.33809932	3.61653860
H	3.81550416	-5.68953653	3.77996784
C	1.32056418	-6.18410699	2.31008999
H	2.24024712	-6.28770324	1.72309803
H	0.77692087	-7.13328274	2.24208340
H	0.70556188	-5.41616924	1.82723137
C	-0.14371143	-0.93953376	1.39562215
H	0.94458167	-0.87017569	1.28646155
H	-0.49434694	-1.72392391	0.71525874
H	-0.57095810	0.00977776	1.05301947

C	-0.74362140	0.10839851	3.56670908
H	-1.78041831	0.45372174	3.48356767
H	-0.50503858	0.03412528	4.63379355
H	-0.10131312	0.88619743	3.13824955
C	0.33132392	4.52838549	0.96824321
H	-0.43732004	4.72014393	1.72555664
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H	0.74179477	5.49728226	0.66187513
C	0.49628105	2.41208036	-0.32238243
H	0.80137840	2.05888702	0.66922158
H	-0.13615384	1.63634575	-0.76889052
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C	-2.51069529	5.58416553	-5.55706931
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H	0.54073335	4.31832101	-6.05935928
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L3*2H₂O (II)

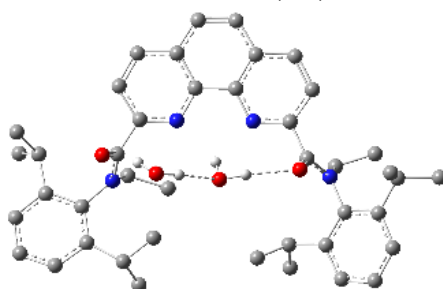


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C	-1.59999210	-1.26499183	-2.21297669
C	-3.34019066	3.55316068	0.91679687
C	-2.79088079	0.51174550	-1.33903501
C	-0.50758033	-2.22703785	-2.07774672
C	-3.48668499	-0.39503386	-3.45605014
H	-4.15270288	-0.41300151	-4.32385459
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C	-3.24999352	3.45811558	-1.58064406
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H	-1.48861536	5.65772679	2.85089961

C	-2.20958738	4.27607517	1.35841818
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C	-3.67861430	0.51842779	-2.43849652
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C	-2.94025793	1.41455216	-0.11560124
C	1.78484996	-3.22441630	0.59484227
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C	-2.13265267	-2.24561945	-4.43069826
H	-2.77370649	-2.25126447	-5.31702268
C	-2.41499582	-1.31036228	-3.38597304
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C	0.16959993	3.47182318	1.62168871
C	-0.32227371	5.53148105	0.21201056
C	2.84635876	-0.18712165	0.04671777
C	2.02475941	0.67121249	-0.93396600
C	3.60033382	0.72756294	1.03668149
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C	5.72925140	-2.75913696	-1.89005805
H	6.48972317	-3.38339520	-2.36944872
C	5.42198247	-4.71011407	-0.39052655
C	4.34604071	-5.77404405	-0.11810928
C	6.41455609	-4.59244446	0.78701477
H	6.01309107	-5.09467582	-1.24194224
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H	2.51235037	-4.48049128	3.13838475
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C	3.56062233	-2.81556842	2.22131307
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H	0.54302109	-0.94693312	3.07324526
O	0.95560730	-1.62152629	3.66190630
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H	5.92656244	-4.21330286	1.69591845
H	1.59601068	0.06182408	-1.74283349
H	2.63499697	1.47177833	-1.38475239
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H	3.64843060	-5.48411264	0.67691959
H	4.83917792	-6.71244487	0.18491406
H	2.87580299	1.36007097	1.57521091
H	4.31185654	1.38170918	0.50650248
H	4.15953169	0.14153160	1.78262858
H	-6.78177315	0.93762852	1.93153470
H	-6.22047099	2.01062462	3.24108502
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H	-0.14173215	6.20885191	1.06244874
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L3*2H₂O (III)

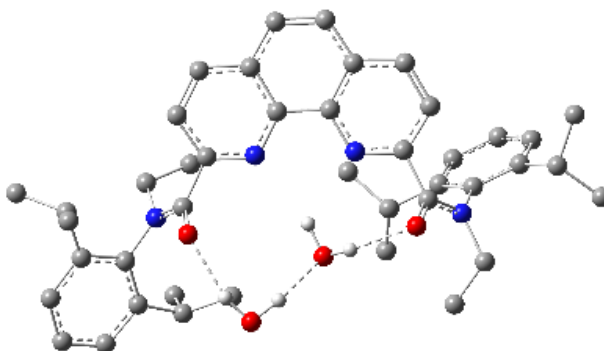


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C	-1.75908225	2.50255223	-1.29127729
C	3.86493407	2.77933483	0.61250632
C	0.29134027	3.30261149	-0.60871248
C	-2.74398165	1.42955281	-1.27961265
C	-1.10499575	4.75397345	-1.91721604
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C	-3.36437614	-0.67918235	-0.59112830
C	2.98188740	2.99991489	-1.71264663
H	2.01024006	2.88128367	-2.21528217
H	3.57099101	2.09357842	-1.93314568
C	5.43232658	1.22541524	1.57864242
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C	4.31057206	1.44843081	0.76972368
C	4.48887560	3.85762623	1.27677136
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C	0.07833414	4.55123661	-1.23734044
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C	1.48567852	3.07651415	0.30572329
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C	3.72029912	4.22638660	-2.24885209
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C	3.59627248	0.25744234	0.14010782
H	2.79420088	0.64370803	-0.50888106
C	2.91380128	-0.61110464	1.21572052
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H	-3.74993828	-5.52755761	-2.94315923
H	2.79211131	6.64488029	2.46595943
H	3.96557798	5.64929744	3.36792040
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H	5.03770665	0.02921108	-1.50812576
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L3*2H₂O (IV)

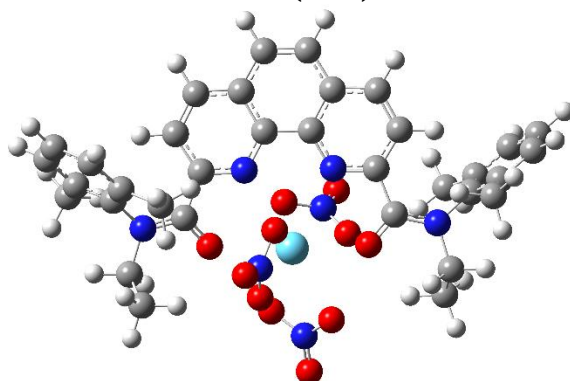


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H	4.16590377	3.93480802	-2.53982392
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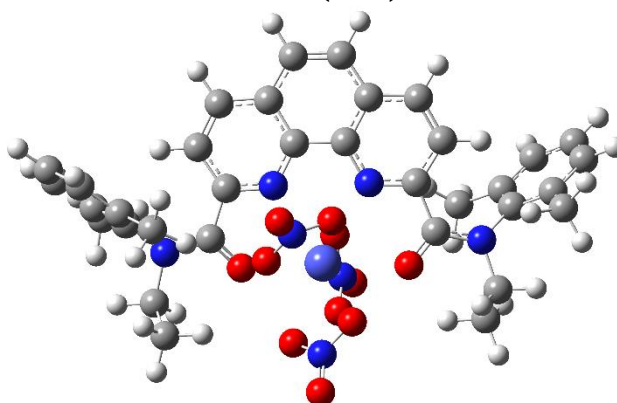


