

Electronic Supplementary Information

2-Methylpyrrolidine Derived 1,10-Phenanthroline-2,9-diamides: New Ligands for Ln(III)/Am(III) Separation

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1. Experimental part

1.1 Materials

Ar-saturated solvents, purified and dried using standard techniques were used¹.

Lanthanides nitrates $\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$, $\text{Nd}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$, $\text{Eu}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$, $\text{Lu}(\text{NO}_3)_3 \cdot x\text{H}_2\text{O}$ and (\pm)-2-methylpyrrolidine were purchased from Sigma and used without further purification. Water content x in lutetium nitrate was determined as $x = 3$. Deuterated solvents for NMR spectra were purchased from commercial sources and used without further purification. Triethylamine was purified by simple distillation, previously held for 12 hours over sodium hydroxide. 3-Nitrobenzotrifluoride (“F-3”) analytical grade was purchased from Rhodia (France) and was used as a solvent in the extraction experiments without further purification.

Dichlorides of 1,10-phenanthroline-2,9-dicarboxylic acids for synthesis of ligands **L3** and **L4** may be prepared according to knowing procedures.²

Syntheses of ligands **L1** and **L2** were reported earlier.^{2,3}

1.2 Methods

All syntheses were performed in argon inert atmosphere.

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 (¹³C).

IR spectra were recorded on FTIR spectrometer Nicolet iS5 (Thermo Scientific) using an internal reflectance attachment with diamond optical element – attenuated total reflection (ATR) with 45° angle of incidence. Resolution 4 cm⁻¹, the number of scans is 32.

HRMS ESI - mass spectra were recorded on the MicroTof Bruker Daltonics and Orbitrap Elite instruments.

Single crystals of **L1**, **L3** and **L4** were obtained upon slow isothermal (25°C) recrystallization of corresponding substances from acetonitrile-dichloromethane (50/50) mixture.

X-ray diffraction data for **L1**, **L3** and **L4** were collected at 120 K with a Bruker APEXII DUO CCD diffractometer; those for **L3*** $\text{Nd}(\text{NO}_3)_3$ and **L4*** $\text{Nd}(\text{NO}_3)_3$, at 100 K with a Bruker D8 Quest CMOS diffractometer, both using graphite monochromated Mo-K α radiation ($\lambda = 0.71073$ Å). Using Olex2⁴, the structures were solved with the ShelXT⁵ structure solution program using Intrinsic Phasing and refined with the XL⁶ refinement package using Least-Squares minimization against F^2 in anisotropic approximation for non-hydrogen atoms. Positions of hydrogen atoms were calculated, and they were refined in isotropic approximation within the riding model. Crystal data and structure refinement parameters for **L1**, **L3**, **L4**, **L3*** $\text{Nd}(\text{NO}_3)_3$ and **L4*** $\text{Nd}(\text{NO}_3)_3$ are given in Table S1. CCDC 2076146 (for **L1**), 2072998 (for **L3**), 2072997 (for **L4**), 2164120 (for

L3*Nd(NO₃)₃) and 2164121 (for **L4***Nd(NO₃)₃) contain the supplementary crystallographic data for this paper.

Detailed crystallographic data provided here in Chapter 3.

UV–VIS spectra were recorded at the temperature 25.0 ± 0.1 °C in the wavelength region of 200–400 nm (0.5 nm interval) on a Shimadzu UV 1800 spectrophotometer controlled by LabSolutions UV-Vis software with thermostatic attachment (Shimadzu TCC-100) using quartz cuvettes with an optical path length of 10 mm. A stock solution of the ligand was prepared (ca. 10^{-4} mol/L) by dissolving respective ligand in CH₃CN, and then a working ligand solution (ca. 10^{-5} mol/L) was prepared from the initial solution. A working titrant solution (10^{-3} mol/L) was prepared by dissolving respective lanthanide (III) nitrate hydrate Ln(NO₃)₃·6H₂O (Ln = La, Nd, Eu, Lu) in CH₃CN. 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. The titration was carried out by adding 2 µl aliquots of the working metal cation solution to 2 mL of the working ligand solution in the titration cell. The titration continued until no obvious change was observed in the spectra. The stability constants of the Ln(III) complexes were calculated using the HypSpec2014 program.

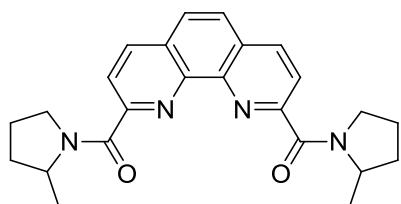
1.3 Solvent extraction experiments

For solvent extraction experiments 0.5 mL of organic solution of the ligand in “F-3” and 0.5 mL of aqueous phase containing nitric acid and radionuclides or lanthanides were treated with a vortex shaker for 30 minutes in 1.5 mL polypropylene vial at temperature 25 ± 1 °C. Then samples were centrifuged (5 minutes, 6000 rpm) and aliquots of each phase were taken for determination of radionuclide or lanthanide concentration. Content of ²⁴¹Am ($E_{\gamma} = 59.5$ keV) and ¹⁵²Eu ($E_{\gamma} = 121.8$ keV) was determined by gamma-spectrometry using a high-pure germanium detector GR 3818 (Canberra Ind.). The distribution coefficients were calculated as the ratio of count rates for the corresponding organic and aqueous phases, and separation factors were calculated as the ratio of distribution coefficients for the two elements. Content of ²⁴¹Am ($E_{\alpha} = 5637$ keV) and ²⁴⁴Cm ($E_{\alpha} = 5901$ keV) was determined by alpha spectrometer Model 7401 with Si detectors (Canberra Ind.). The content of lanthanides in the initial aqueous phase and in the equilibrium aqueous phase after extraction was determined by ICP-OES (Agilent ICP-OES 720). For ²⁴⁴Cm and lanthanides the activity/concentration in the organic phase was calculated as the difference between the concentrations in the initial and equilibrium aqueous phases. All extraction experiments were repeated three times. Errors for $0.01 < D < 100$ are within 10%.

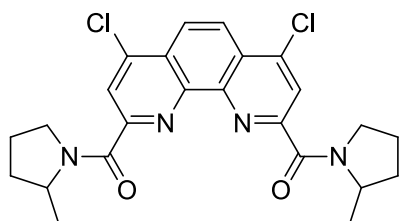
1.4 Synthesis and analytical data

General method for synthesis of diamides

A solution of (\pm)-2-methylpyrrolidine (12.5 mmol) and 1.74 ml of triethylamine (12.5 mmol) in 10 ml of methylene chloride was added at -10°C under vigorous stirring to a suspension of 5 mmol of the corresponding chloride in 50 ml of methylene chloride. Then the reaction mixture was allowed to reach room temperature followed by refluxing for 4 hours. Next, the reaction mixture was diluted with 50 ml of methylene chloride, washed with water (2×50 ml), dried over sodium sulfate, and the solvent was distilled off. The residue was purified by recrystallization from a mixture of hexane/ethyl acetate or by silica gel column chromatography (eluent: hexane/acetone = 7/3), obtaining the desired product in the form of a white or slightly colored solid.



(2-methylpyrrolidin-1-yl)(9-((2-methylpyrrolidin-1-yl)carbonyl)-1,10-phenanthrolin-2-yl)methanone (MePyrrDAPhen). Yield 57% (1.15 g), yellowish powder, m.p. $211\text{-}214^{\circ}\text{C}$, Rf 0.24 (acetone:hexane 1:2); ^1H NMR (400 MHz, CDCl_3) δ 8.39-7.80 (group of m, 6H, phenanthroline CH), 5.68-5.17 (group of m, 1H, pyrrolidine ring CH), 4.55-3.65 (group of m, 4H, pyrrolidine ring CH_2 + 1H, pyrrolidine ring CH), 2.33-1.60 (groups of m, 8H, pyrrolidine ring CH_2), 1.47-0.81 (groups of m, 6H, CH_3); ^{13}C NMR (101 MHz, CDCl_3) δ 166.4-165.9 (group of CO), 154.7-154.0, 144.8-144.4, 137.2-136.9, 129.4-129.2, 127.5-127.4, 123.7-123.2 (groups of phenanthroline carbons), 54.6-53.9 (group of pyrrolidine ring CH carbons), 49.6-49.3, 47.3-46.9, 34.2-33.8, 32.3-32.1, 25.2-24.8, 22.0-21.7 (groups of pyrrolidine ring CH_2 and CH_3 carbons), 19.7-19.5 (group of CH_3 carbons); IR (ν , cm^{-1}) 3066, 3037, 2965, 2896, 2868 (C-H stretching vibrations), 1616 (C=O), 1546, 1505, 1455, 1418, 1398 (C=C, C=N); HRMS (ESI-TOF) (m/z) $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{24}\text{H}_{27}\text{N}_4\text{O}_2$ 403.2129, found 403.2130.



(4,7-Dichloro-9-((2-methylpyrrolidin-1-yl)carbonyl)-1,10-phenanthrolin-2-yl)(2-methylpyrrolidin-1-yl)methanone (MePyrrDAPhenCl). Yield 60% (1.41 g), yellowish powder, m.p. $225\text{-}227^{\circ}\text{C}$, Rf 0.67 (acetone:hexane 1:2); ^1H NMR (400 MHz, CDCl_3) δ 8.43-8.22 (m, 4H,

phenanthroline CH), 5.65-5.20 (group of m, 2H, pyrrolidine ring CH), 4.55-1.60 (groups of m, 12H, pyrrolidine ring CH₂), 1.46-0.87 (groups of m, 6H, CH₃); ¹³C NMR (101 MHz, CDCl₃) δ 165.2-164.4 (group of CO), 154.9-154.1, 144.8-144.3, 145.4-145.3, 143.9-143.7, 127.6-127.4, 124.5-124.1 (groups of phenanthroline carbons), 54.8-54.1 (group of pyrrolidine ring CH), 49.6-49.4, 47.5-47.2, 34.1-33.8, 32.3-32.1, 25.1-24.9 (groups of pyrrolidine ring CH₂), 22.0-21.7 (groups of CH₃ and pyrrolidine ring CH₂), 19.7-19.5 (group of CH₃); IR (ν, cm⁻¹) 3071, 3042, 2966, 2880 (C-H stretching vibrations), 1622 (C=O), 1570, 1529, 1455, 1448, 1415 (C=C, C=N); HRMS (ESI-TOF) (m/z) [M+H]⁺ calculated for C₂₄H₂₅Cl₂N₄O₂ 471.1349, found 471.1343.

General method for synthesis of complexes

A solution of 0.1 mmol of lanthanide nitrate in 1 ml of dry acetonitrile was added dropwise to a solution of 0.1 mmol of ligand in 1 ml of chloroform. After that the reaction mixture was concentrated *in vacuo* (~20 Torr) to 1/5 of the initial volume and treated with 2 ml of diethyl ether. The resulting precipitate of the complex was filtered, washed with a fresh portion of ether, dried in air, then at 80°C at ~2 Torr.

Complex L3*La(NO₃)₃. Yield 66.8 mg (91.8%). Gray-yellow powder. T_{decomp.} 193°C. IR (ν, cm⁻¹) 1597(CO), 1456, 1313 (ONO₂).

Complex L3*Nd(NO₃)₃. Yield 68.7 mg (93.8%). Gray-green powder. T_{decomp.} 199°C. IR (ν, cm⁻¹) 1595(CO), 1464, 1301 (ONO₂).

Complex L3*Eu(NO₃)₃. Yield 72 mg (96 %). White powder. T_{decomp.} 325°C. IR (ν, cm⁻¹) 1597 (CO), 1470, 1300 (ONO₂).

Complex L3*Lu(NO₃)₃. Yield 71.5 mg (93.7%). Gray-yellow powder. T_{decomp.} 184°C. IR (ν, cm⁻¹) 1600(CO), 1465, 1301 (ONO₂).

Complex L4*La(NO₃)₃ Yield 74.4 mg (93.5%). Light yellow powder. T_{decomp.} 227°C. IR (ν, cm⁻¹) 1601(CO), 1464, 1301 (ONO₂).

Complex L4*Nd(NO₃)₃ Yield 77.8 mg (97%). Light yellow powder. T_{decomp.} 235°C. IR (ν, cm⁻¹) 1599(CO), 1460, 1303 (ONO₂).

Complex L4*Eu(NO₃)₃ Yield 78.5 mg (96.8%). Light yellow powder. T_{decomp.} 238°C. IR (ν, cm⁻¹) 1603(CO), 1464, 1308 (ONO₂).

Complex L4*Lu(NO₃)₃ Yield 81.1 mg (97%). Yellow powder. T_{decomp.} 197°C. IR (ν, cm⁻¹) 1606 (CO), 1463, 1296 (ONO₂).