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L1*Am(NO₃)₃

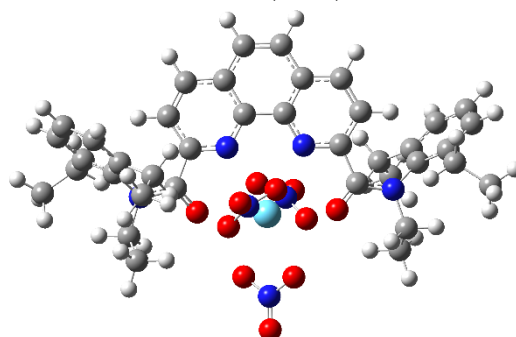


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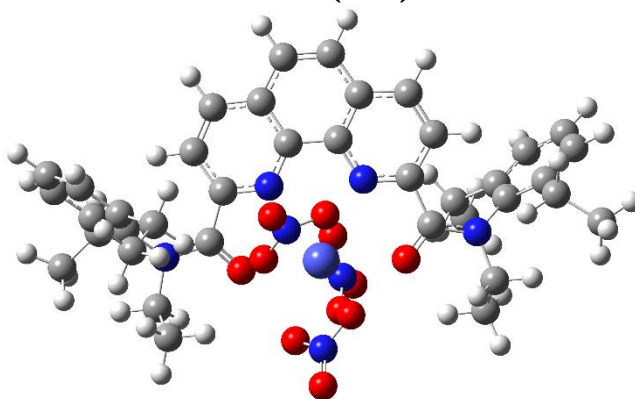


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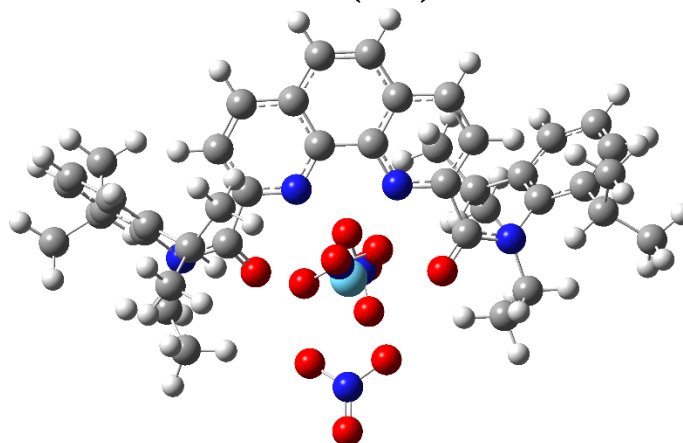


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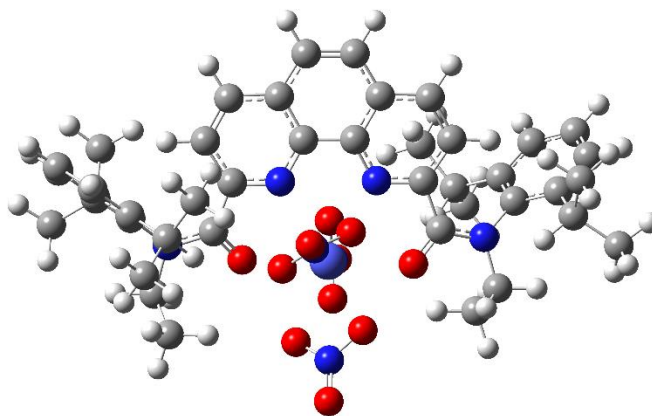


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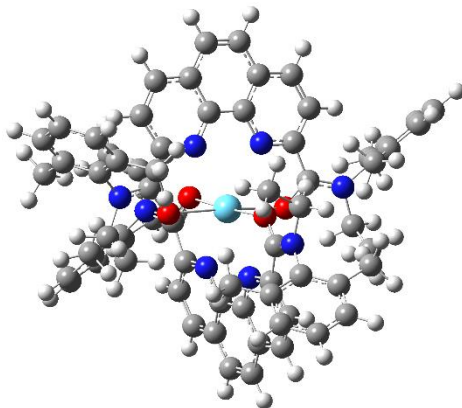
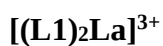
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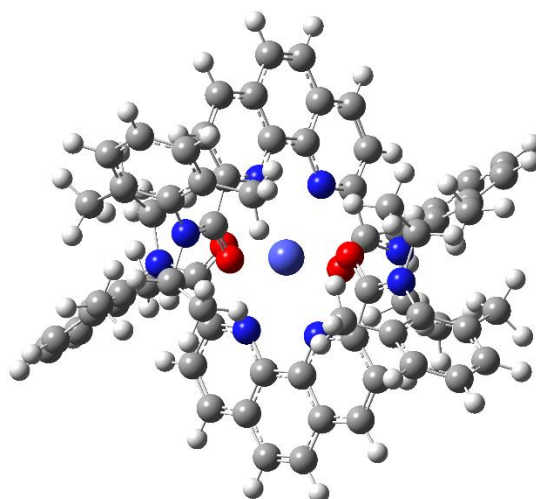
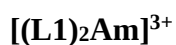


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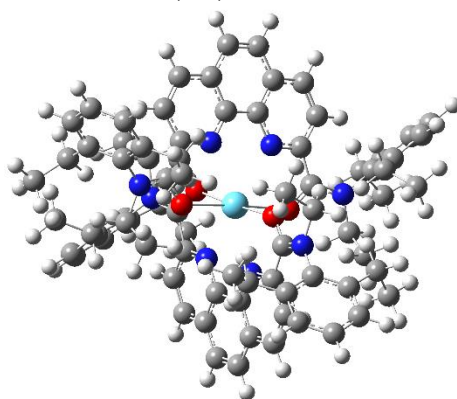
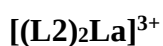


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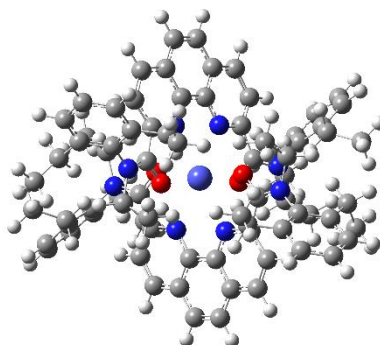
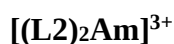
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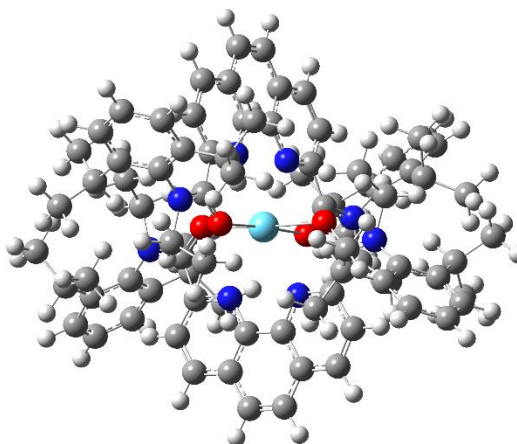
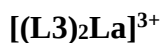
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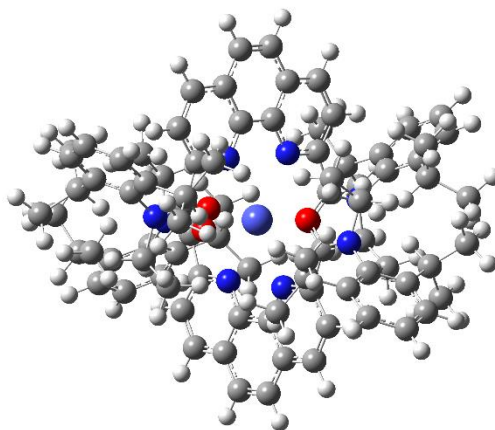
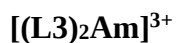
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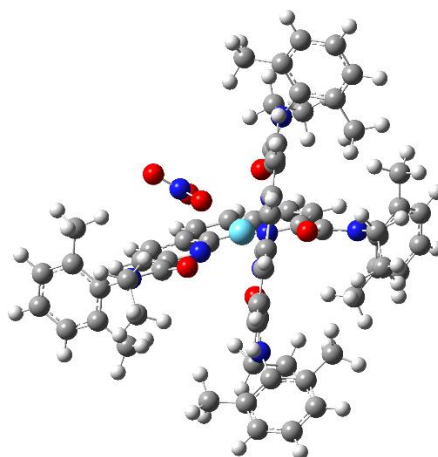
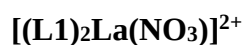
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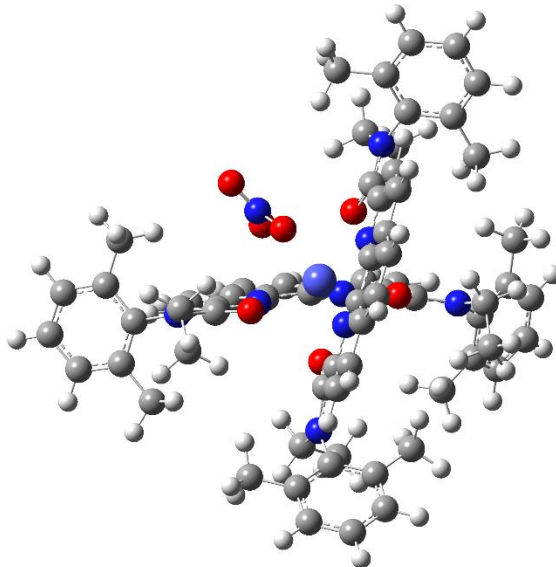
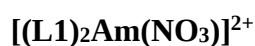


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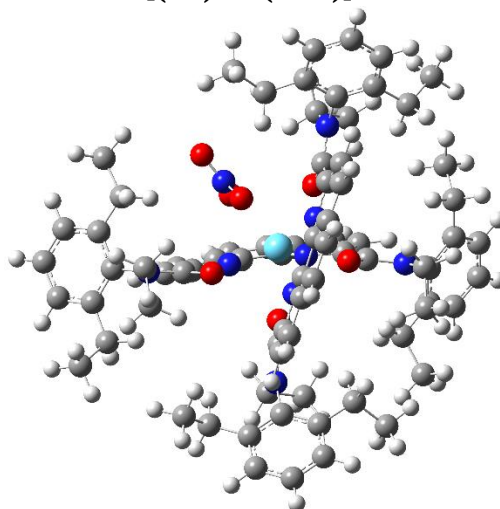
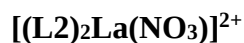


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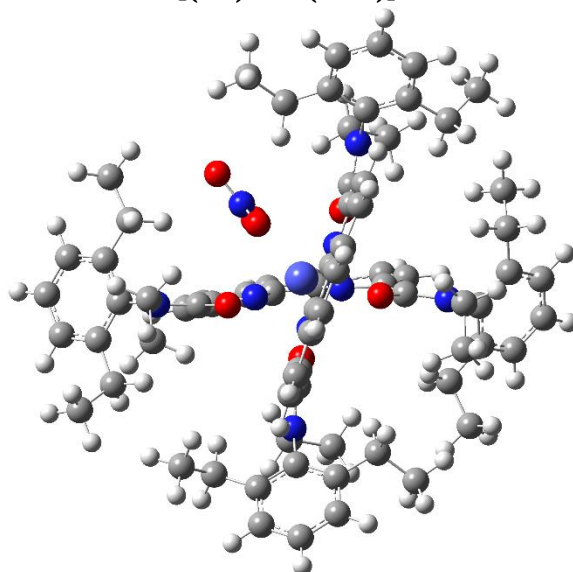
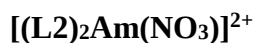


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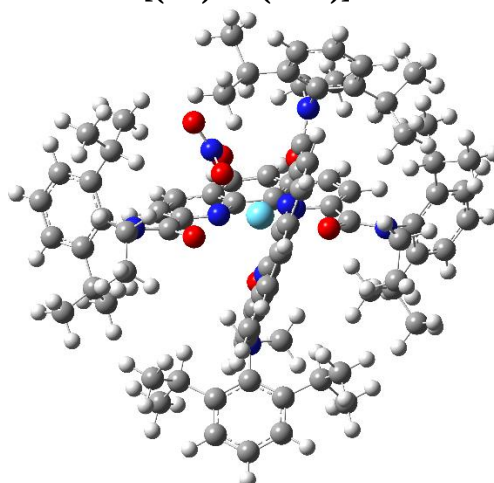
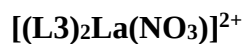


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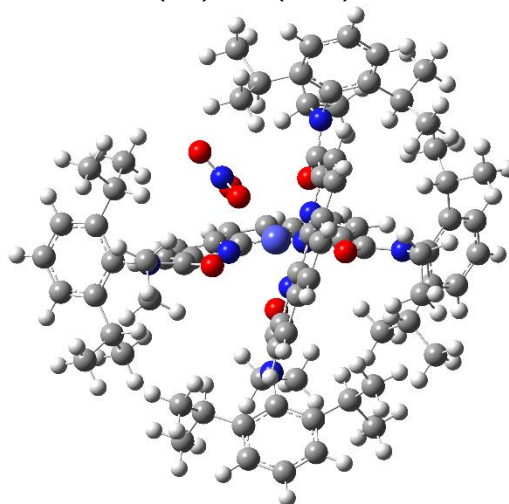
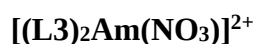
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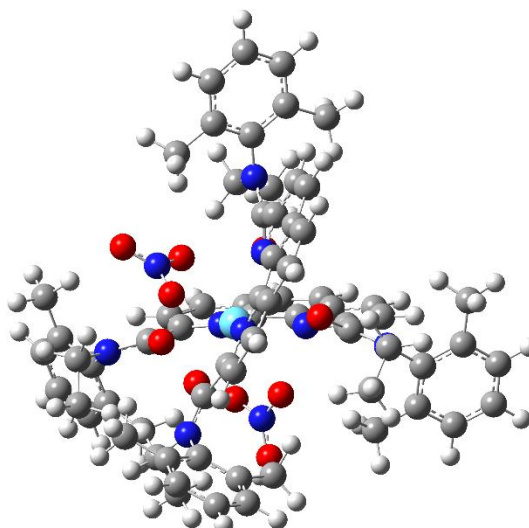
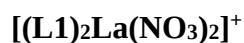
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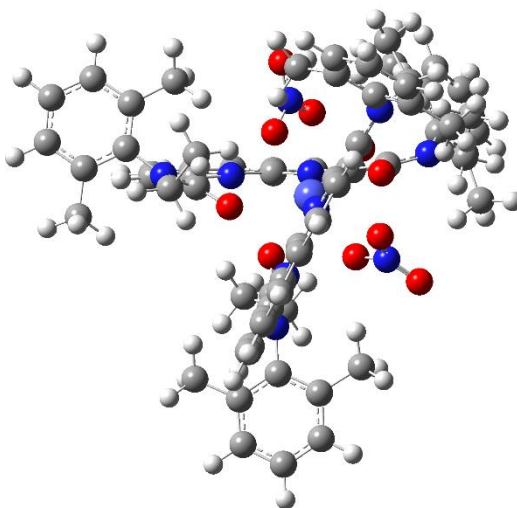