2 NMR, IR and HRMS spectra of synthesized compounds

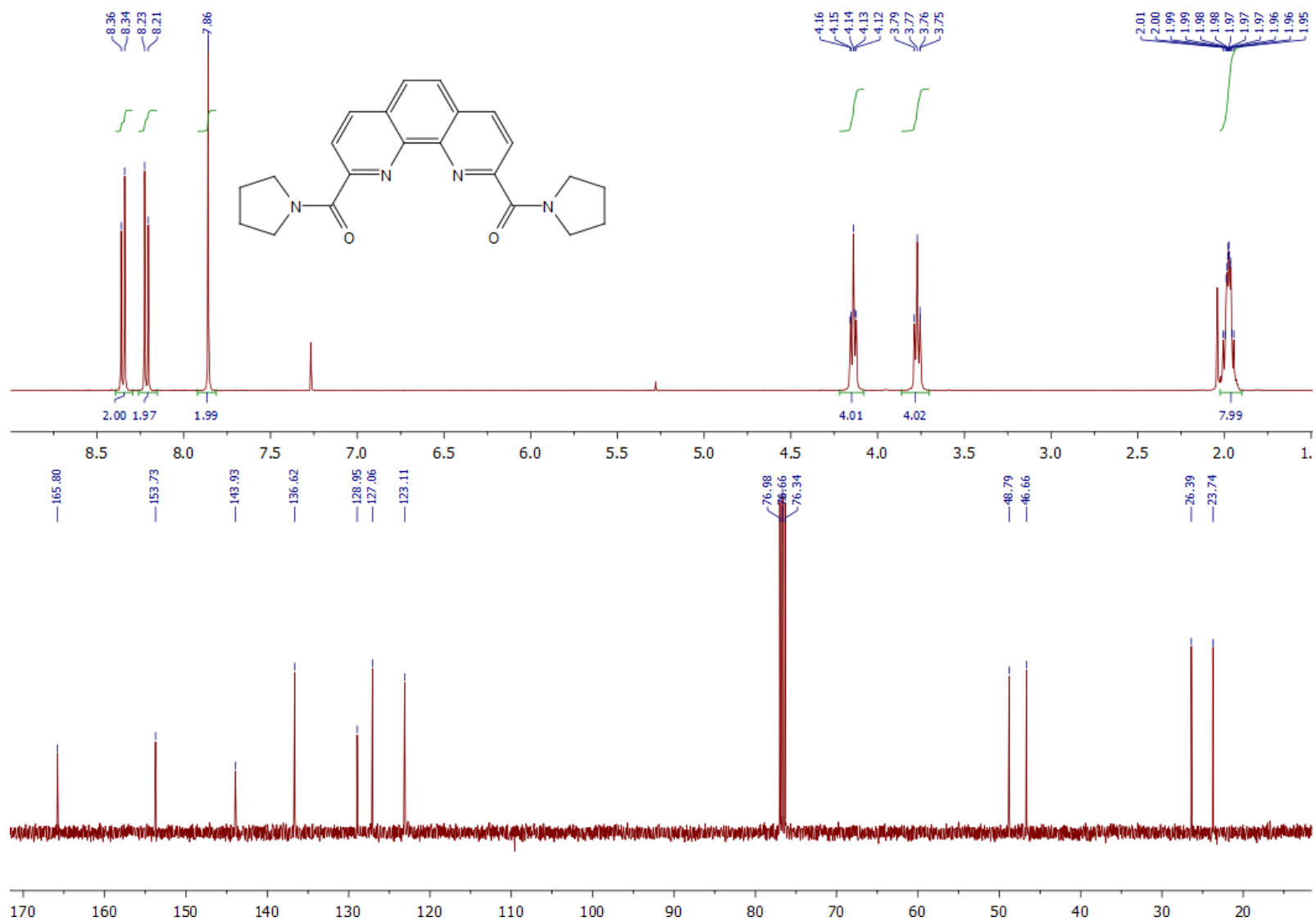


Figure S1. ^1H NMR and ^{13}C NMR spectra of L1 in CDCl_3 at 25°C

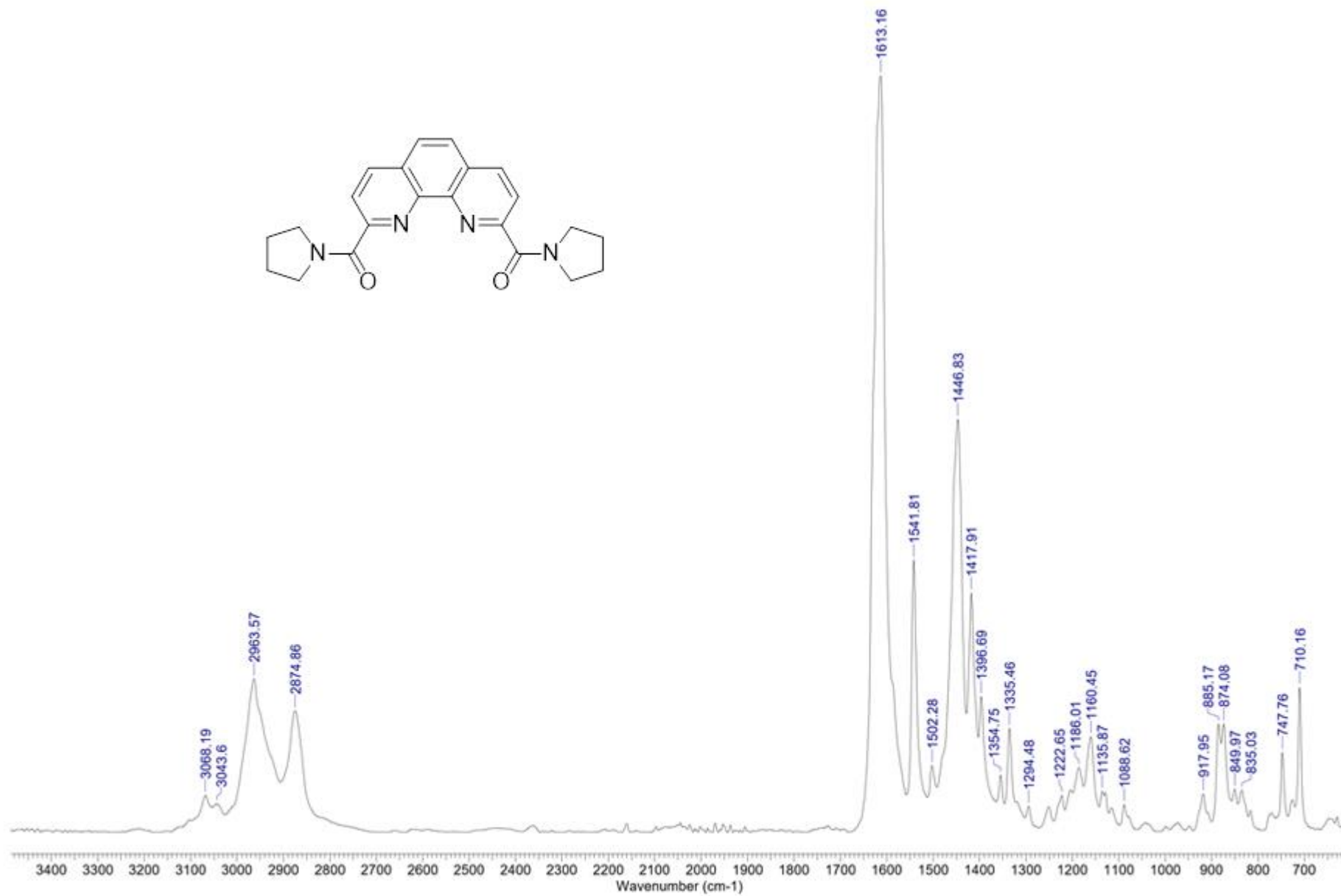


Figure S2. Solid-state IR spectra of L1

Display Report

Analysis Info

Analysis Name D:\Data\Kolotyrkina\2020\Muzalevsky\0916033.d
Method tune_50-1600.m
Sample Name /MUSE PVS-066
Comment C22H22N4O2 mH 375.1815 calibrant added CH3CN

Acquisition Date 16.09.2020 18:58:59

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

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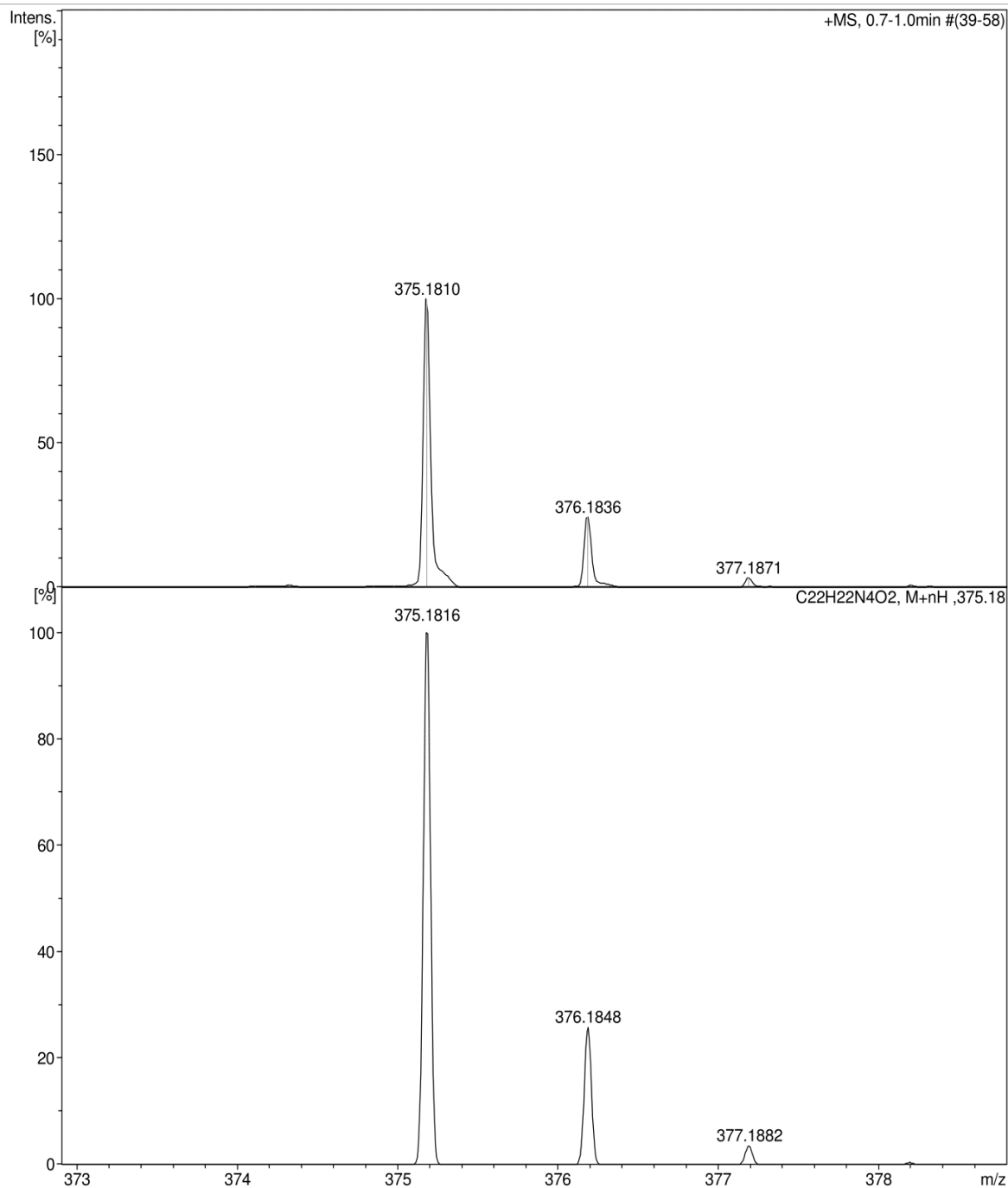


Figure S3. HRMS spectra of L1

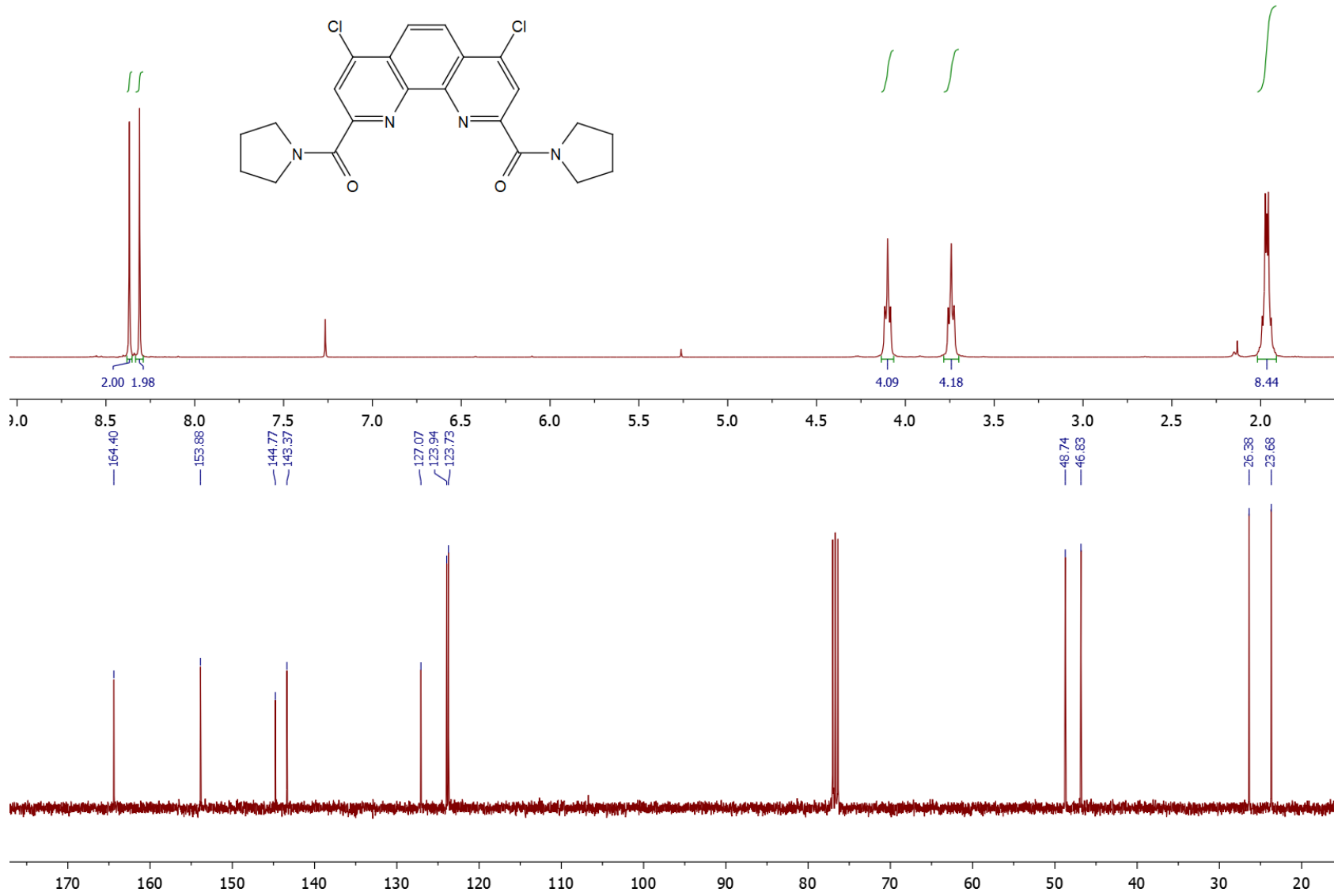


Figure S4. ¹H NMR and ¹³C NMR spectra of L2 in CDCl₃ at 25°C

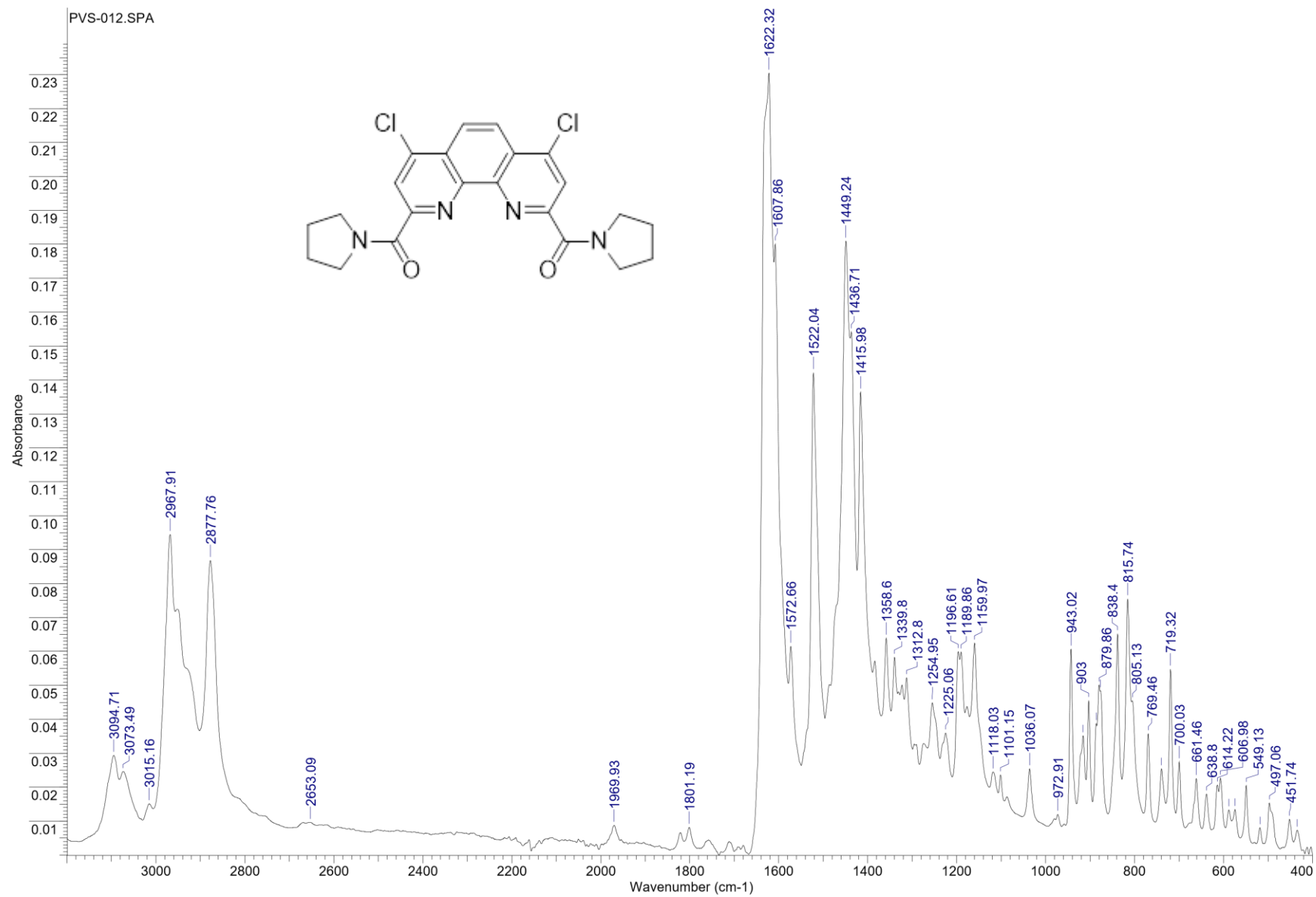


Figure S5. Solid-state IR spectra of L2

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Analysis Info

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Method tune_50-1600.m
Sample Name /MUSE PVS-012
Comment C22H20Cl2N4O2 mH 443.1036 clb added CH3CN

Acquisition Date 11.07.2019 11:55:25
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

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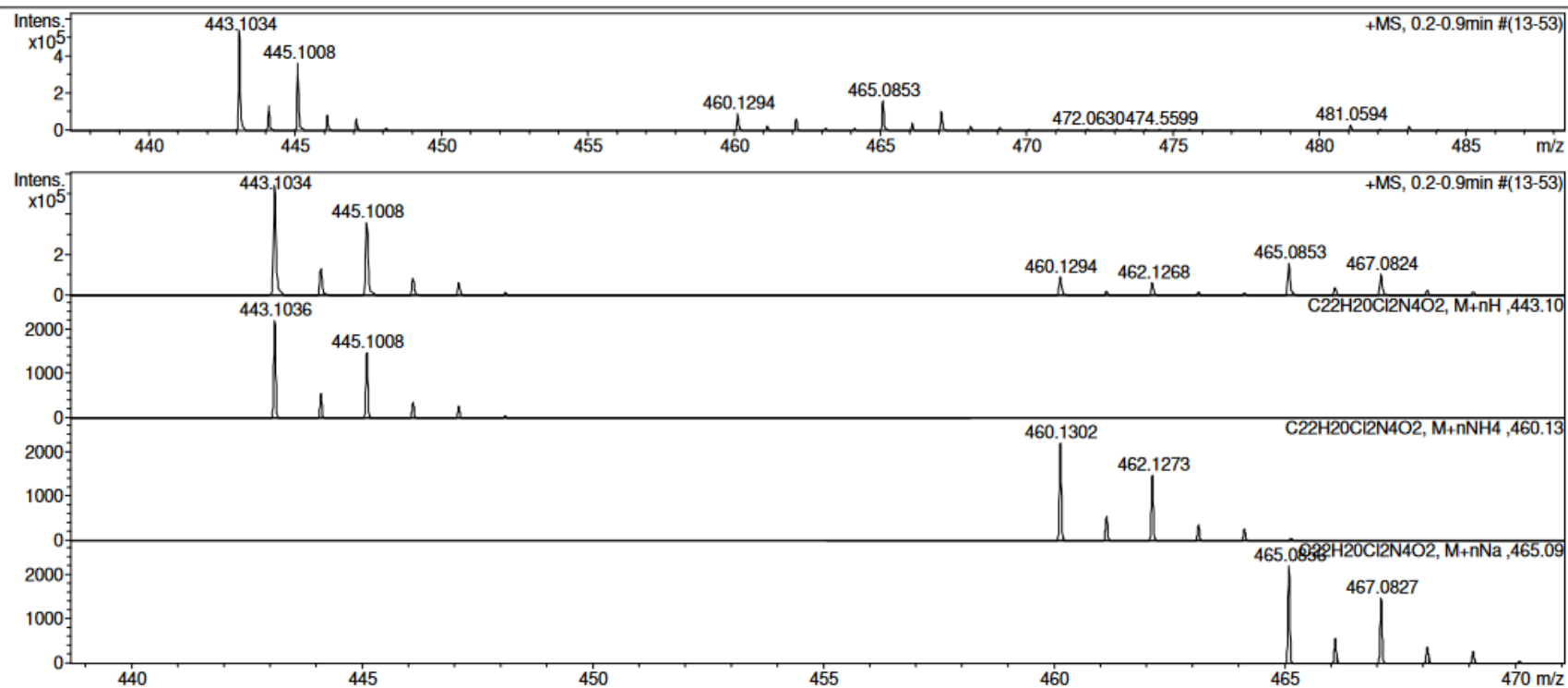


Figure S6. HRMS spectra of L2

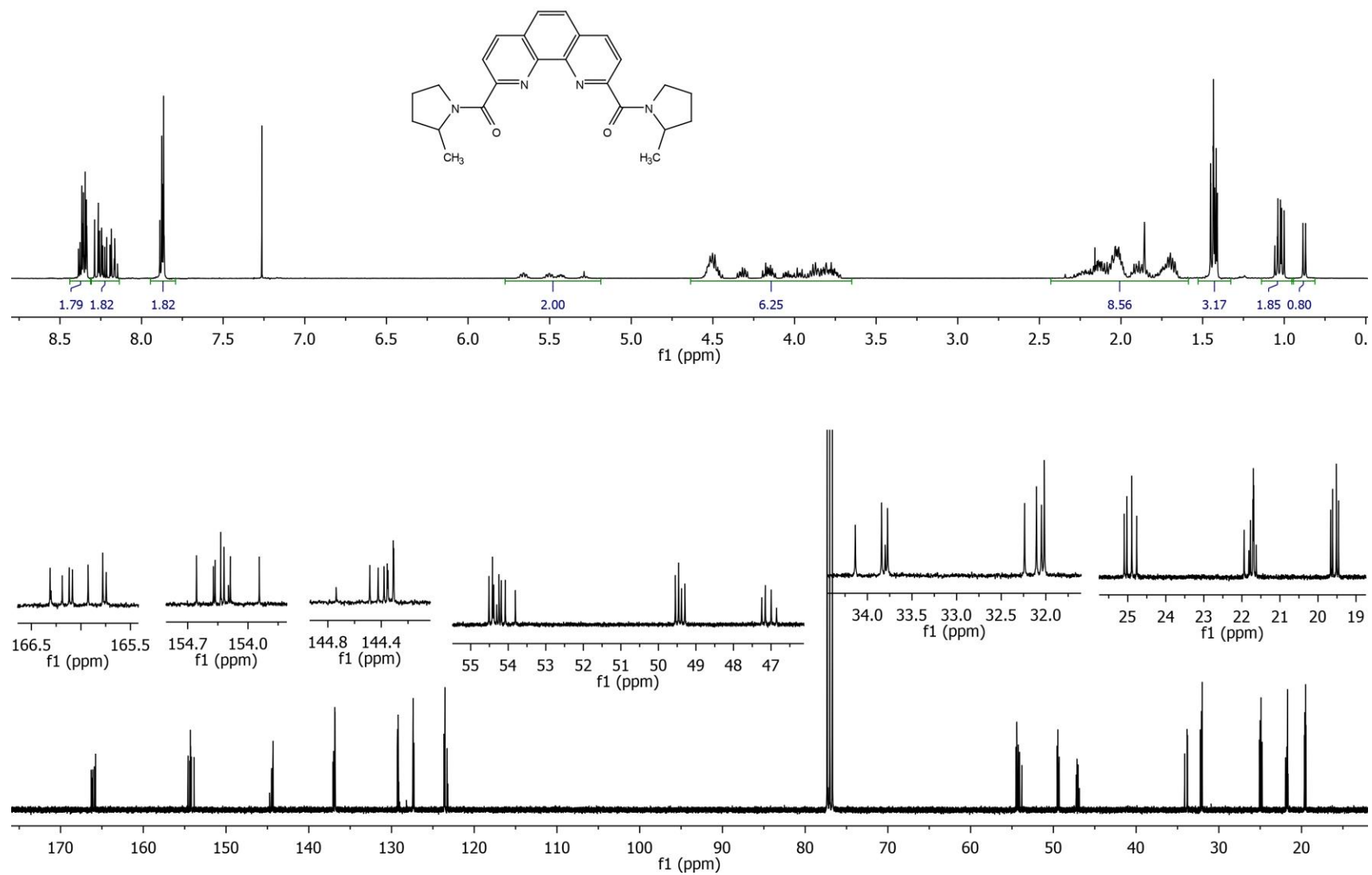


Figure S7. ^1H NMR and ^{13}C NMR spectra of L3 in CDCl_3 at 25°C

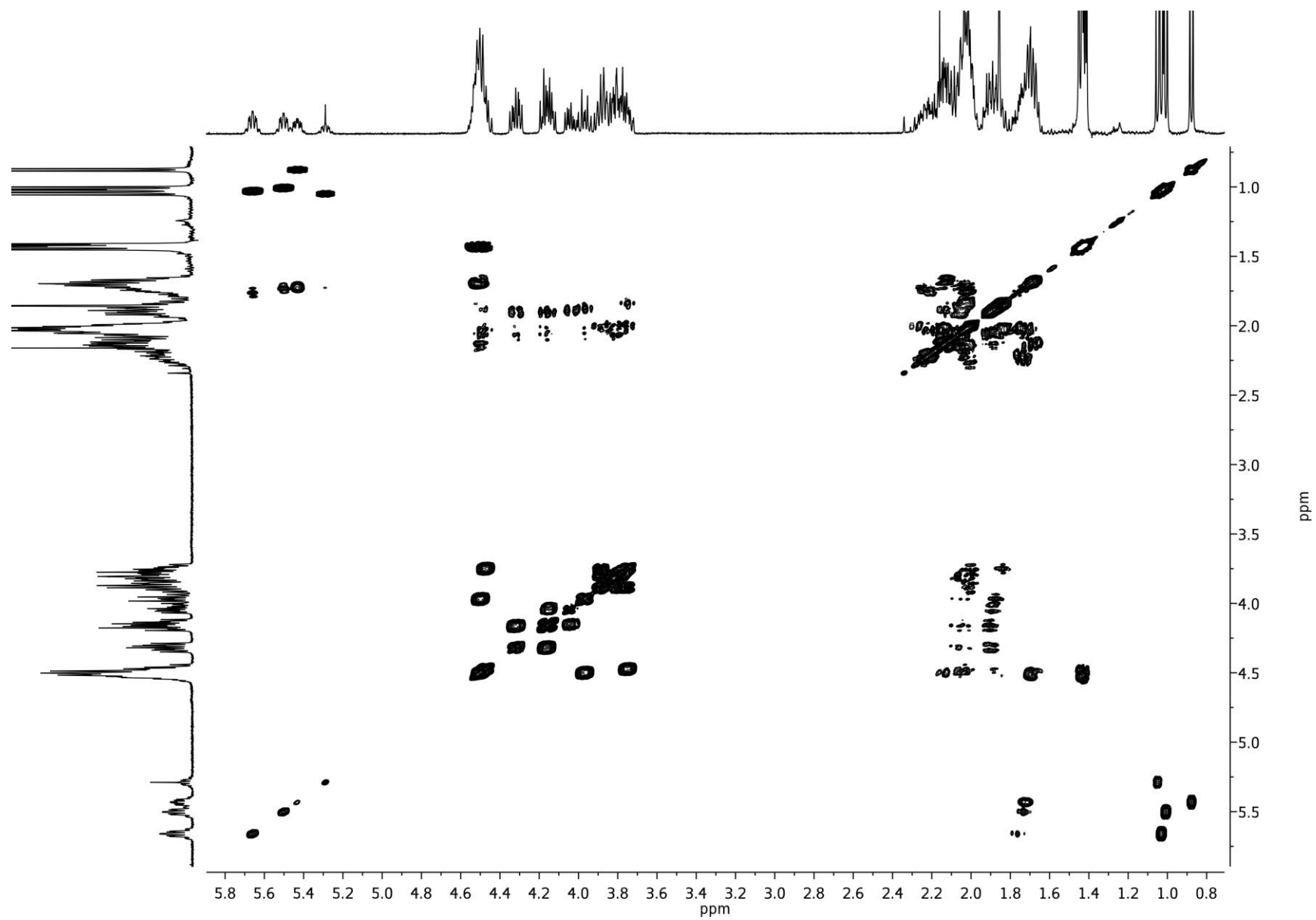


Figure S8. Fragmental view of ¹H/¹H COSY spectra of L3 in CDCl₃ at 25°C

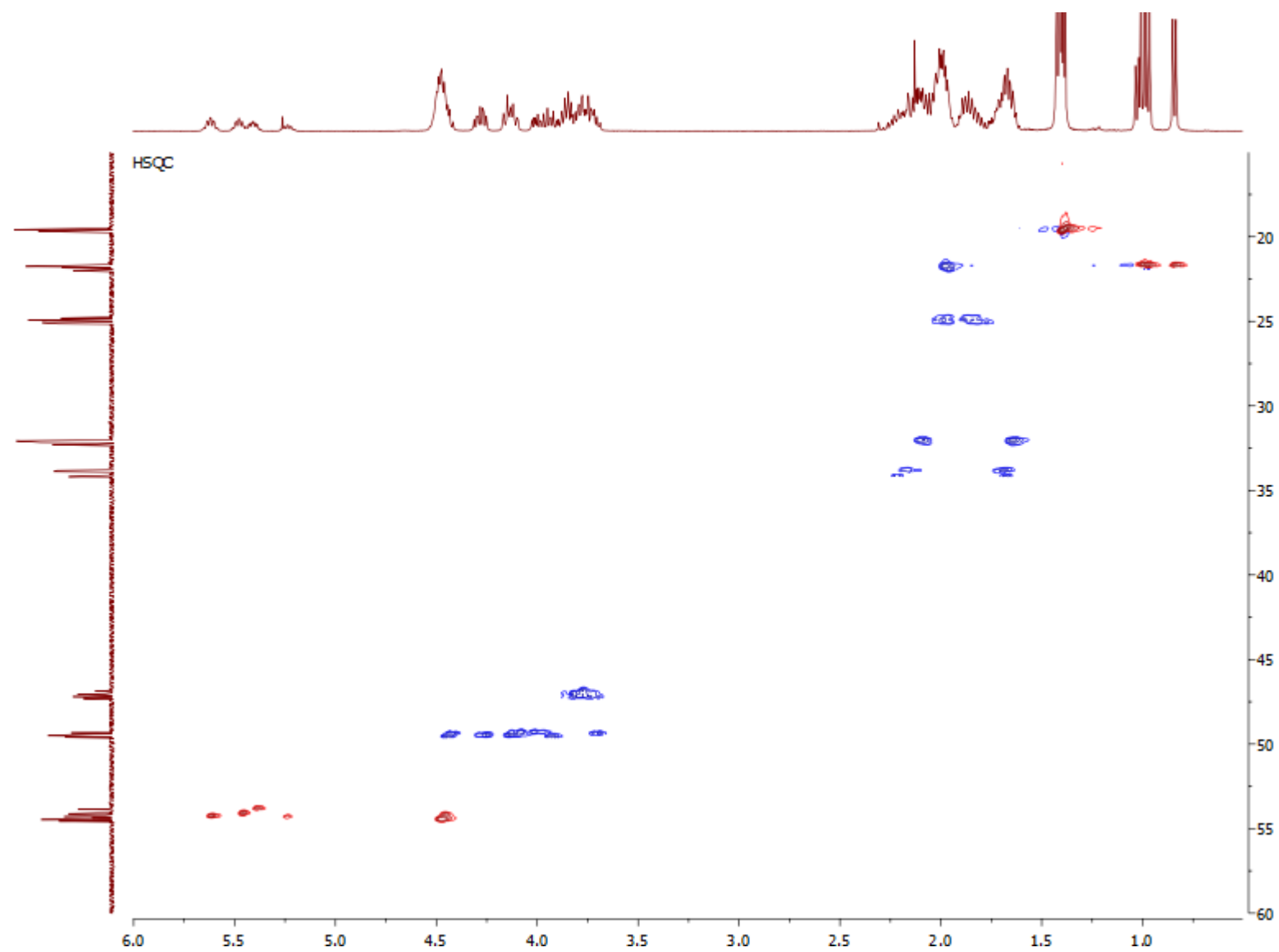


Figure S9. Fragmental view of $^1\text{H}/^{13}\text{C}$ HSQC spectra of **L3** in CDCl_3 at 25°C

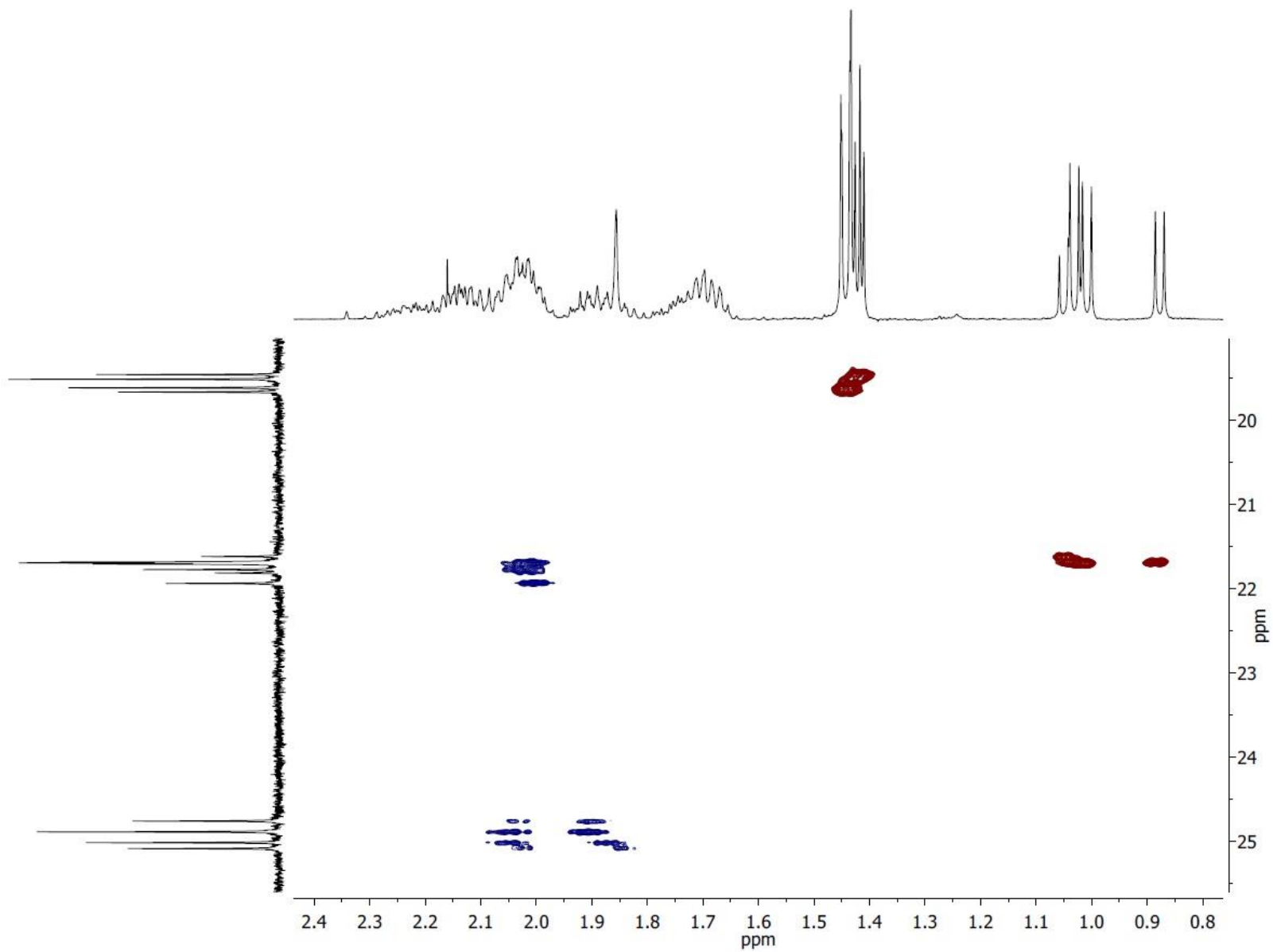


Figure S10. Fragmental view of $^1\text{H}/^{13}\text{C}$ HSQC spectra of **L3** in CDCl_3 at 25°C