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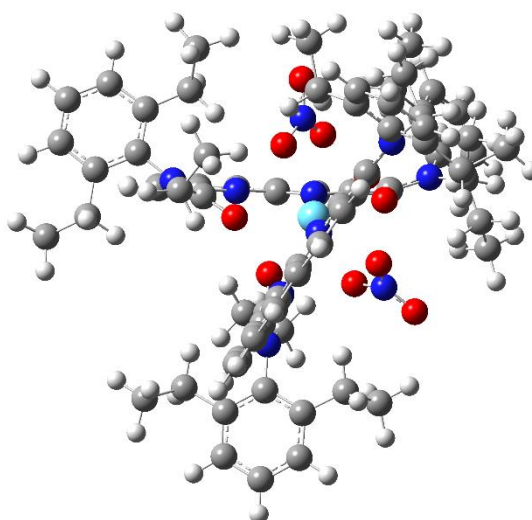
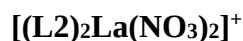
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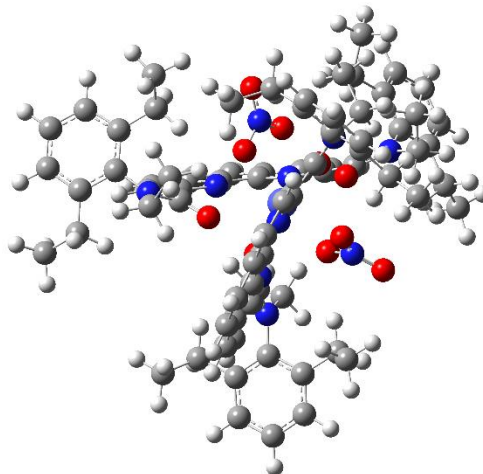
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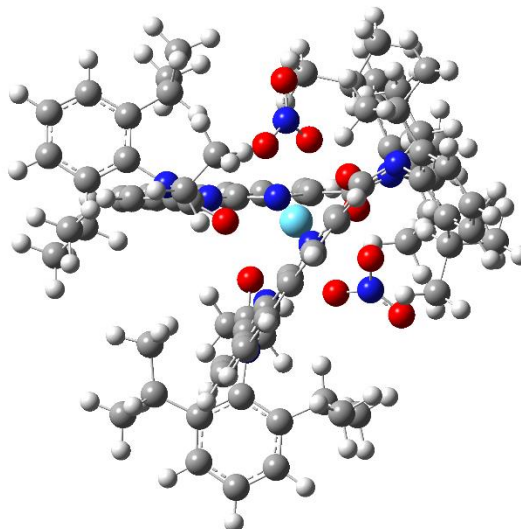
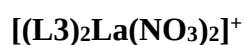
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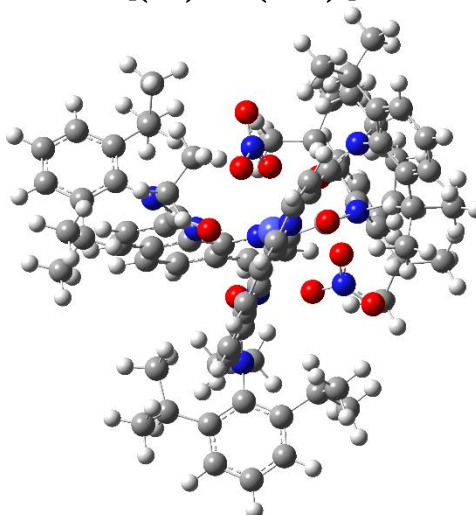
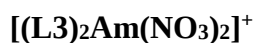
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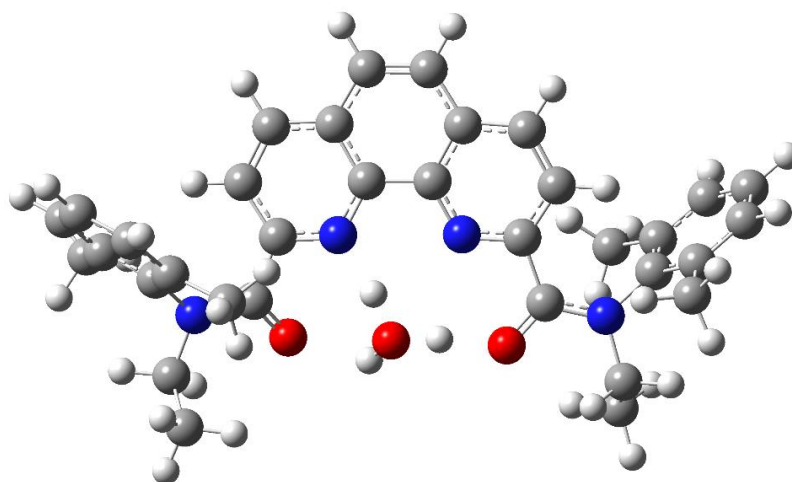
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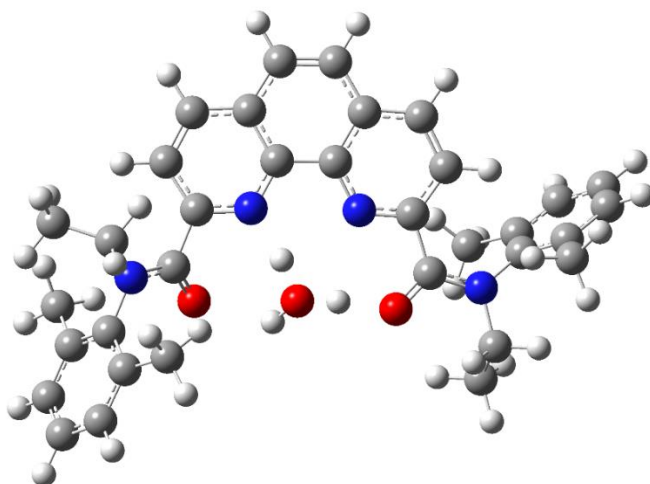


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C	-4.94512566	-2.99618578	0.45318922
C	-6.19784894	-3.21420225	-0.13674485
H	-7.02613150	-2.54957304	0.12374760
C	-6.40217986	-4.25915230	-1.03457230
H	-7.38831849	-4.41210545	-1.47957175
C	-5.34865648	-5.10935052	-1.36633019
H	-5.50601291	-5.92266161	-2.08015971
C	-4.07825556	-4.93796640	-0.80277725
C	-2.94823028	-5.85439661	-1.20191292
H	-2.78973982	-6.65362251	-0.45776990
C	-4.75745294	-1.82992964	1.39174342
H	-4.13045007	-2.08697271	2.25634521
H	3.74607684	6.75699326	1.02286749
H	2.94782810	5.37024804	1.82047188
H	5.16763306	0.64586908	-1.42219884
H	4.39775356	0.68122664	0.18366576
H	-4.27733566	-0.97850003	0.87910605
H	-5.73179117	-1.48158719	1.76294010
H	-3.17421962	-6.34478578	-2.15949442
H	-1.99532777	-5.31267923	-1.30251768
H	0.77889535	0.08537352	0.54879601
O	1.05259113	-0.76080433	1.17834943
H	1.18506650	-0.28599369	2.03596672
H	0.24179546	-1.44615383	1.18785825

L1*H3O⁺ (conformation II)

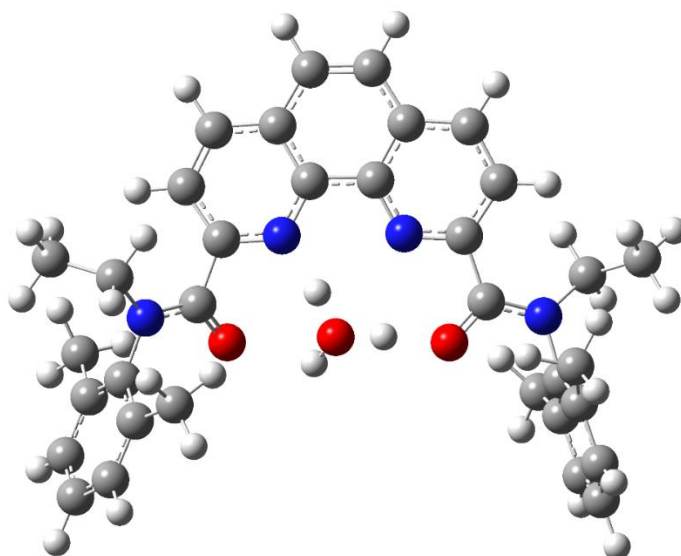


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N	-1.23089089	-0.43765256	-1.04338939
N	0.42402507	1.66216142	-0.64369095
N	-2.36781502	-3.71465494	-0.04330921
N	3.41491522	2.92905544	0.76947492
C	-1.97883084	-1.51976569	-1.22529037
C	-2.92012043	-1.59333090	-2.28258733
H	-3.49695370	-2.49816098	-2.46613711
C	-3.11279068	-0.48029105	-3.08528149

H	-3.84867763	-0.51090648	-3.89333067
C	-2.36820138	0.69921685	-2.86165549
C	-2.54112298	1.92088359	-3.58985795
H	-3.29536573	1.96154018	-4.38035160
C	-1.79585700	3.02872129	-3.29038075
H	-1.95588927	3.96420462	-3.83299227
C	-0.78720763	2.99366319	-2.27149636
C	-0.00357988	4.10757543	-1.89742637
H	-0.17425021	5.07416454	-2.37963316
C	0.96554140	3.97512590	-0.91797878
H	1.55694615	4.83603317	-0.60379340
C	1.18196214	2.71503816	-0.32106575
C	-0.55102610	1.78185584	-1.57007099
C	-1.39503422	0.63302701	-1.82823384
C	2.14117795	2.44714366	0.83776608
C	4.05822246	3.48185576	-0.44171167
H	4.95066177	2.86936726	-0.64687147
H	3.37654238	3.33191067	-1.29170874
C	4.47269598	4.94654826	-0.31368076
H	3.60680399	5.61638844	-0.19322117
H	5.01440742	5.25143791	-1.22254609
H	5.14305573	5.09004553	0.54675582
C	4.27667174	2.70223703	1.91656380
C	4.17118063	3.56361133	3.02664227
C	5.05184181	3.36545786	4.09650640
H	4.98821902	4.02834880	4.96368092
C	5.99370634	2.33857010	4.07153083
H	6.67416886	2.20041791	4.91518849
C	6.05309870	1.47555969	2.98070437
H	6.76981152	0.64957646	2.97564424
C	5.19383061	1.63372273	1.88481688
C	5.25728989	0.64884476	0.74253018
H	5.90004299	1.00861376	-0.07972728
C	3.11980582	4.64122859	3.09970745
H	2.11358369	4.19270502	3.14893852
C	-1.62200329	-2.59343110	-0.19961707
C	-1.84384608	-4.76055564	0.87831834
H	-2.25862874	-5.71495103	0.52515334
H	-0.75145275	-4.78031271	0.75554729
C	-2.21195952	-4.53836223	2.34461041
H	-1.81475447	-3.58091241	2.71058326
H	-1.76645342	-5.34557255	2.94707207
H	-3.30119023	-4.56988478	2.49538032
C	-3.68374479	-3.93787267	-0.59488577
C	-4.78745889	-3.22776416	-0.07563202
C	-6.05253013	-3.50703487	-0.61078305
H	-6.92121895	-2.97192224	-0.21747344
C	-6.21774710	-4.45150473	-1.62110600

H	-7.21405835	-4.65506216	-2.02089148
C	-5.11244561	-5.13632450	-2.12311772
H	-5.24077929	-5.86949381	-2.92423456
C	-3.82702688	-4.89795717	-1.62125553
C	-2.64402943	-5.63238216	-2.20175289
H	-2.35620041	-6.49672712	-1.57905139
C	-4.64647827	-2.16635551	0.98733029
H	-3.92932848	-2.45071146	1.76923842
H	5.68858963	-0.30092181	1.09042806
H	4.26223944	0.43721461	0.32291503
H	3.26202366	5.25455020	4.00052747
H	3.14754786	5.30853116	2.22496772
H	-4.29922865	-1.21250514	0.55374040
H	-5.61876480	-1.97463004	1.46308163
H	-2.88823791	-6.02078079	-3.20077536
H	-1.75827834	-4.98437884	-2.28535894
H	0.70516323	0.34206433	0.00529369
O	1.05794785	-0.53018943	0.56099123
H	1.18424369	-0.13848086	1.45918182
H	0.29921496	-1.27539327	0.52567847

L1*H3O⁺ (conformation III)

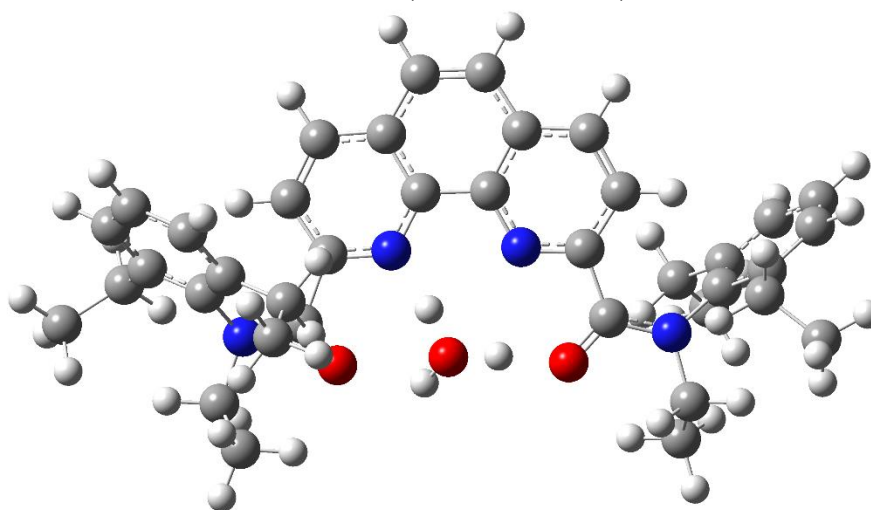


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O	0.99151963	2.17683847	1.42009435
N	-1.44556902	-0.42428812	-1.54232134
N	0.05749670	1.77600075	-1.13501601
N	-2.69575549	-3.53238903	-0.27309678
N	2.75693514	3.34309931	0.54937691
C	-2.08019700	-1.57338494	-1.73366503
C	-2.77973574	-1.83186223	-2.93800891
H	-3.21611679	-2.80867246	-3.14495476
C	-2.89116600	-0.82149444	-3.88093420
H	-3.44608234	-0.99403612	-4.80710284

C	-2.28320025	0.43387477	-3.65290815
C	-2.38975239	1.56583355	-4.52489673
H	-2.99383893	1.47929238	-5.43205458
C	-1.76872233	2.74727455	-4.22057614
H	-1.88276387	3.61399407	-4.87705743
C	-0.94336572	2.87720392	-3.05442176
C	-0.27836787	4.06614127	-2.68003993
H	-0.41069969	4.97193295	-3.27824538
C	0.53313177	4.08060860	-1.55865472
H	1.03027733	5.00002771	-1.24723471
C	0.71668747	2.89390213	-0.81620881
C	-0.77101428	1.75684170	-2.20081249
C	-1.51366074	0.54232727	-2.46338037
C	1.51697491	2.77863970	0.48066211
C	3.53413125	3.85310367	-0.60043998
H	4.48503266	3.29717534	-0.62390203
H	2.99729507	3.58897631	-1.52322856
C	3.83213175	5.35022896	-0.53809302
H	2.91855369	5.96251487	-0.59520397
H	4.48170063	5.62667309	-1.38318577
H	4.36065266	5.60460108	0.39273713
C	3.45479207	3.26621925	1.82085246
C	3.13604029	4.19749648	2.82901092
C	3.86341283	4.14489499	4.02386159
H	3.63402779	4.86426793	4.81465434
C	4.86056554	3.19063956	4.21719489
H	5.41809337	3.16541597	5.15655063
C	5.13027901	2.25501298	3.22208783
H	5.88863808	1.48460540	3.38727598
C	4.43078353	2.26796544	2.00771491
C	4.71581968	1.20608695	0.97318687
H	5.43643987	1.55167324	0.21155741
C	2.02110739	5.19833232	2.66360380
H	1.04919946	4.68272709	2.58985189
C	-1.84580590	-2.51540541	-0.55702786
C	-4.05413833	-3.71650569	-0.83144802
H	-4.72869913	-3.84384672	0.02920795
H	-4.35789681	-2.78354309	-1.32635715
C	-4.19192123	-4.92662457	-1.75347019
H	-3.56510237	-4.84440706	-2.65548248
H	-5.24183019	-5.02185160	-2.07145465
H	-3.91271949	-5.85064966	-1.22561778
C	-2.33166608	-4.43645920	0.80806343
C	-1.41347399	-5.47189278	0.54381181
C	-1.13111116	-6.37292883	1.57719070
H	-0.42671019	-7.18783033	1.38974494
C	-1.72507860	-6.23924835	2.83091381
H	-1.49144435	-6.95256896	3.62486151