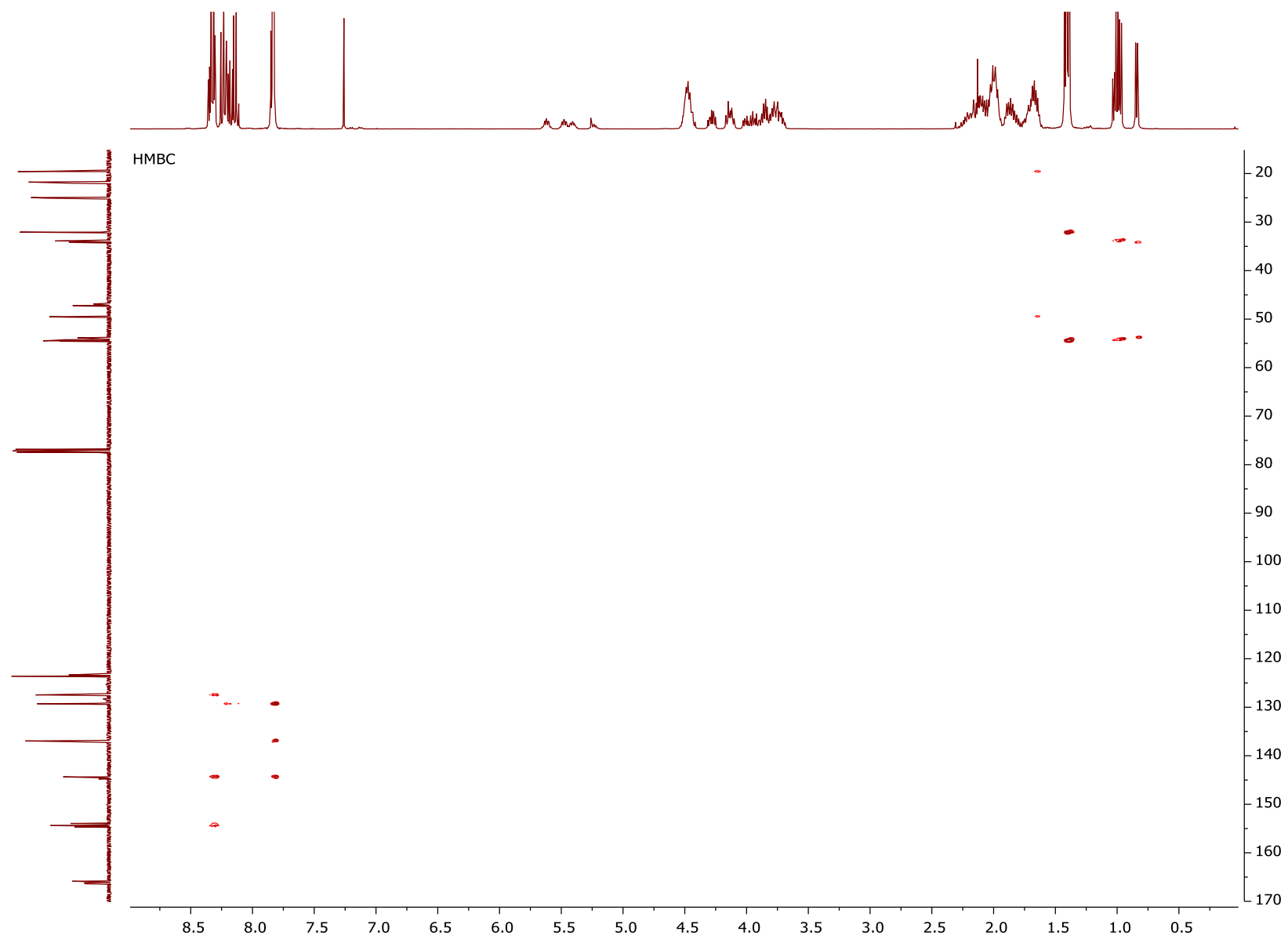


Figure S11. $^1\text{H}/^{13}\text{C}$ HMBC spectra of **L3** in CDCl_3 at 25°C

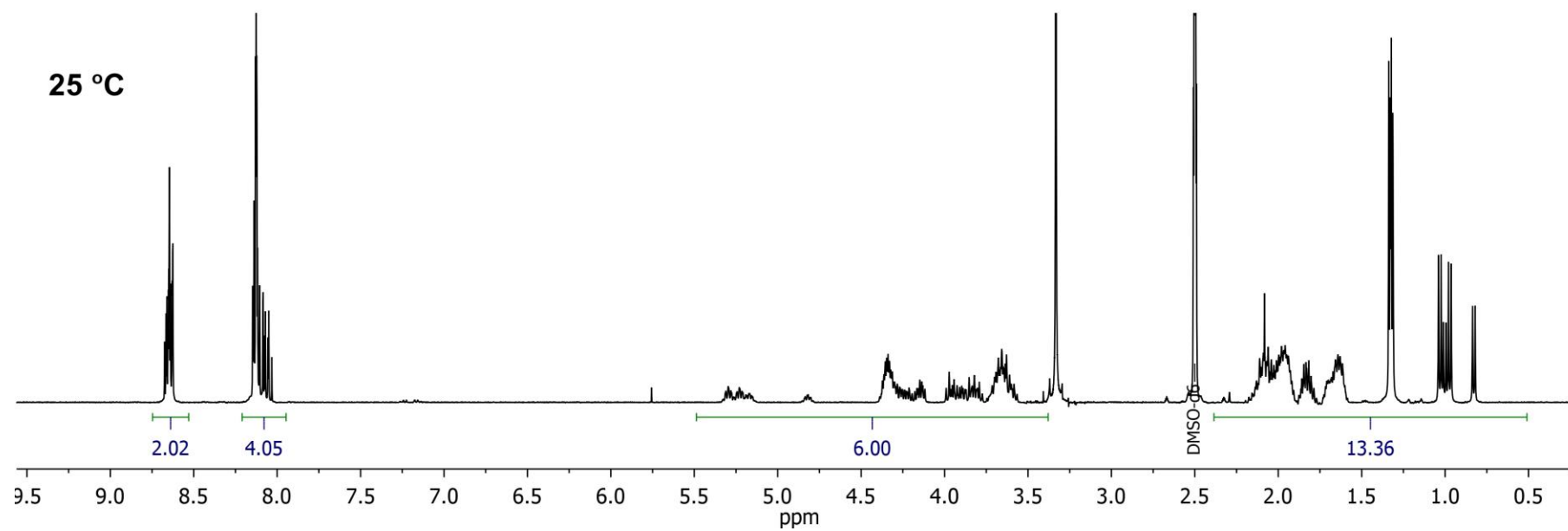
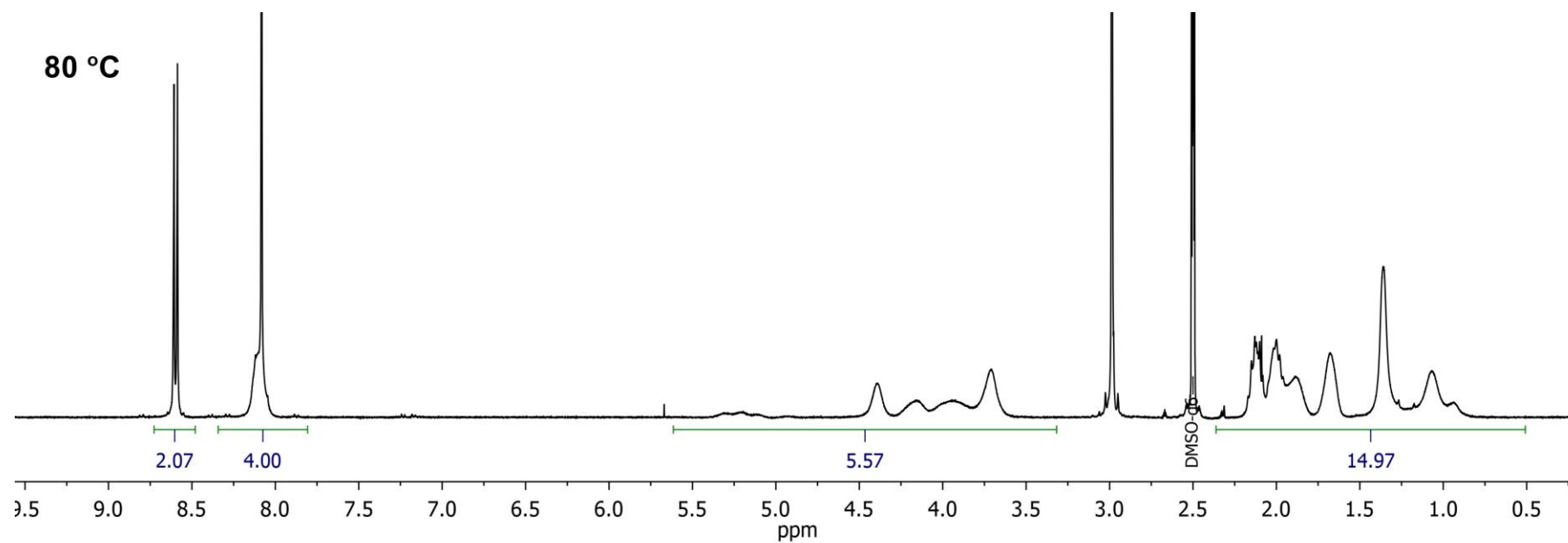