C	-2.59940476	-5.18456659	3.07797754
H	-3.04017332	-5.06084507	4.07105871
C	-2.91866262	-4.25893179	2.07523292
C	-3.83978562	-3.10600018	2.39204360
H	-4.89301099	-3.34280762	2.16014971
C	-0.70980070	-5.59705194	-0.78349312
H	-1.41277171	-5.61192270	-1.62986194
H	5.16062414	0.32327414	1.45466742
H	3.80244935	0.88544501	0.44956819
H	1.98162319	5.87342030	3.52996792
H	2.14535887	5.81274827	1.75890911
H	-0.02133190	-4.74909492	-0.93570869
H	-0.11781693	-6.52239044	-0.81645066
H	-3.79551256	-2.87431099	3.46606545
H	-3.57011404	-2.19640583	1.83529452
H	0.32467638	0.51432154	-0.34723635
O	0.66556591	-0.30295715	0.28734390
H	0.65381807	0.12422890	1.17676156
H	-0.02364639	-1.11481740	0.20410531

L2*H3O⁺ (conformation I)

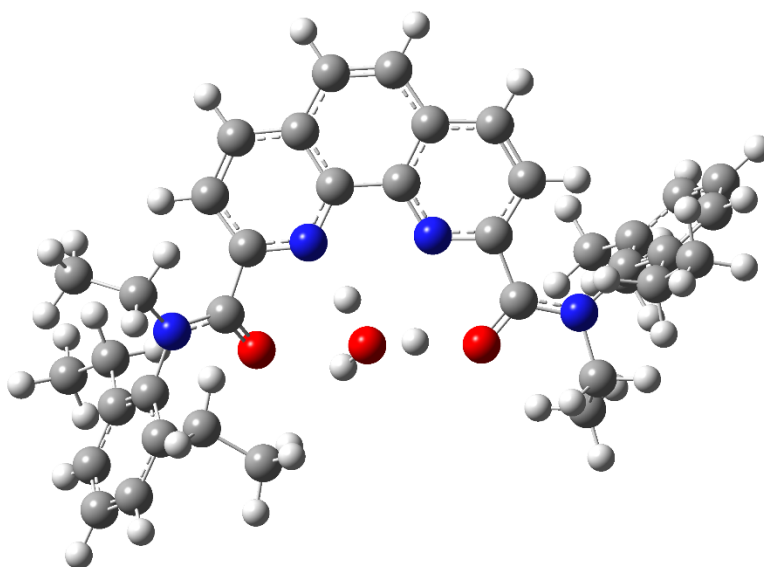


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N	0.50131287	1.53438120	-0.28002679
N	-2.59987666	-3.62379333	0.64586911
N	3.44264575	2.94164957	1.20451480
C	-2.03720150	-1.57331650	-0.71559176
C	-2.93761278	-1.68812233	-1.80375548
H	-3.55324962	-2.57550374	-1.93928882
C	-3.03669838	-0.63799103	-2.70219018
H	-3.73795223	-0.69959025	-3.53879377
C	-2.24134307	0.51807412	-2.54125201
C	-2.31827755	1.67855168	-3.37722477

H	-3.03449817	1.68709059	-4.20333306
C	-1.52850873	2.76960900	-3.13700577
H	-1.61302281	3.66116481	-3.76402663
C	-0.56883401	2.77342387	-2.07157551
C	0.25762626	3.87498817	-1.76008289
H	0.16427336	4.80047007	-2.33475551
C	1.17601706	3.78463057	-0.72972567
H	1.81080844	4.63363333	-0.48086520
C	1.29885969	2.57475636	-0.01396385
C	-0.42722888	1.61850565	-1.25854550
C	-1.31849475	0.49371642	-1.46016931
C	2.20890645	2.35888298	1.19504946
C	4.25112490	2.77180477	2.43882962
H	4.92331593	3.63883605	2.49639419
H	3.55117838	2.80630773	3.28645590
C	5.05611990	1.47325418	2.46628899
H	4.39373354	0.59721903	2.41083171
H	5.61733249	1.41816738	3.41224998
H	5.78043283	1.43327535	1.63950148
C	4.07070689	3.55010466	0.05606262
C	4.44690418	2.75255636	-1.05009112
C	5.02724291	3.39616178	-2.15305182
H	5.30816261	2.80067435	-3.02597005
C	5.25432044	4.76851972	-2.15691318
H	5.70711752	5.24634015	-3.02909456
C	4.89951096	5.53304254	-1.04724689
H	5.07162839	6.61339021	-1.05362417
C	4.30240959	4.94751423	0.07447852
C	3.89272646	5.84014153	1.23093936
C	4.25263486	1.24878981	-1.11095161
H	3.55807830	1.01982735	-1.93947144
C	-1.77127922	-2.57865578	0.40270113
C	-2.17922204	-4.59472269	1.69320444
H	-2.67573484	-5.54277714	1.44484485
H	-1.09147198	-4.72497454	1.59566573
C	-2.53672580	-4.16205165	3.11416590
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H	-2.17885829	-4.92831614	3.81955751
H	-3.62436430	-4.06494817	3.24350203
C	-3.90616016	-3.81372103	0.05764437
C	-4.98232383	-2.98638242	0.45145152
C	-6.22501023	-3.19967366	-0.16267055
H	-7.06861019	-2.56132344	0.11312694
C	-6.40279329	-4.19908868	-1.11463785
H	-7.37986288	-4.34074964	-1.58302815
C	-5.33189501	-5.01492412	-1.47381768
H	-5.47072145	-5.79421133	-2.22883293
C	-4.06669409	-4.84356797	-0.89934433

C	-2.92822359	-5.73404266	-1.35791720
C	-4.85590700	-1.87099579	1.47190082
H	3.27642143	6.66418968	0.82845326
H	3.25017608	5.28433847	1.93110081
H	3.77214146	0.88508133	-0.19163147
H	-3.82667599	-1.81935899	1.85458130
H	-5.04622146	-0.91007081	0.96035086
H	-2.87870800	-5.68664146	-2.46017233
H	-1.96786368	-5.34502598	-0.98680028
H	0.71076951	0.23549276	0.42989930
O	1.01945741	-0.62559353	1.03069531
H	1.17096044	-0.17267749	1.89665314
H	0.21894746	-1.32308339	1.04901750
C	-5.82743378	-2.00726215	2.65704495
H	-6.87758162	-1.99319655	2.32907088
H	-5.66074899	-2.94901357	3.20239332
H	-5.68539437	-1.17300178	3.36128969
C	-3.09531109	-7.20643335	-0.93854526
H	-4.03022815	-7.63068359	-1.33511099
H	-2.25825242	-7.80978141	-1.32241900
H	-3.11976819	-7.31674345	0.15692577
C	5.08650136	6.45381582	1.98626690
H	4.73031700	7.10779437	2.79712972
H	5.72904791	5.67763107	2.43074407
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C	5.56248469	0.47047072	-1.32896552
H	6.27465759	0.65525782	-0.51008581
H	5.35891872	-0.61081537	-1.36896828
H	6.05524044	0.75533442	-2.27049885

L2*H3O⁺ (conformation II)