Figure S12. ^1H NMR spectra of **L3** in DMSO-d_6 at 25°C and 80°C

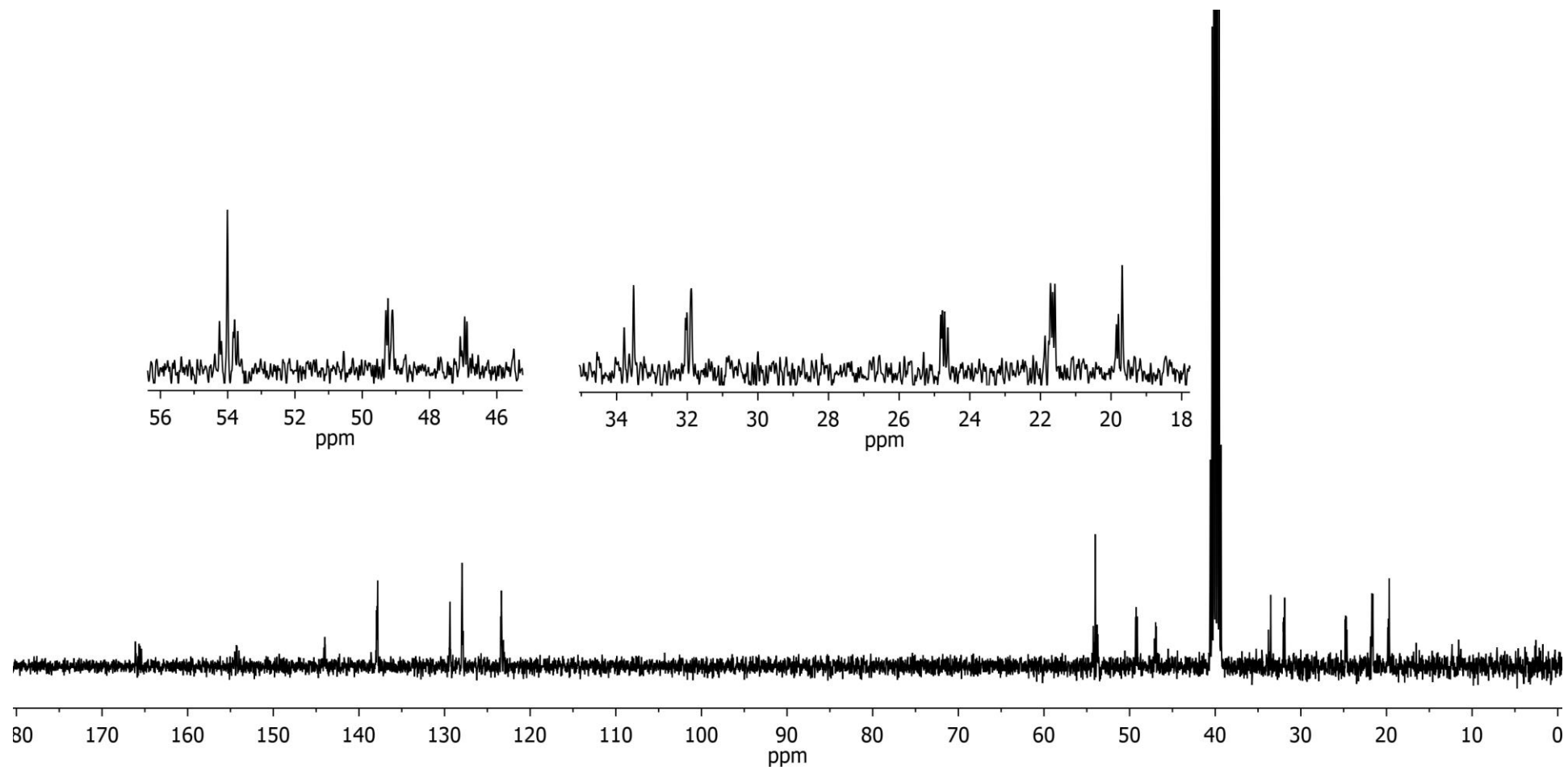


Figure S13. ^{13}C NMR spectra of L3 in DMSO-d_6 at 25°C

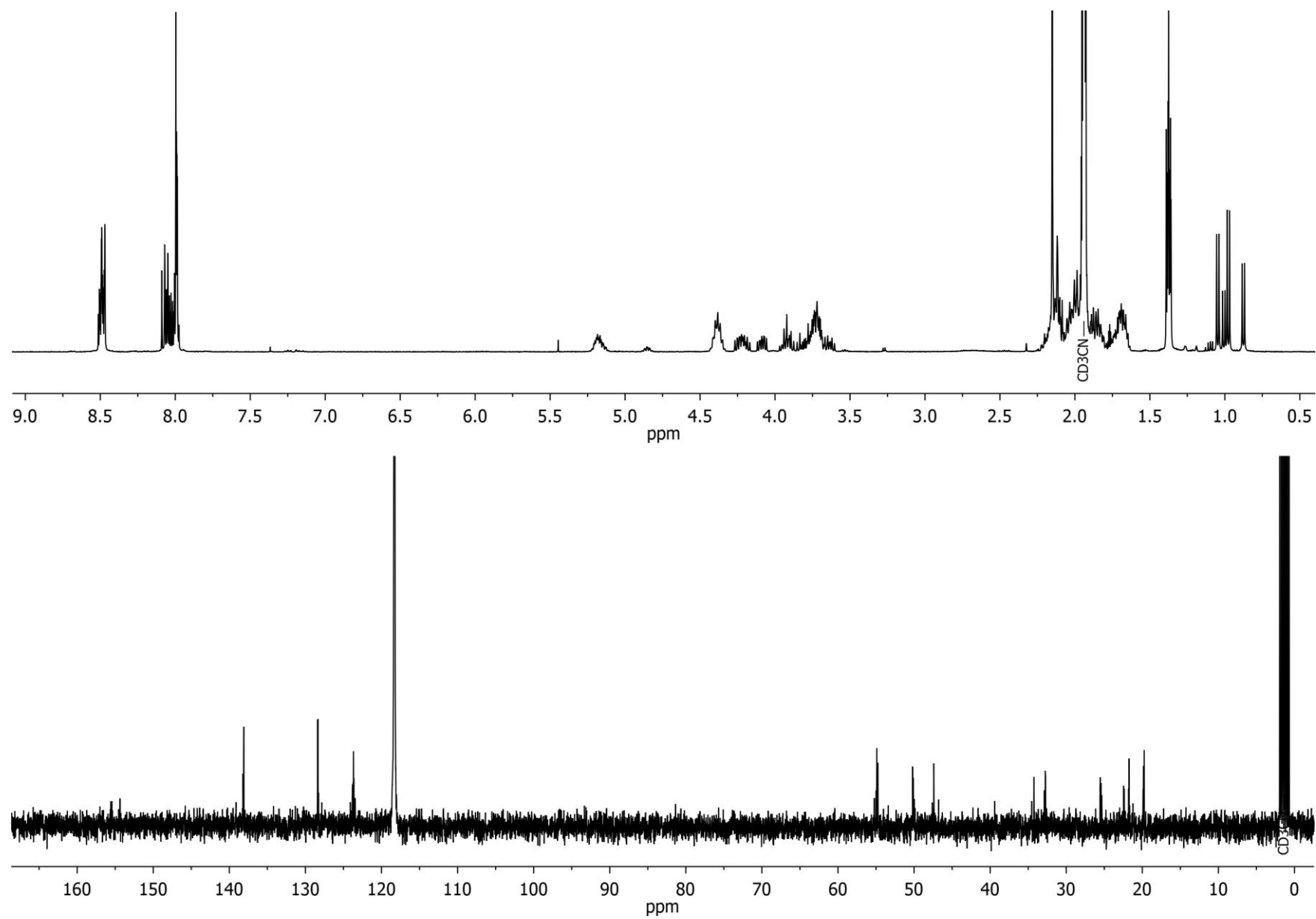


Figure S14. ¹H NMR and ¹³C NMR spectra of L3 in CD₃CN at 25°C

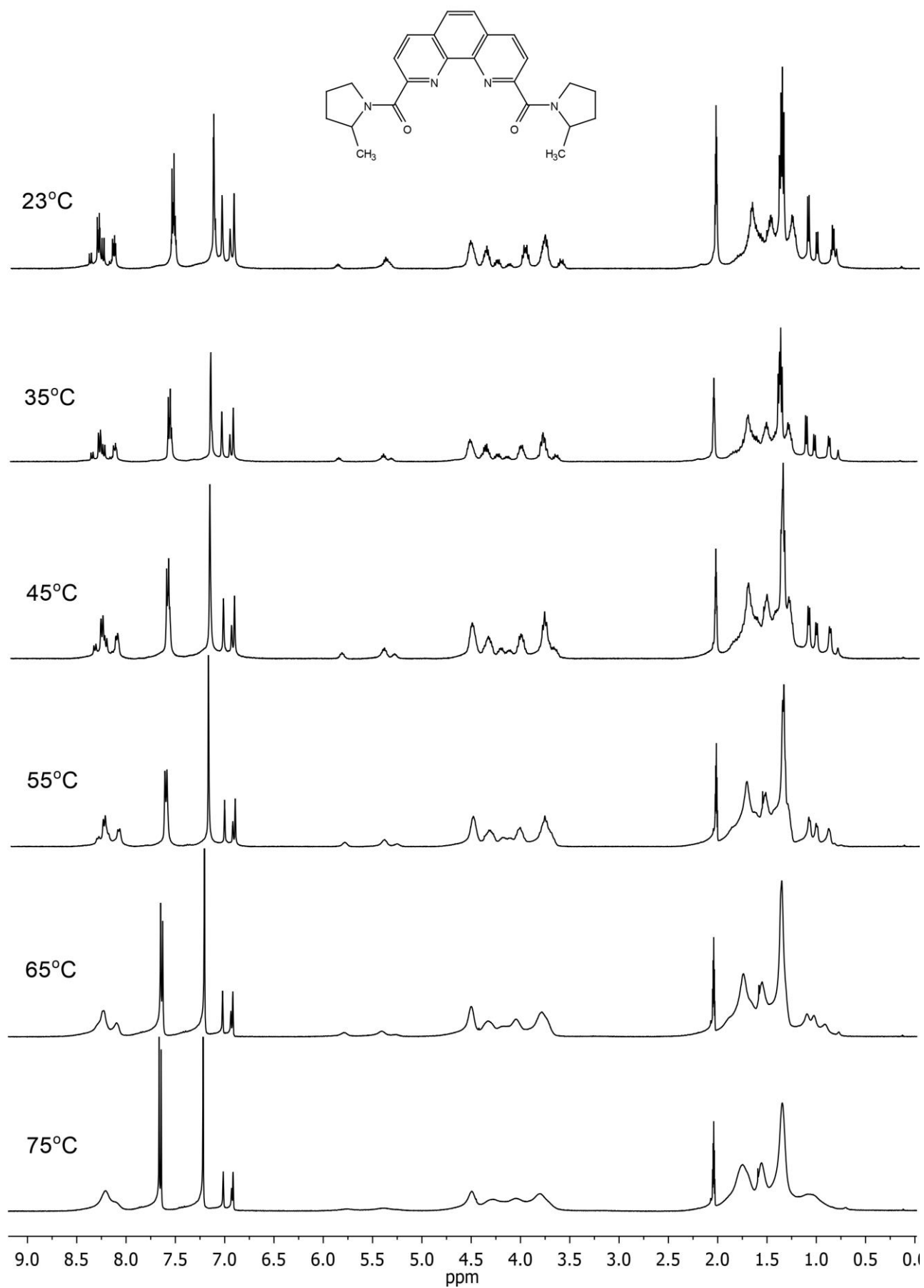


Figure S15. ¹H NMR spectra of L3 in toluene-d₈ at different temperatures

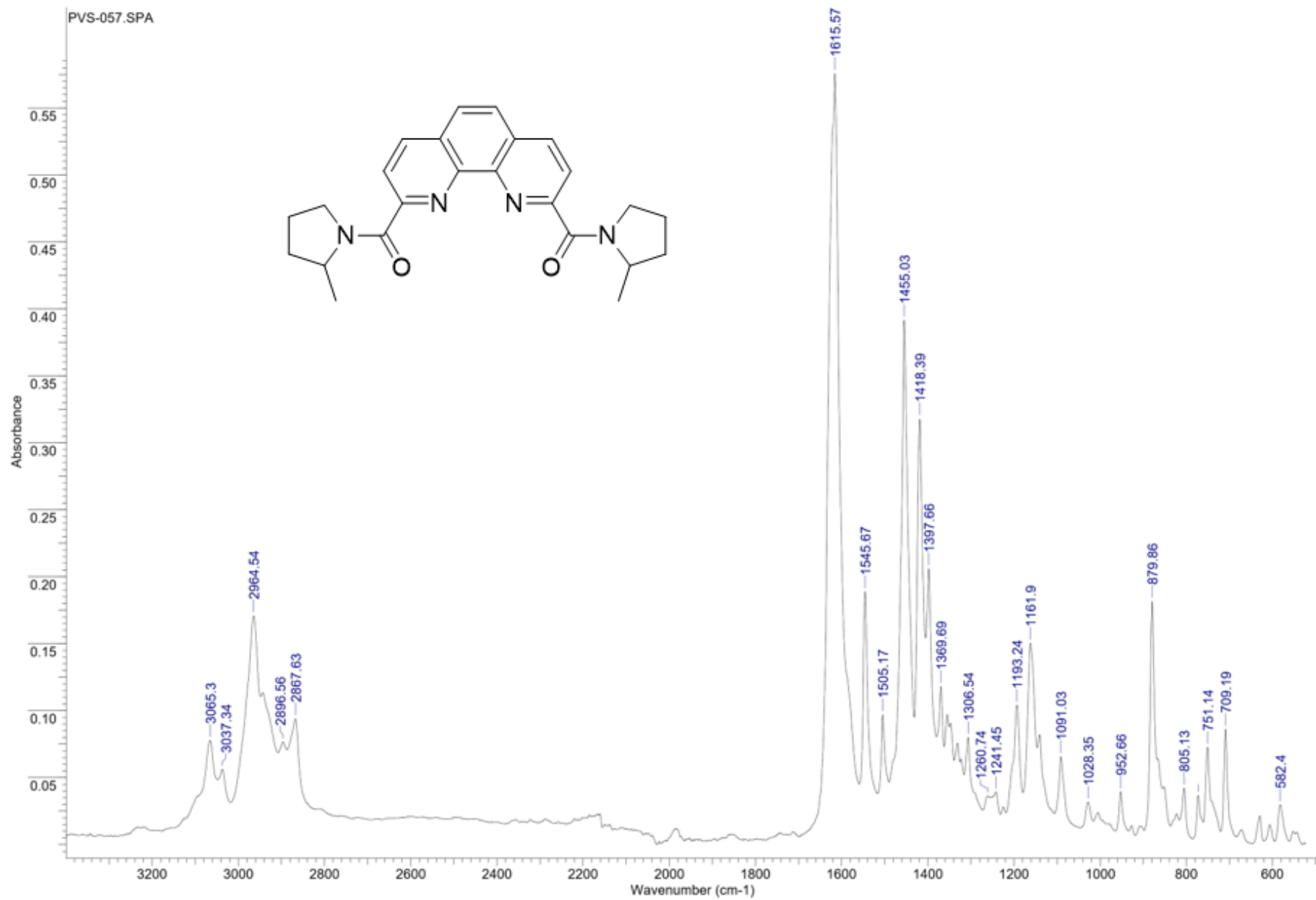


Figure S16. Solid-state IR spectra of L3 at 25°C

Display Report

Analysis Info

Analysis Name D:\Data\Kolotyrkina\2020\Muzalevsky\0730052.d
Method tune_50-1600.m
Sample Name /MUSE PVS-057
Comment C24H26N4O2 mH 403.2128 clb added CH3CN

Acquisition Date 30.07.2020 20:43:23
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

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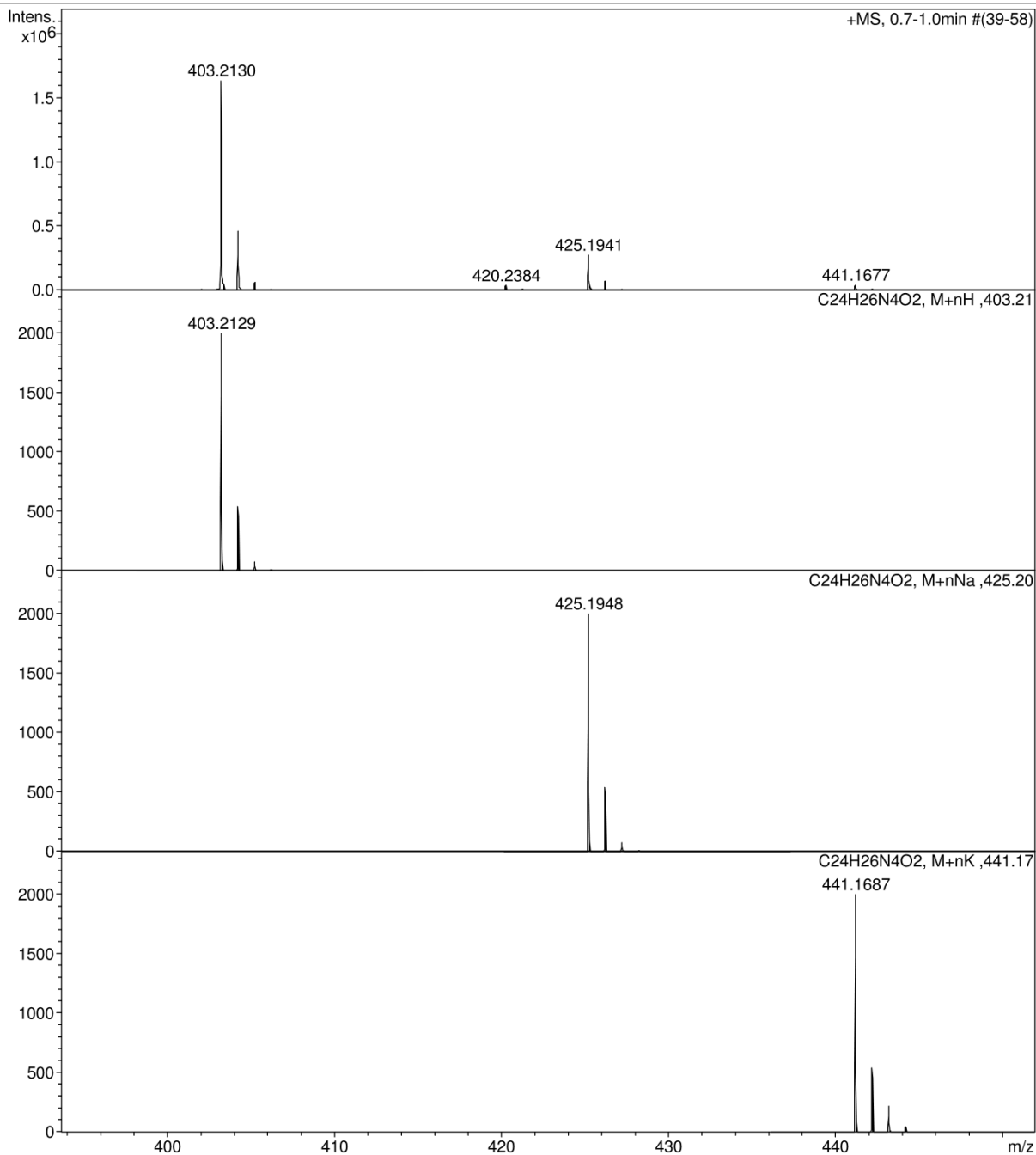


Figure S17. HRMS spectra of L3.