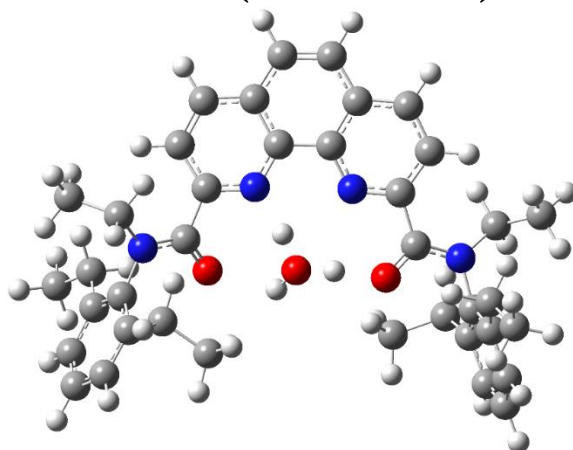


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N	3.52980068	3.01028947	0.59811143
C	-2.03675597	-1.32499953	-1.33510186
C	-3.00171765	-1.35809038	-2.37305281
H	-3.62091435	-2.23628066	-2.54488434
C	-3.16360653	-0.23800837	-3.17254744
H	-3.91679616	-0.23791272	-3.96508615
C	-2.36919629	0.91046082	-2.96336551
C	-2.51474316	2.13952985	-3.68467213
H	-3.28222095	2.20820871	-4.46034942
C	-1.72913814	3.22093513	-3.39356205
H	-1.86860666	4.16451139	-3.92777430
C	-0.70512848	3.14745681	-2.39250437
C	0.11159612	4.23768286	-2.02099691
H	-0.04119634	5.21267039	-2.49202192
C	1.09032713	4.07222442	-1.05693025
H	1.70266043	4.91717794	-0.74080570
C	1.28797157	2.80077324	-0.47705658
C	-0.49029969	1.92403991	-1.70361217
C	-1.37795271	0.80454434	-1.95017139
C	2.26542003	2.50543438	0.66054413
C	4.16154651	3.61855464	-0.59488412
H	5.07678440	3.04130963	-0.80415545
H	3.49153378	3.46894967	-1.45405449
C	4.53622478	5.09064124	-0.42968569
H	3.65573191	5.73965765	-0.30237898
H	5.07923003	5.42626673	-1.32692233
H	5.19646298	5.23015979	0.43916155
C	4.40633594	2.79088576	1.73849184
C	4.29440656	3.64950100	2.85612037
C	5.21790343	3.48852188	3.89376279
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C	6.27581307	1.65281956	2.73867337
H	7.03977442	0.87064752	2.70232176
C	5.36517254	1.76291739	1.67685697
C	5.41542501	0.72755177	0.57113785
H	6.45713698	0.63231144	0.21866412
C	3.17961223	4.67623162	2.93711436
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C	-2.00455541	-4.52478052	0.84297349
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H	-0.91968925	-4.63398846	0.69751030

C	-2.31167985	-4.17973256	2.29958994
H	-1.84171330	-3.22892535	2.58632459
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H	-3.39451803	-4.12302752	2.48027761
C	-3.75601476	-3.75995428	-0.76943892
C	-4.91978174	-3.11506456	-0.30513940
C	-6.12769953	-3.40922716	-0.95861304
H	-7.04423793	-2.91405564	-0.62681183
C	-6.17690473	-4.31258354	-2.01309186
H	-7.12883004	-4.52602996	-2.50556410
C	-5.01145090	-4.94532102	-2.45148736
H	-5.06198286	-5.64469641	-3.28772262
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C	-2.49452167	-5.31961453	-2.34488841
H	-2.08163560	-5.96663326	-1.54982377
C	-4.92644242	-2.10447180	0.82513127
H	-3.90699275	-1.96091534	1.21119828
H	4.81214053	1.04147746	-0.29337751
H	3.16396260	5.26045094	2.00156823
H	-5.24554707	-1.12945837	0.41437403
H	-1.74194142	-4.52254437	-2.48449219
H	0.73612188	0.42498311	-0.14630362
O	1.04432429	-0.44384030	0.42616488
H	1.20180259	-0.02254696	1.30716435
H	0.24563238	-1.15132255	0.41417992
C	-5.86061935	-2.48585681	1.98666623
H	-6.90615775	-2.57743686	1.65635217
H	-5.56812559	-3.44786324	2.43529493
H	-5.82343978	-1.71543767	2.77226936
C	-2.60642095	-6.13970791	-3.63248956
H	-1.61381503	-6.52148392	-3.91517348
H	-3.27014513	-7.00943953	-3.50779024
H	-2.98517184	-5.53457032	-4.47127138
C	3.23526861	5.63895957	4.12575044
H	2.39728676	6.35055259	4.06819591
H	3.14947107	5.10776167	5.08651066
H	4.17005954	6.22149002	4.13696591
C	4.91509634	-0.65044154	1.04607327
H	3.86146474	-0.59504640	1.35838485
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H	5.50433816	-1.01297310	1.90189063

L2*H3O⁺ (conformation III)

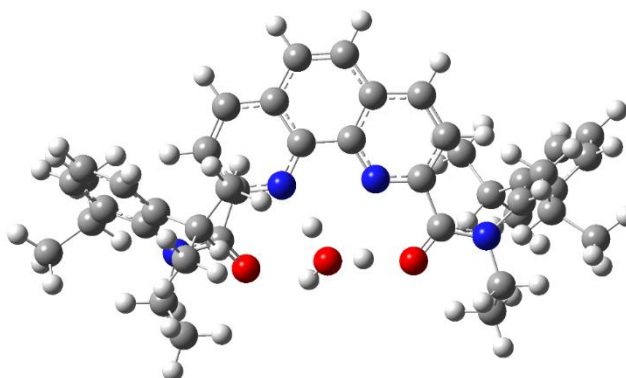


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C	-2.16422562	-1.53517793	-2.01438689
C	-2.85392782	-1.80054072	-3.22282313
H	-3.28185855	-2.78055241	-3.43166761
C	-2.96685313	-0.79229437	-4.16767591
H	-3.51593961	-0.96967815	-5.09638884
C	-2.36963658	0.46766725	-3.93759056
C	-2.48544535	1.59885037	-4.80926954
H	-3.08583579	1.50637615	-5.71831742
C	-1.87942008	2.78680662	-4.50088236
H	-2.00241838	3.65380911	-5.15537875
C	-1.05861000	2.92351978	-3.33244134
C	-0.41526134	4.12134625	-2.95026231
H	-0.56420976	5.02886571	-3.54187771
C	0.39334469	4.14334166	-1.82716296
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C	0.60193173	2.95504409	-1.09326702
C	-0.87018970	1.80277782	-2.48234185
C	-1.60369297	0.58210864	-2.74607067
C	1.41543773	2.84815791	0.19740447
C	3.36292799	4.09151269	-0.84344447
H	4.35562655	3.61279468	-0.85710501
H	2.86375047	3.80526529	-1.78062281
C	3.54967345	5.60513316	-0.74915705
H	2.59752139	6.15504694	-0.81186816
H	4.19135417	5.94044667	-1.57890637
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C	3.31510136	3.45130708	1.55850177
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H	5.94395841	1.90923605	3.06297578
C	4.37130101	2.53685855	1.72648261
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H	-3.62406431	-4.81364621	-2.96099471
H	-5.30151960	-5.00520115	-2.38518103
H	-3.97122425	-5.82668592	-1.53476278
C	-2.43855367	-4.39527311	0.53575436
C	-1.54801948	-5.46099197	0.27793708
C	-1.32145830	-6.37713551	1.31079186
H	-0.64811931	-7.21906809	1.14218912
C	-1.94409691	-6.23541774	2.55134191
H	-1.76280646	-6.97201249	3.33784208
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C	-3.85057093	-2.97329932	2.14973509
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H	-1.56264013	-5.48031168	-1.87042628
H	4.18840485	1.62061908	-0.22969325
H	1.79960301	5.77699714	1.43117343
H	-0.16821000	-4.68720600	-1.14645824
H	-4.26798329	-2.49460578	1.25097882
H	0.23644158	0.54847433	-0.63491843
O	0.56829436	-0.25865680	0.00594231
H	0.56335976	0.19529526	0.88335214
H	-0.12937256	-1.06656057	-0.06513382
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H	1.30504678	5.81113180	4.48000202
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C	4.31124608	0.04851093	1.24614746
H	3.22756777	-0.00847316	1.42859949
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L3*H3O⁺ (conformation I)

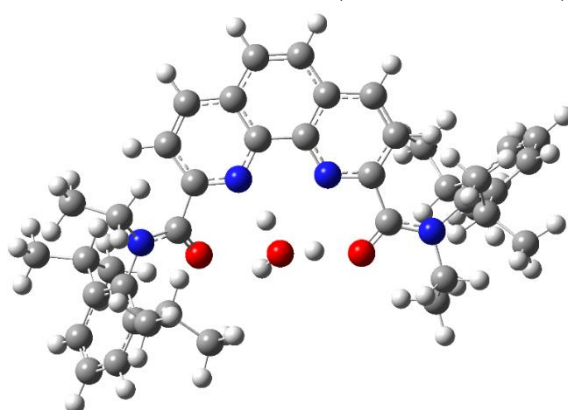


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C	-2.96340403	-1.76060315	-1.63984445
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C	-3.02649426	-0.74509939	-2.58028193
H	-3.73811093	-0.81121405	-3.40779716
C	-2.18520097	0.38360673	-2.47094761
C	-2.22435817	1.51015429	-3.35472022
H	-2.94383976	1.50964003	-4.17803507
C	-1.39460309	2.58043046	-3.16309695
H	-1.44876644	3.44738608	-3.82690852
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C	0.43453999	3.67621004	-1.83865517
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C	-0.32882486	1.47132933	-1.23681077
C	-1.25852573	0.36880183	-1.39263422
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C	4.35688588	2.59425047	2.46232153
H	5.07534904	3.42333166	2.51495741
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H	-2.23534650	-7.83642415	-1.00679744