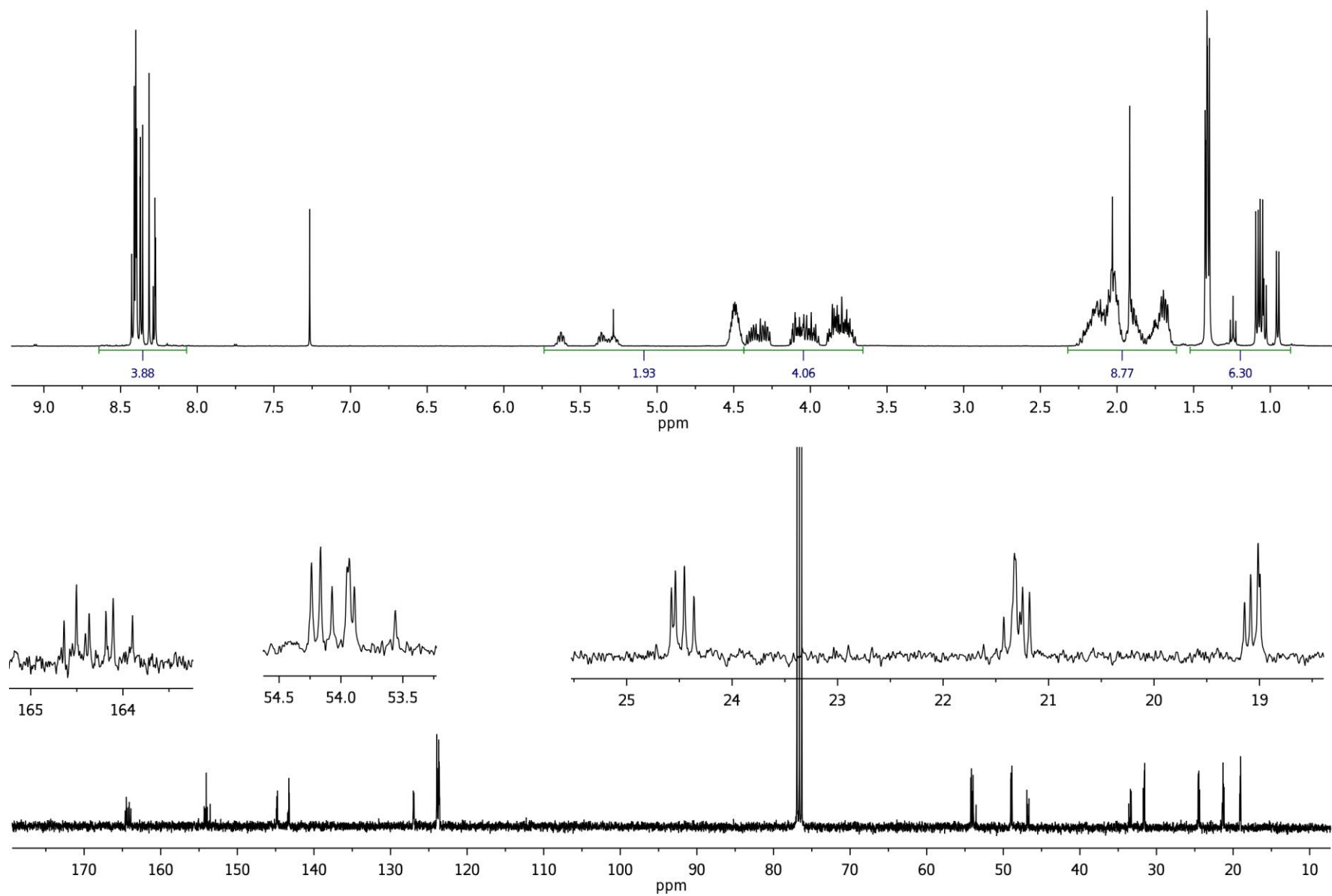


Figure S18. ^1H NMR and ^{13}C NMR spectra of **L4** in CDCl_3 at 25°C

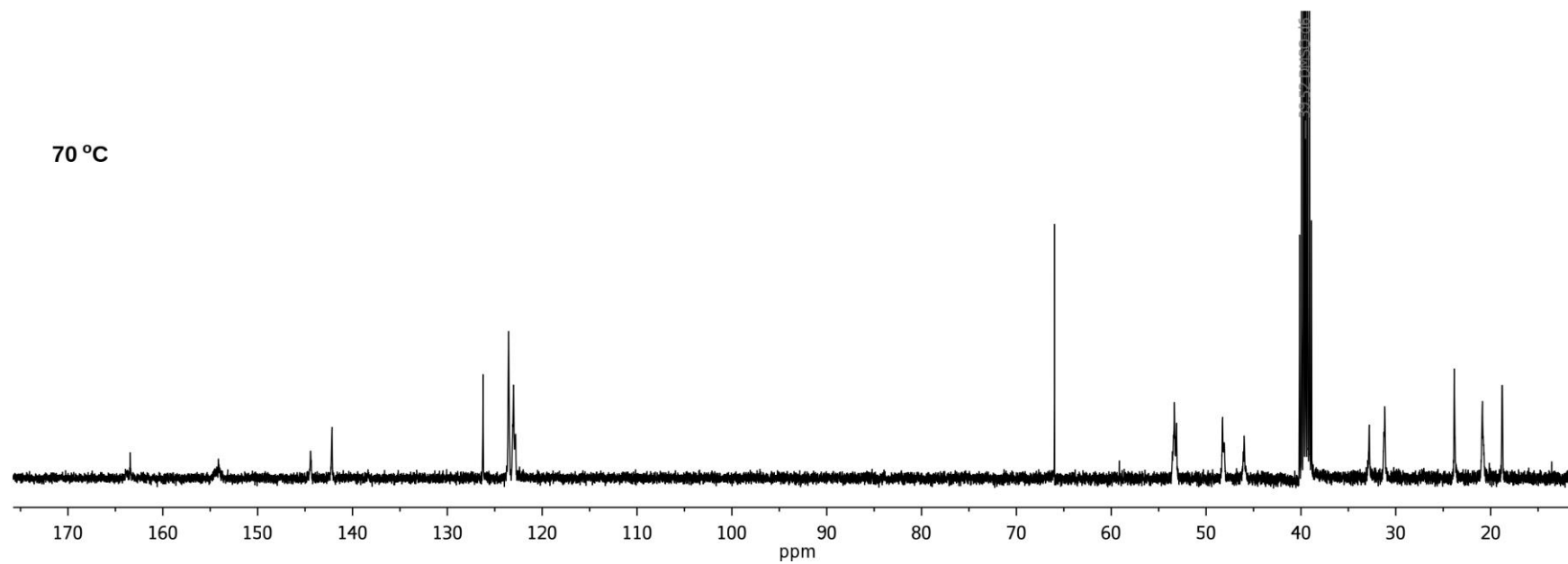
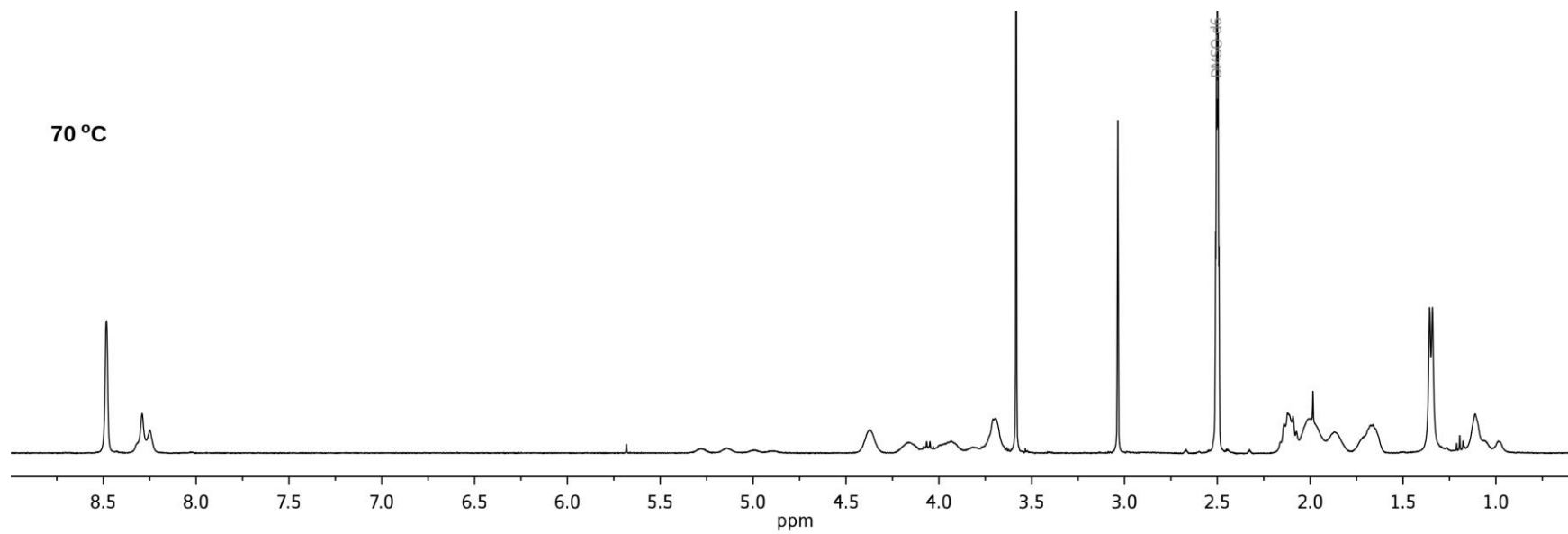


Figure S19. ^1H NMR and ^{13}C NMR spectra of **L4** in DMSO-d_6 at 70°C

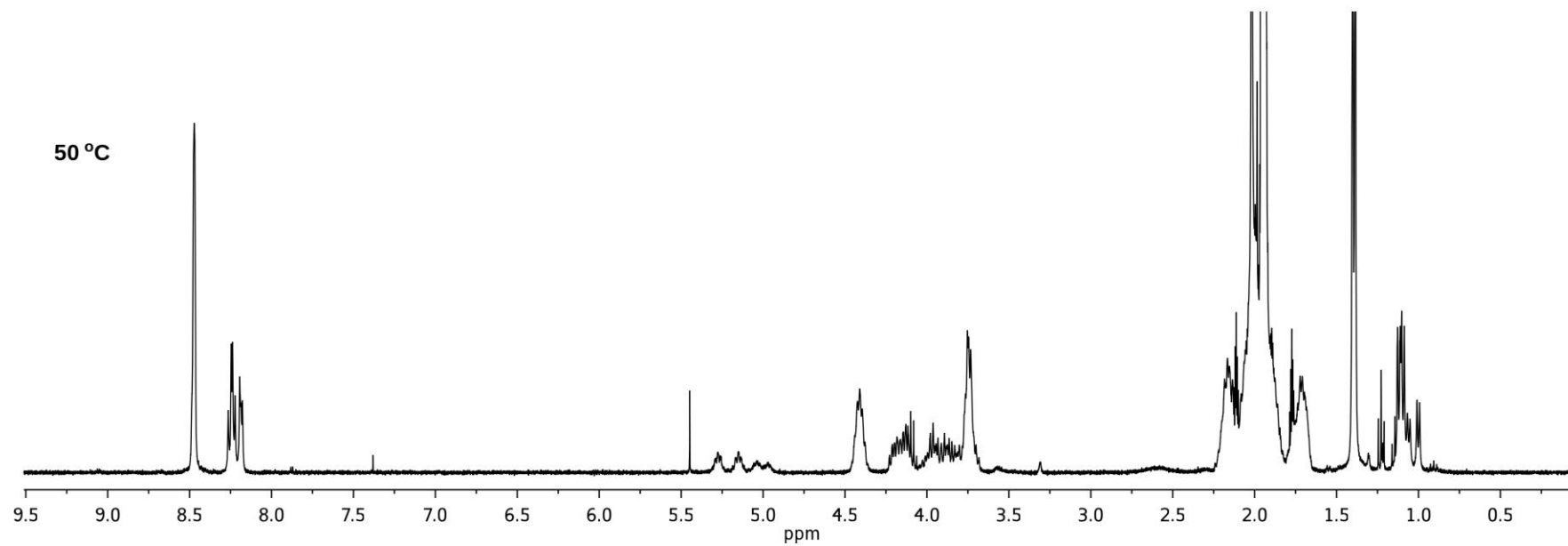
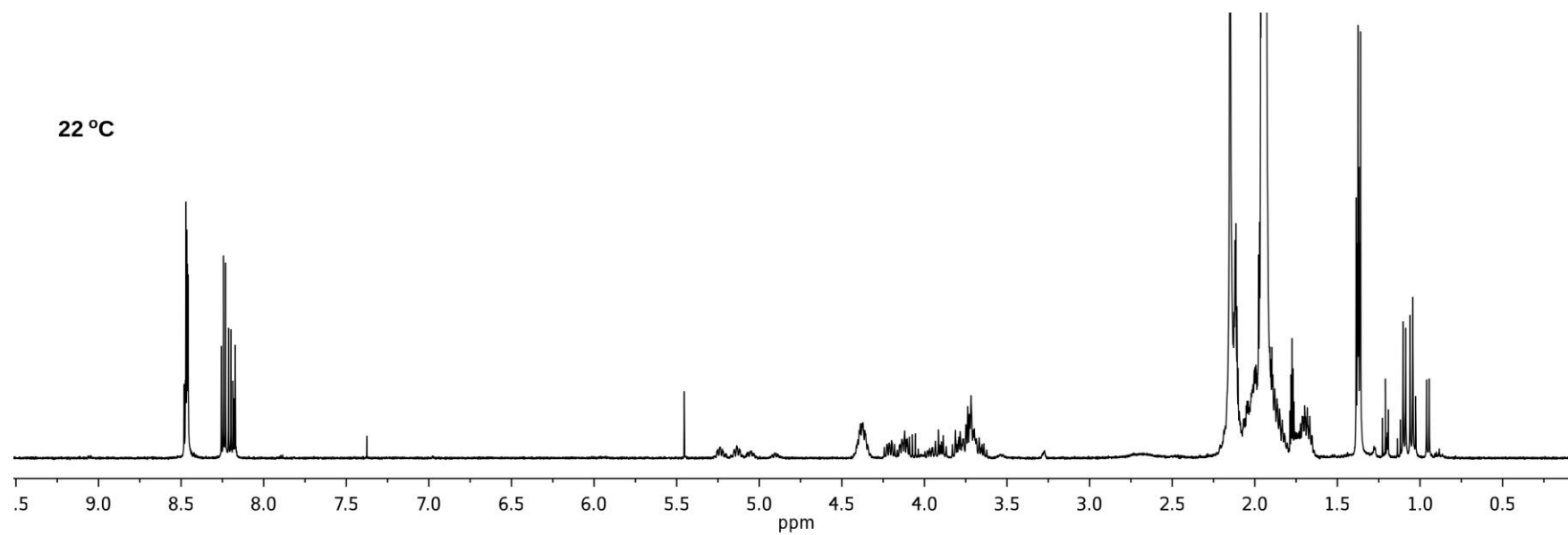