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H	6.59442549	0.91639062	-0.37644519
H	5.88447529	-0.44909061	-1.28053519
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H	-6.32499733	-0.52499653	0.72447307
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H	2.73150789	1.33756446	-2.37044143
C	2.87640605	6.80693697	1.07383142
H	3.33740508	7.55547591	0.41036384
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L3*H3O⁺ (conformation II)

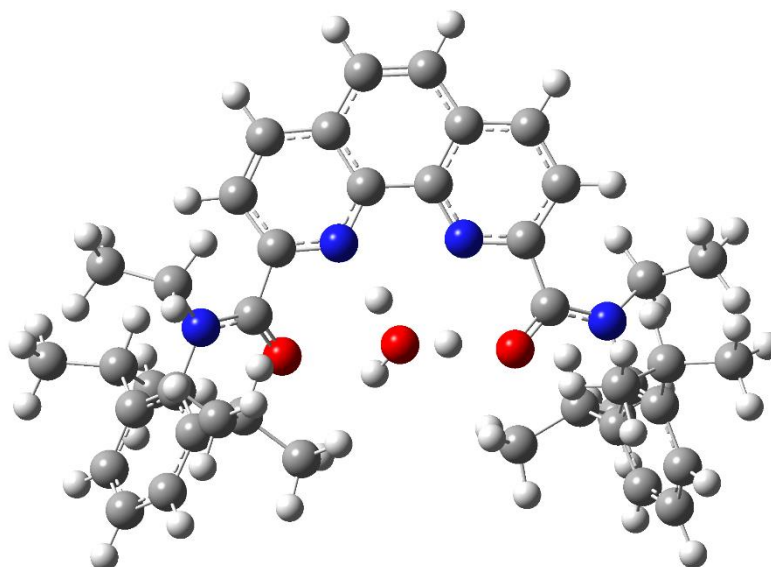


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H	6.86650725	1.54593854	-0.48448281
C	2.13654480	4.66822090	3.84127309
H	1.65565554	3.70108141	3.63335429
H	2.56370325	4.63114459	4.85646237
H	1.36834027	5.45850249	3.82655135

L3*H3O⁺ (conformation III)



O	-0.92057389	-2.24119091	-0.28024176
O	0.80716986	2.27243276	1.03475358
N	-1.57149377	-0.33603448	-1.96128514
N	-0.13699918	1.90619722	-1.51999751
N	-2.73596954	-3.50301355	-0.75507380
N	2.46066952	3.62710223	0.21648635
C	-2.17015798	-1.50105770	-2.17032770
C	-2.85225553	-1.76770177	-3.38281643
H	-3.25678026	-2.75550892	-3.60280049
C	-2.98847412	-0.75037010	-4.31470712
H	-3.53126292	-0.92872271	-5.24692227
C	-2.42189195	0.52062182	-4.06705383
C	-2.56012782	1.65902699	-4.92595784
H	-3.15432078	1.56360287	-5.83874569
C	-1.98203798	2.85676015	-4.60184089
H	-2.12147667	3.72784923	-5.24754183
C	-1.16912167	2.99893353	-3.42854425
C	-0.55127189	4.20580305	-3.03247769
H	-0.71547782	5.11552835	-3.61661151
C	0.25220422	4.23319609	-1.90588603
H	0.70979668	5.16702239	-1.57730013
C	0.47950343	3.04256171	-1.18121470
C	-0.96092205	1.87355058	-2.58938958
C	-1.66337237	0.63919374	-2.87126873
C	1.28265378	2.94604612	0.11689083
C	3.22839130	4.18464510	-0.91984539
H	4.20897827	3.68044217	-0.92407278
H	2.72297736	3.89415190	-1.85236005
C	3.44386327	5.69498455	-0.85085972
H	2.49843285	6.25781312	-0.89847813
H	4.07338733	6.00912452	-1.69785447
H	3.96011255	5.97323690	0.07949274

C	3.14213926	3.61261584	1.50203483
C	2.79500188	4.57848864	2.47193713
C	3.52110608	4.58626694	3.66999243
H	3.27343400	5.32112610	4.43983345
C	4.54875571	3.67573321	3.89863700
H	5.10675320	3.70611027	4.83773427
C	4.85414546	2.71603561	2.93797217
H	5.64511471	1.98824037	3.13680742
C	4.15420444	2.65409959	1.72631783
C	4.46914718	1.53335836	0.74180757
C	1.63716673	5.55189185	2.28911832
C	-1.91759829	-2.45319941	-1.00637731
C	-4.10312464	-3.68743982	-1.29656699
H	-4.76147725	-3.82379897	-0.42341868
H	-4.41545191	-2.75153262	-1.78052069
C	-4.25527942	-4.88836206	-2.22723124
H	-3.63178820	-4.80497890	-3.13133699
H	-5.30801677	-4.97054437	-2.53928105
H	-3.98005539	-5.81871707	-1.70963526
C	-2.35774580	-4.42232029	0.31180139
C	-1.51048870	-5.50951730	0.00916953
C	-1.23125712	-6.41694587	1.03987987
H	-0.57819472	-7.26934422	0.83773409
C	-1.76555759	-6.25117812	2.31423140
H	-1.53848882	-6.97568435	3.10011881
C	-2.57677865	-5.15450318	2.59214391
H	-2.96951819	-5.01788619	3.60291163
C	-2.88545935	-4.21184780	1.60371726
C	-3.70492736	-2.98075036	1.97416123
C	-0.84837954	-5.69012284	-1.35151157
H	-1.32626032	-4.98655547	-2.05302433
H	3.80983474	1.65163856	-0.13409852
H	1.32307022	5.50201340	1.23347215
H	-3.88281845	-2.39591261	1.05642583
H	0.17015030	0.63231767	-0.75639761
O	0.52950962	-0.18276566	-0.13409556
H	0.51316047	0.24191154	0.75673036
H	-0.14084755	-1.00910179	-0.22247108
C	-2.90633825	-2.07607803	2.93437785
H	-3.47119033	-1.15444872	3.14862289
H	-2.71538714	-2.58673966	3.89159478
H	-1.93524701	-1.80274788	2.49446192
C	-1.02884081	-7.10816359	-1.92026133
H	-0.51530723	-7.86145870	-1.30232422
H	-2.09108119	-7.39160914	-1.98317310
H	-0.59689795	-7.16488938	-2.93223570
C	2.02941332	7.00919768	2.58874751
H	1.18051406	7.67844397	2.37503429

H	2.29608175	7.14800804	3.64828921
H	2.88697333	7.33470066	1.97939788
C	4.14906409	0.15904086	1.36266529
H	3.10862795	0.12154020	1.71933810
H	4.29498808	-0.63940546	0.61755357
H	4.80800387	-0.05321509	2.21950566
C	0.64670341	-5.31822742	-1.26688599
H	1.18190489	-6.00913954	-0.59573757
H	1.11275431	-5.38368118	-2.26346708
H	0.77713911	-4.29625236	-0.88114887
C	-5.07572885	-3.34681234	2.57166558
H	-5.65887476	-3.99001440	1.89309698
H	-4.96651715	-3.88434849	3.52682024
H	-5.66068608	-2.43428866	2.76877869
C	5.92789466	1.58453575	0.25038428
H	6.63335972	1.42752955	1.08175612
H	6.10822885	0.79348142	-0.49508333
H	6.17122554	2.55515024	-0.21119381
C	0.43628659	5.11503759	3.15359413
H	0.13948510	4.08196814	2.91947685
H	0.69010466	5.16673283	4.22470790
H	-0.42398873	5.78108746	2.97677024

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