Figure S20. ^1H NMR spectra of **L4** in CD_3CN at 22°C and 70°C

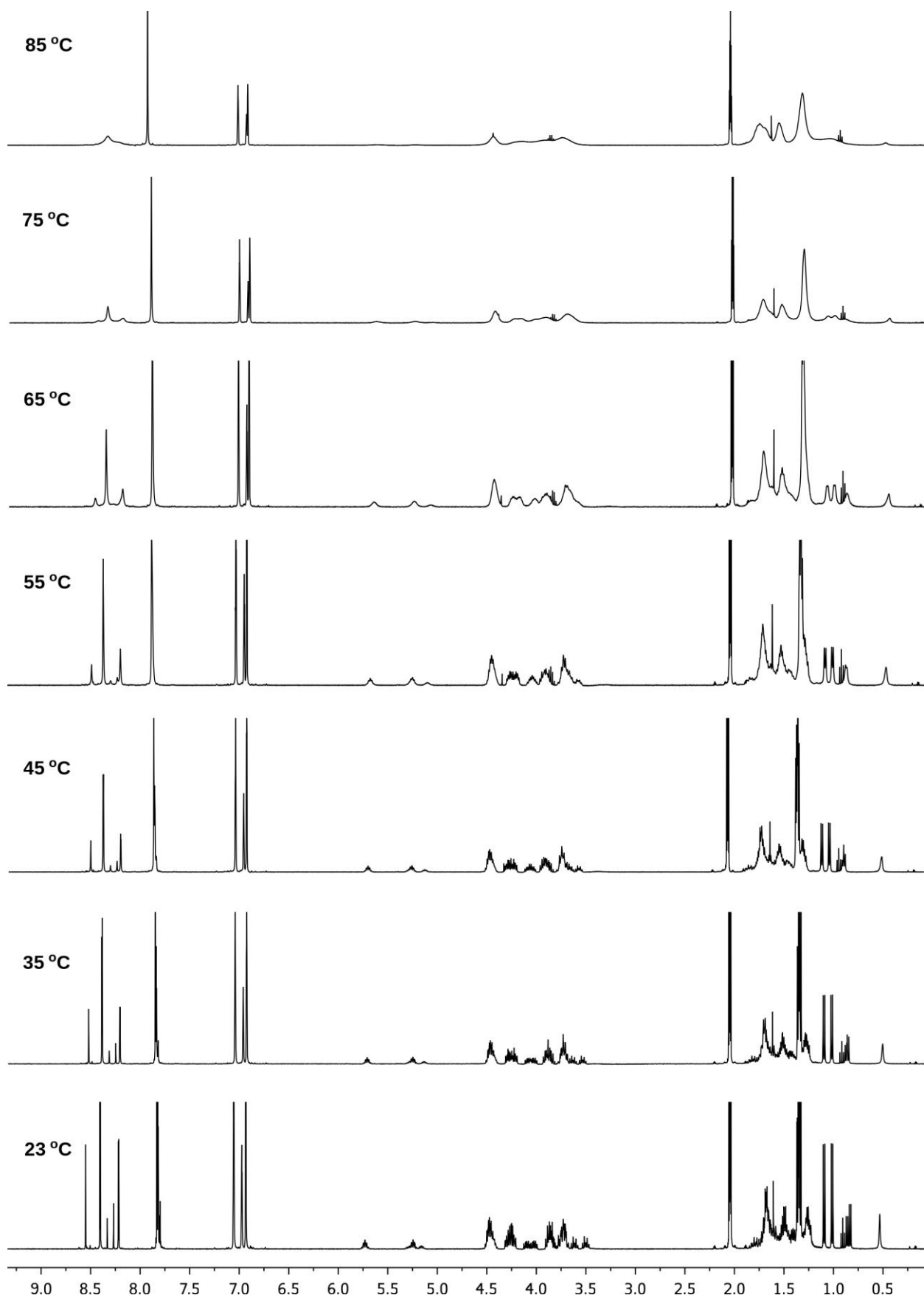


Figure S22. ¹H NMR spectra of L4 in toluene-d₈ at different temperatures

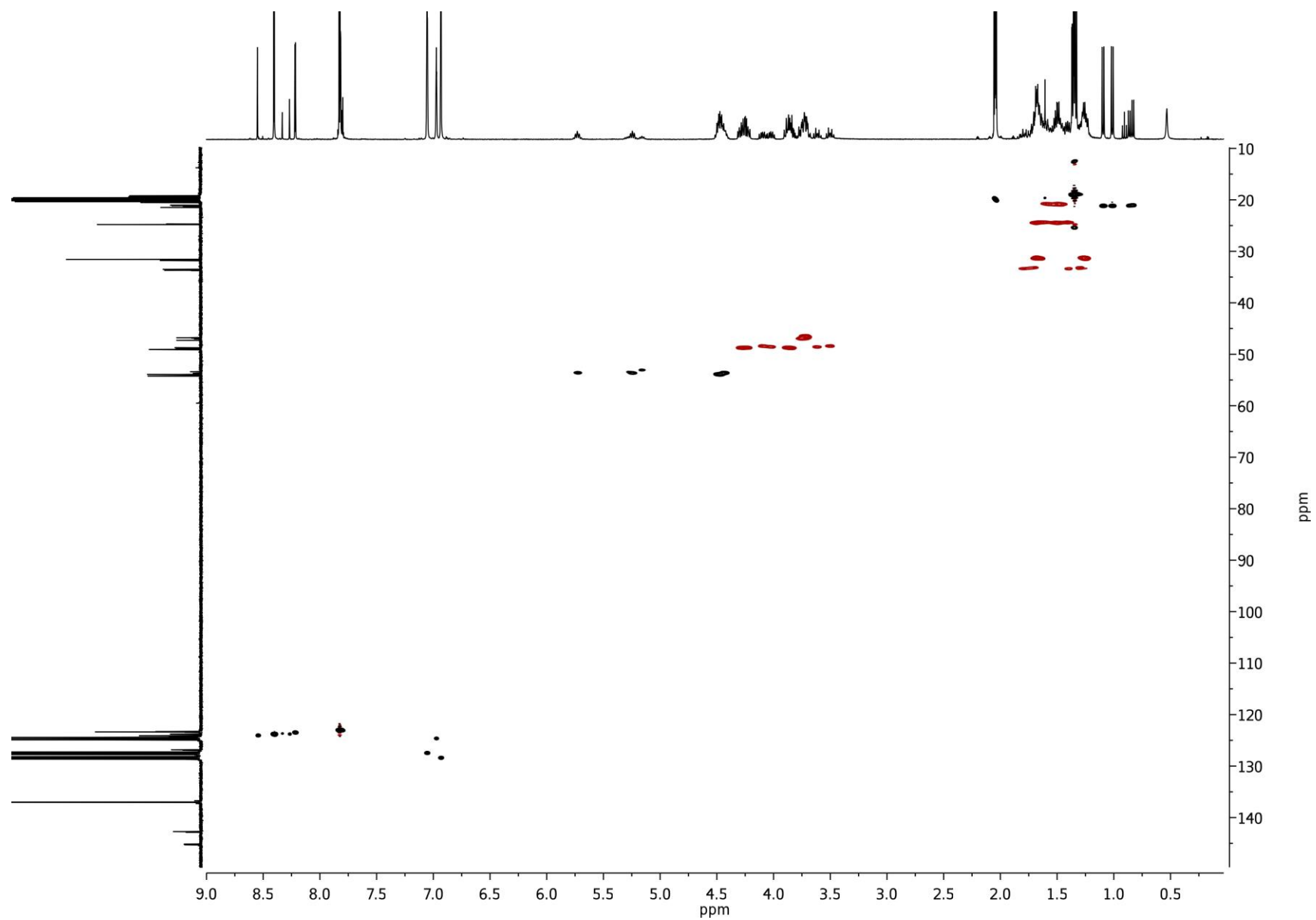


Figure S23. $^1\text{H}/^{13}\text{C}$ HSQC spectra of **L4** in toluene- d_8 at 22°C

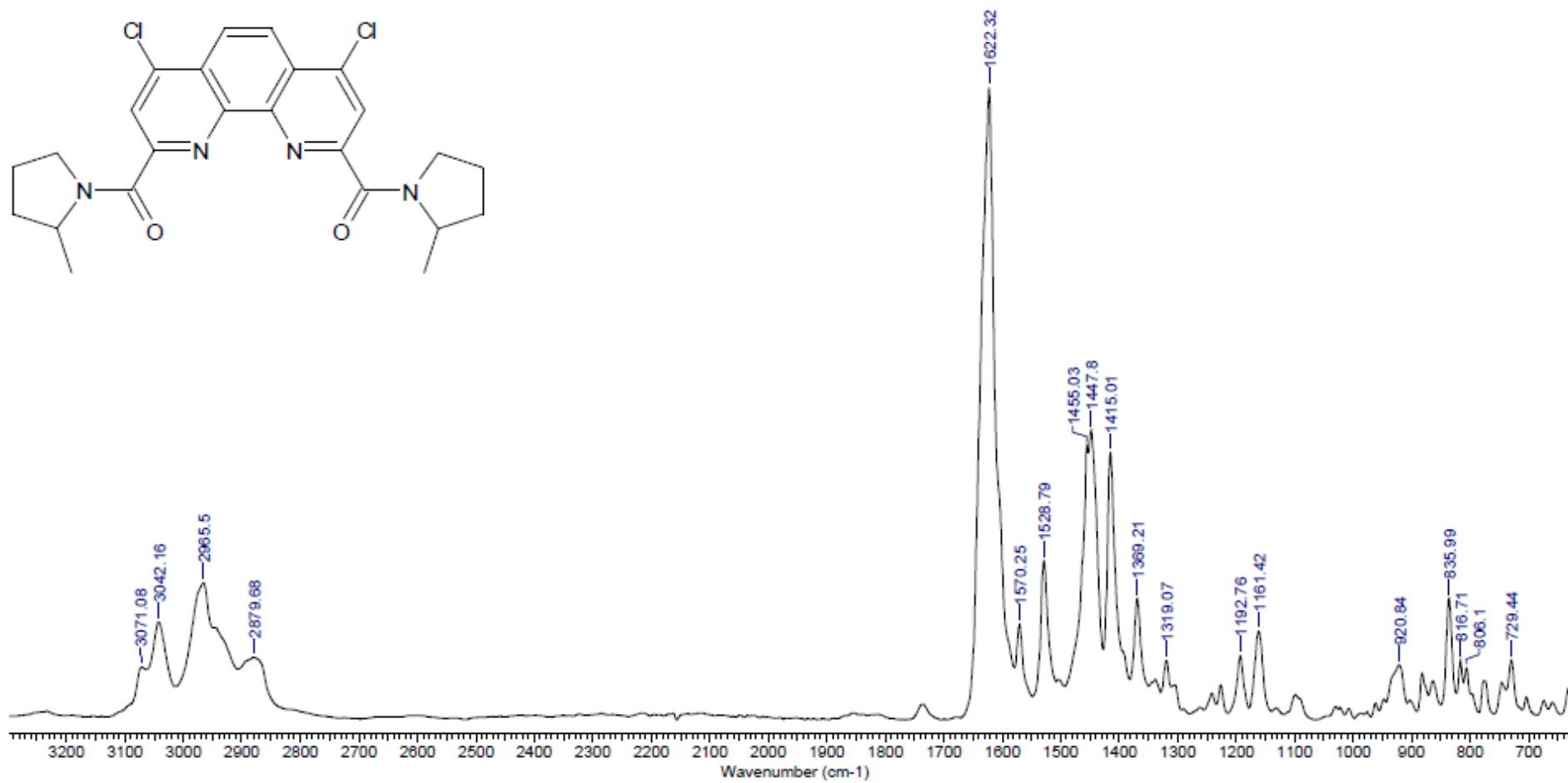


Figure S24. Solid-state IR spectra of L4 at 25°C

Display Report

Analysis Info

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Method tune_50-1600.m
Sample Name /MUSE PVS-048
Comment C24H24Cl2N4O2 mH 471.1349 calibrant added CH3CN

Acquisition Date 15.07.2020 10:22:10

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

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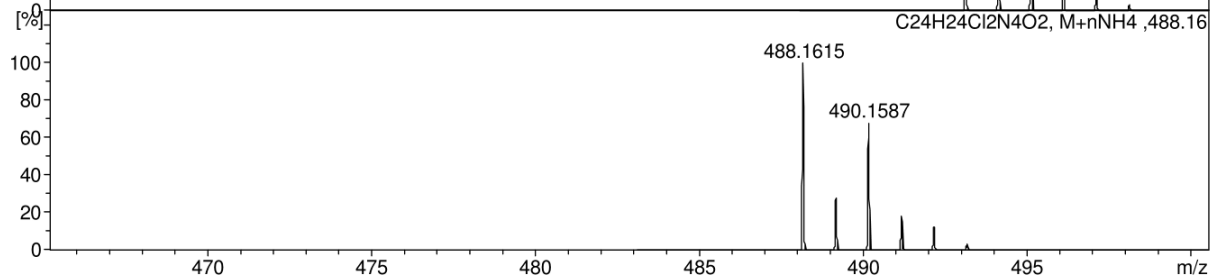
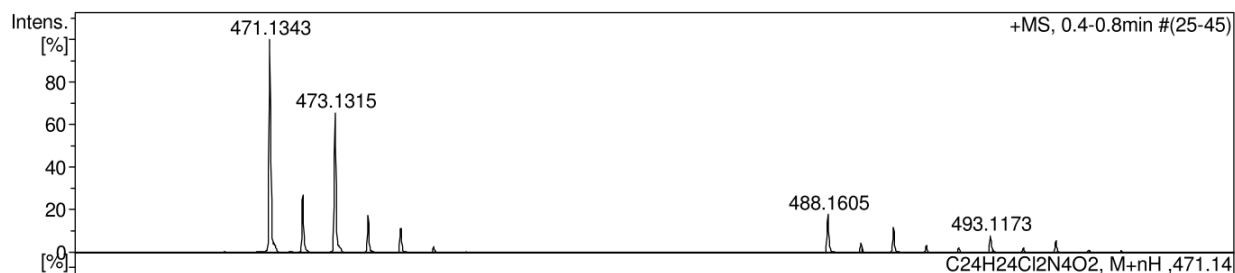
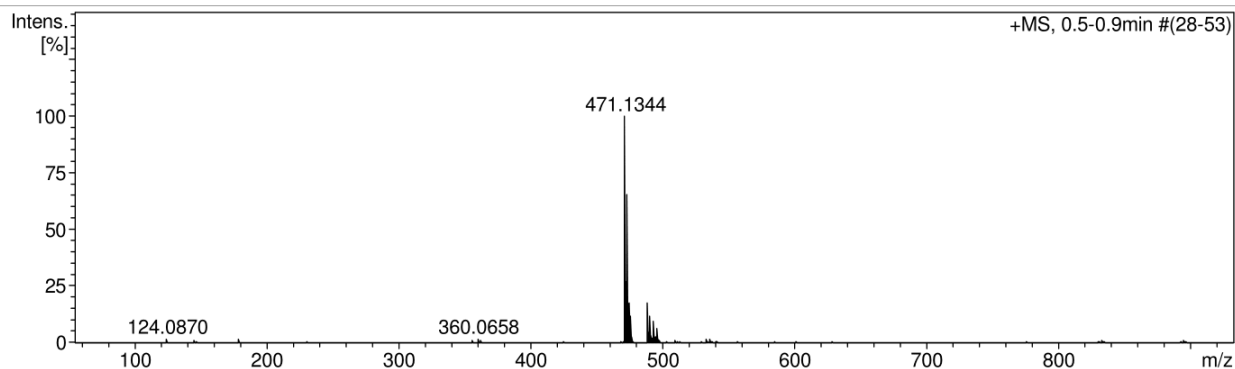


Figure S25. HRMS spectra of L4

IR spectra of complexes

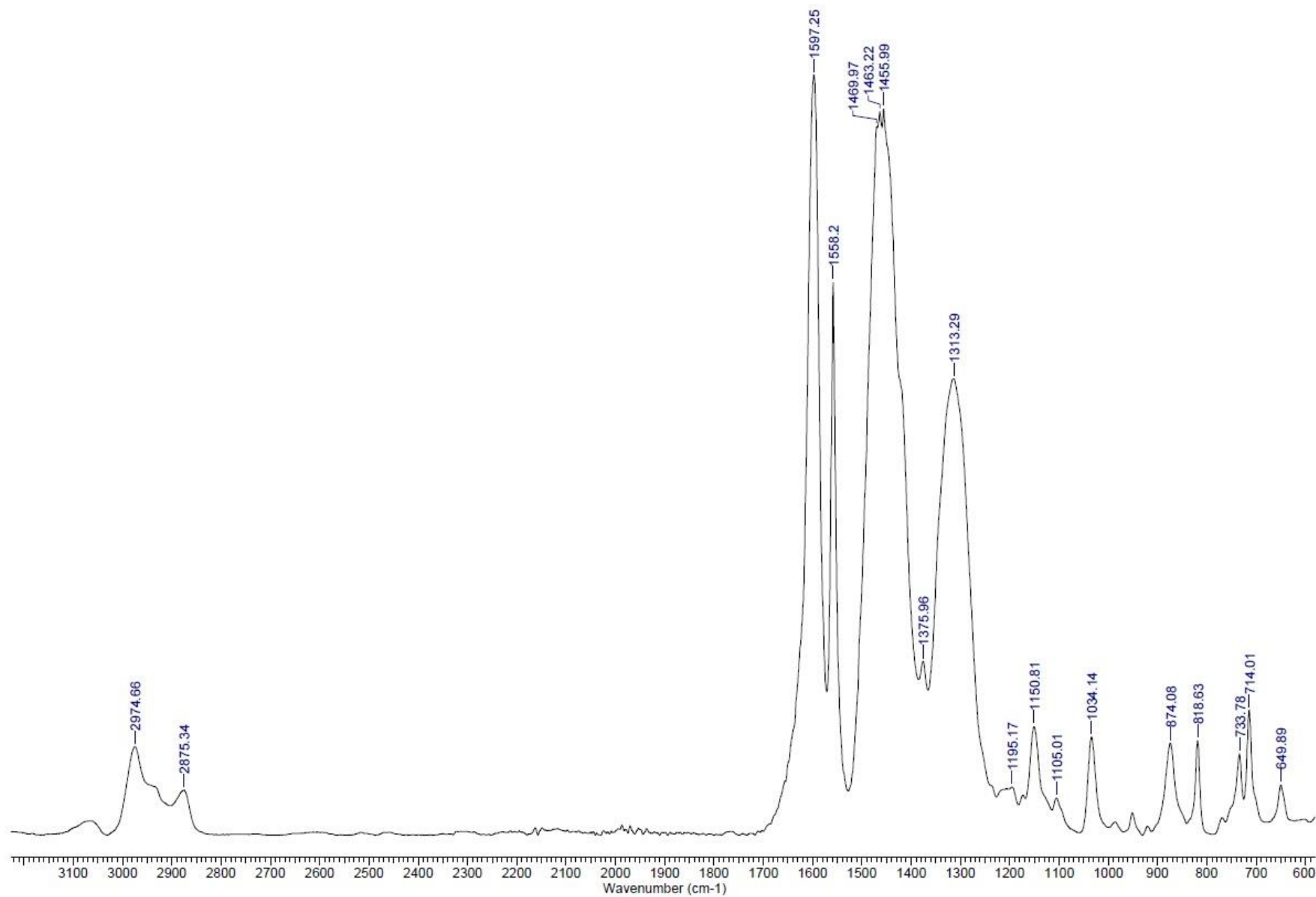


Figure S26. Solid-state IR spectra of complex $L3 \cdot La(NO_3)_3$

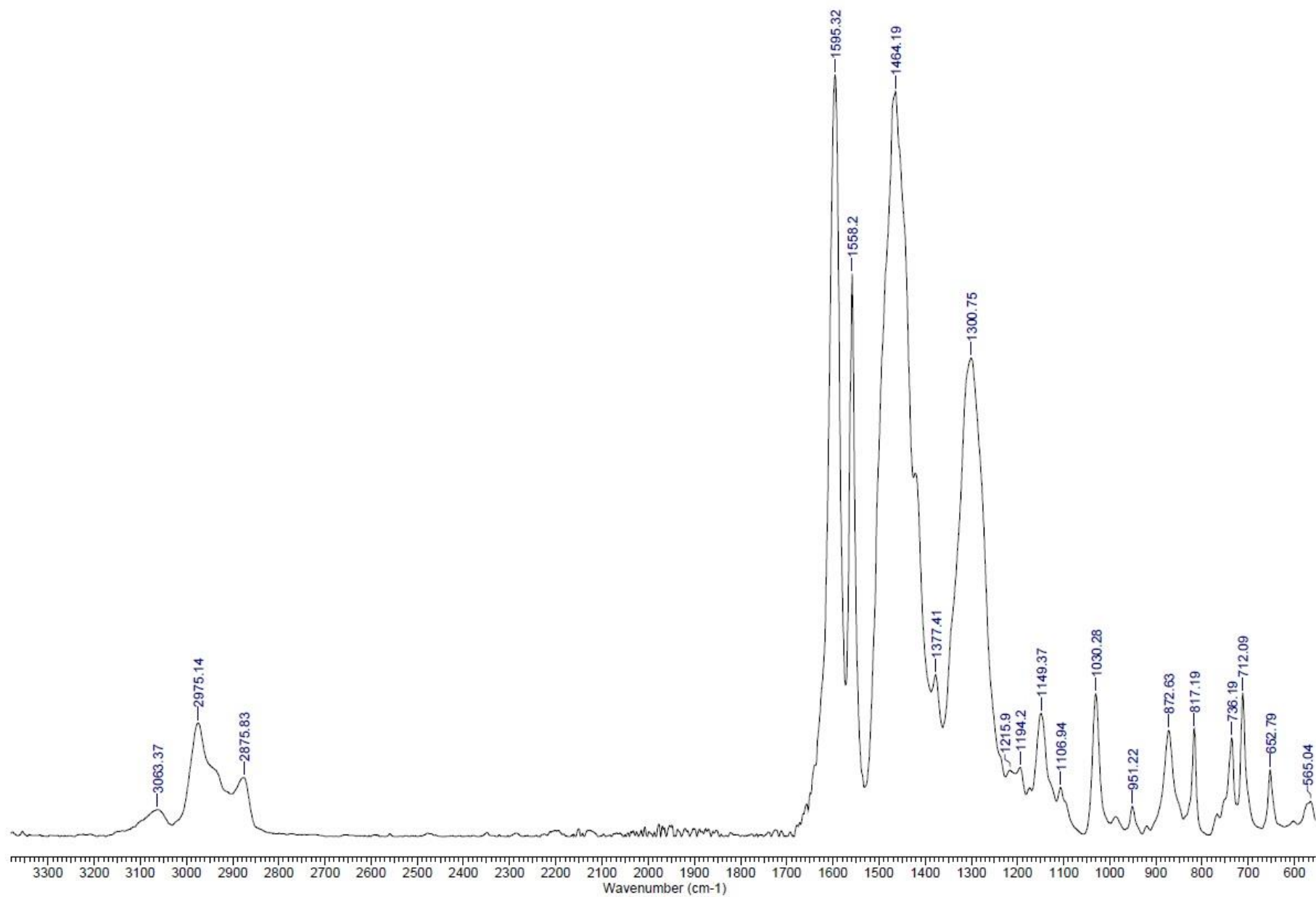


Figure S27. Solid-state IR spectra of complex $L3 \cdot Nd(NO_3)_3$

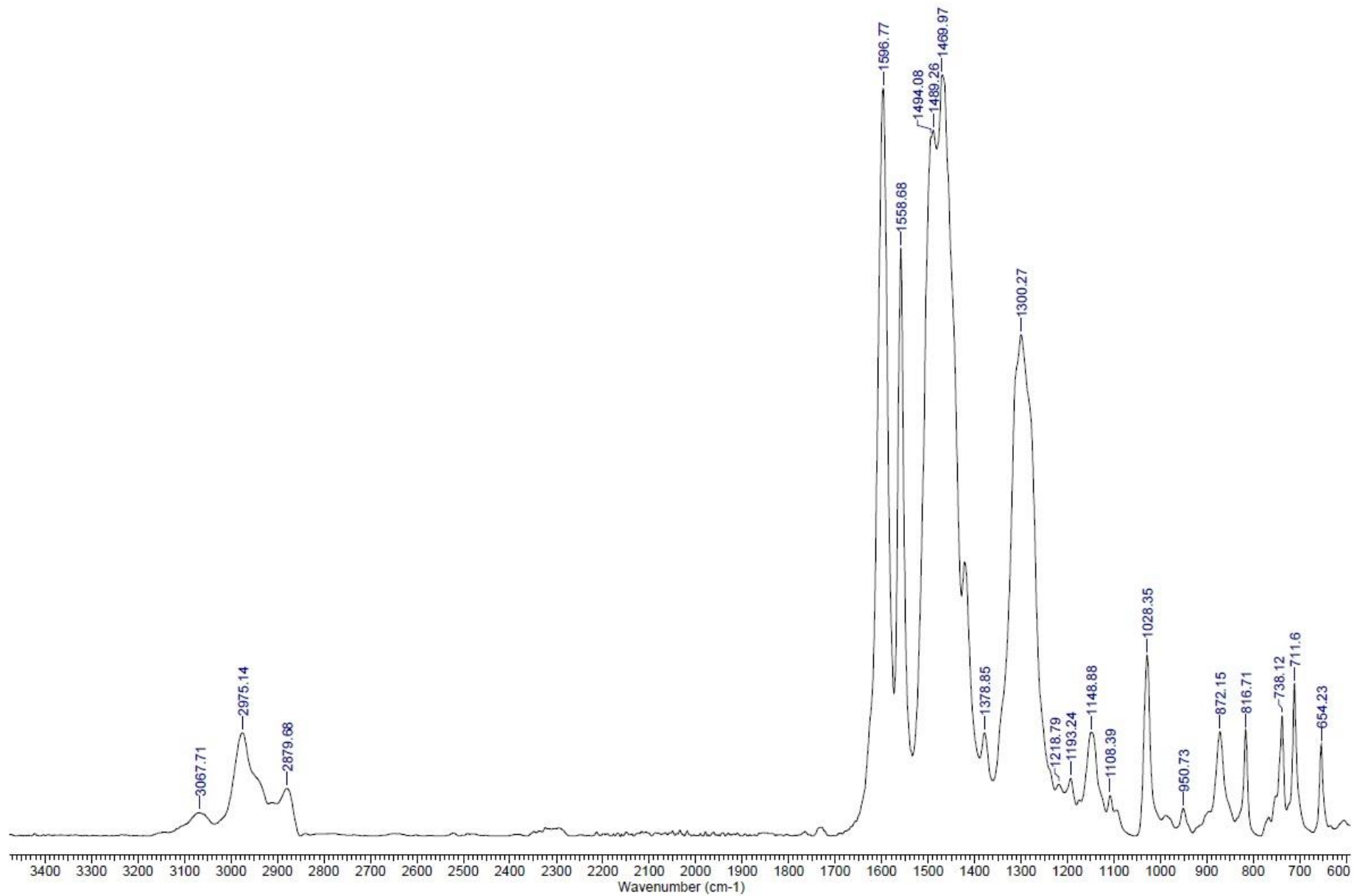


Figure S28. Solid-state IR spectra of complex **L3*Eu(NO₃)₃**

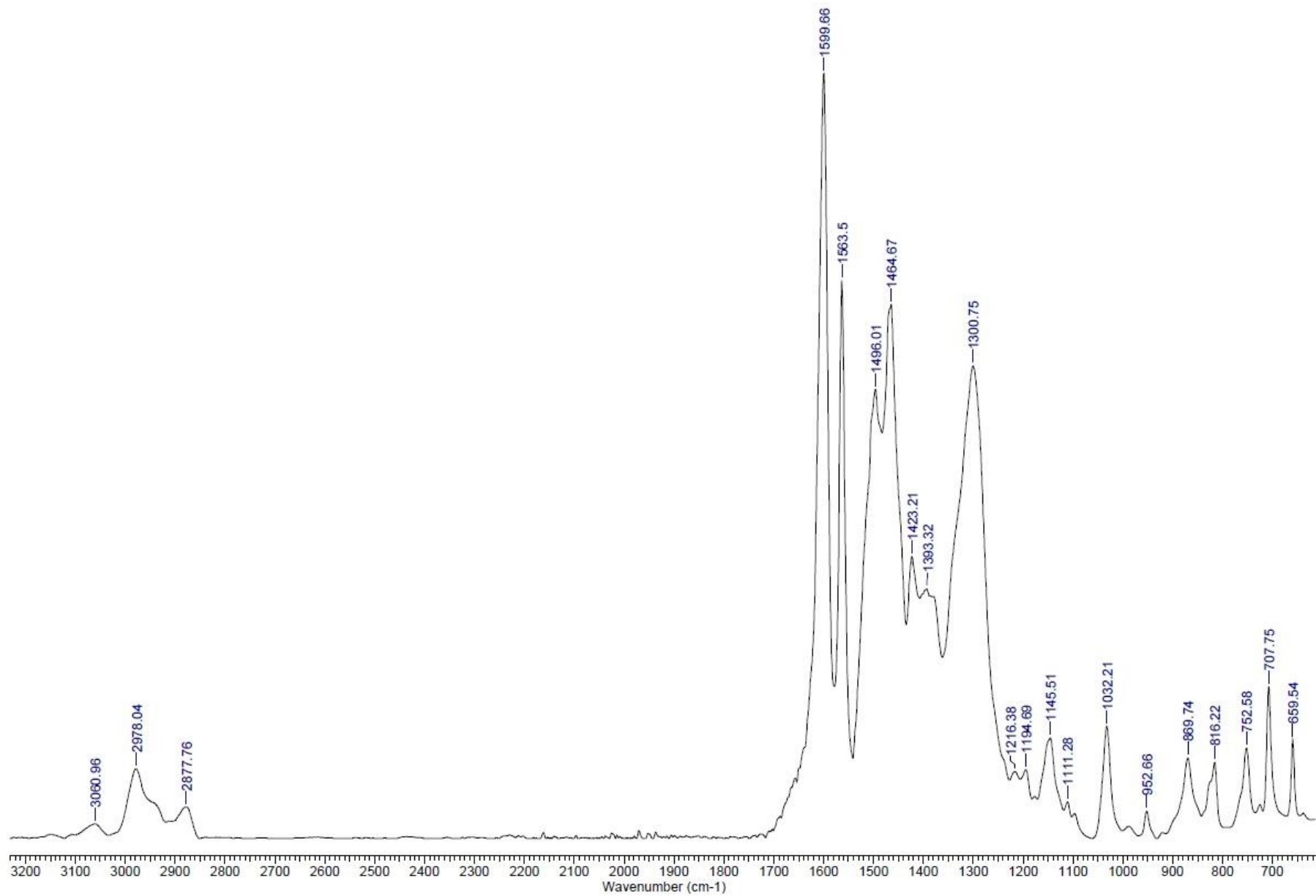


Figure S29. Solid-state IR spectra of complex **L3*Lu(NO₃)₃**

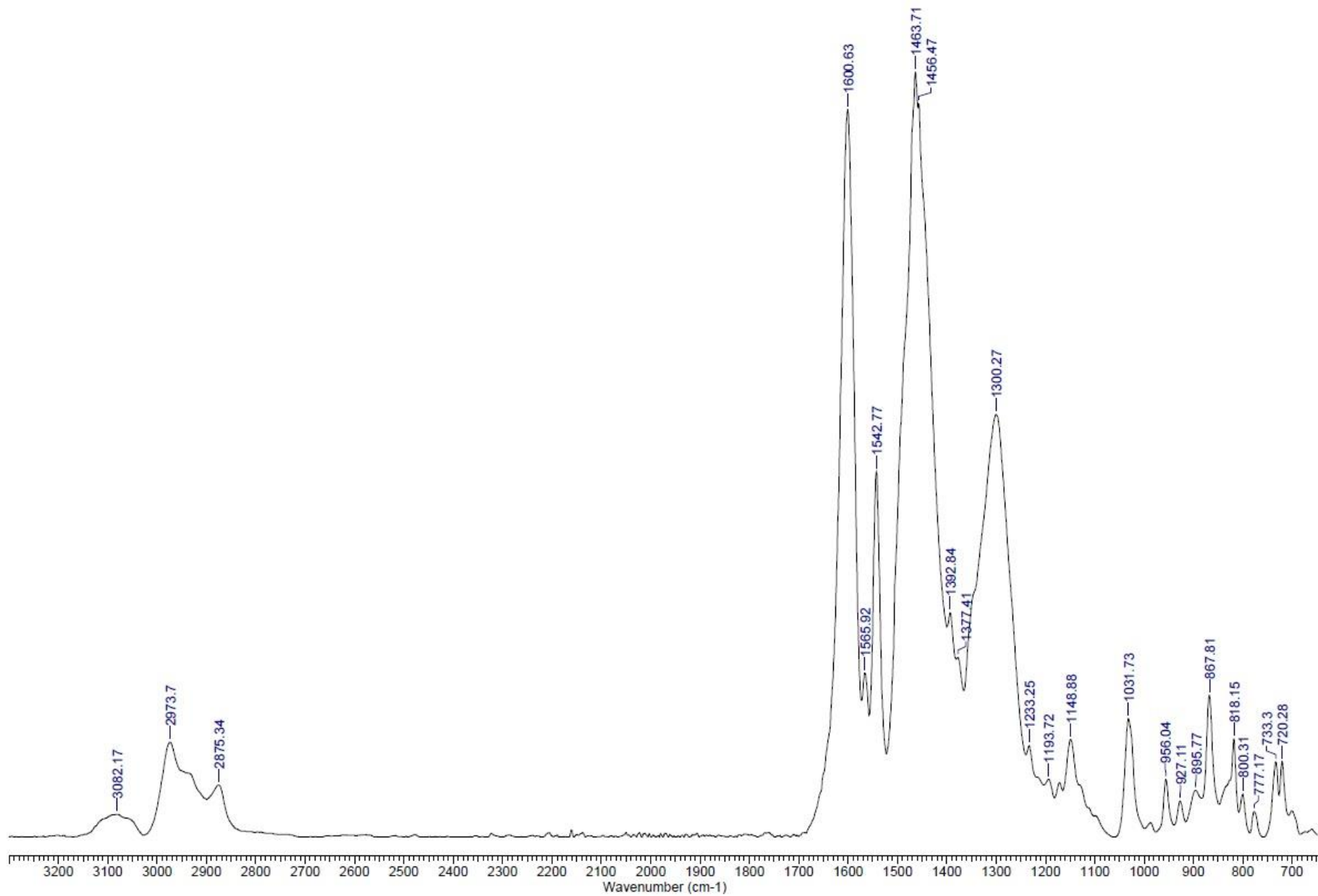


Figure S30. Solid-state IR spectra of complex **L4*La(NO₃)₃**

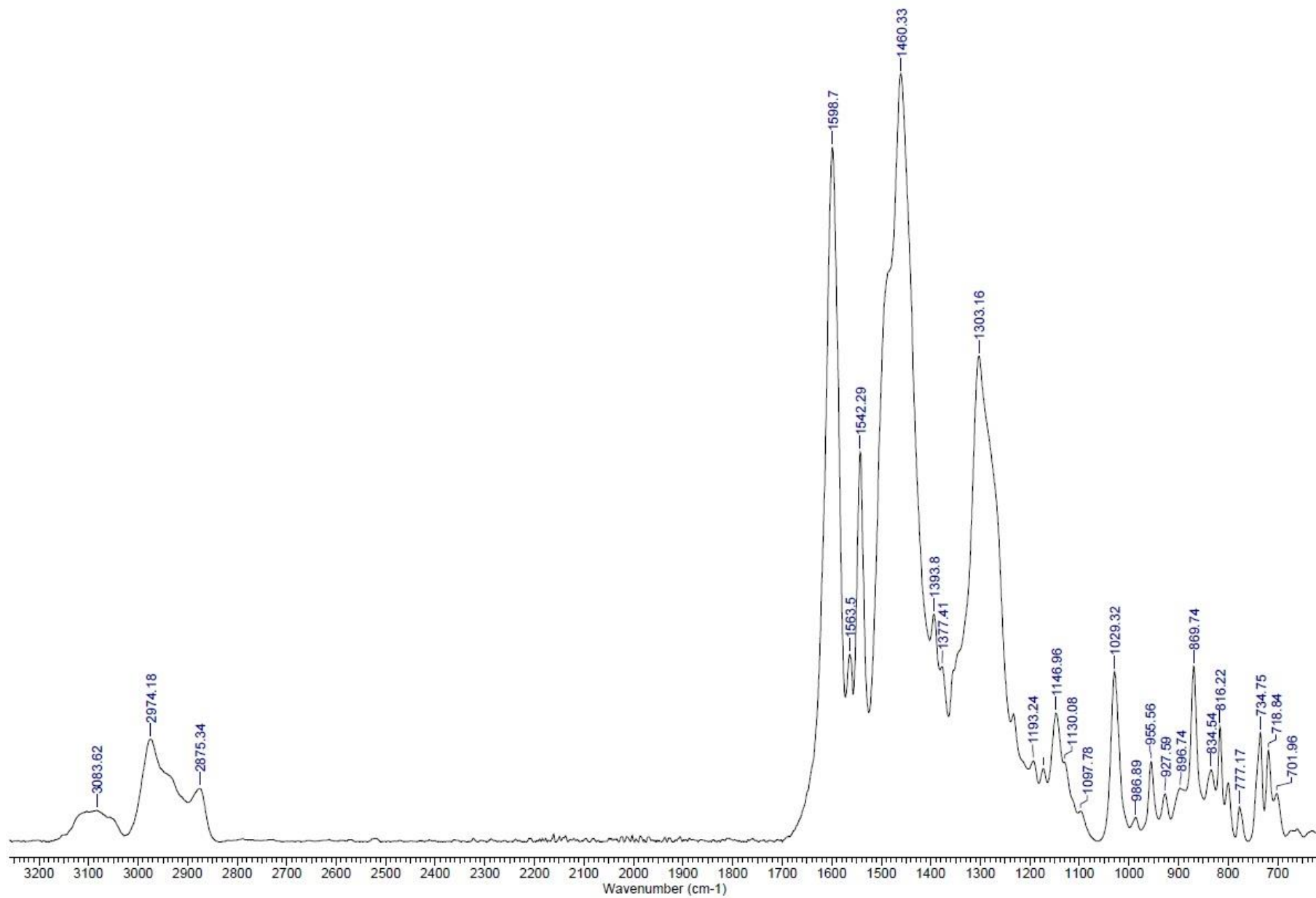


Figure S31. Solid-state IR spectra of complex **L4*Nd(NO₃)₃**

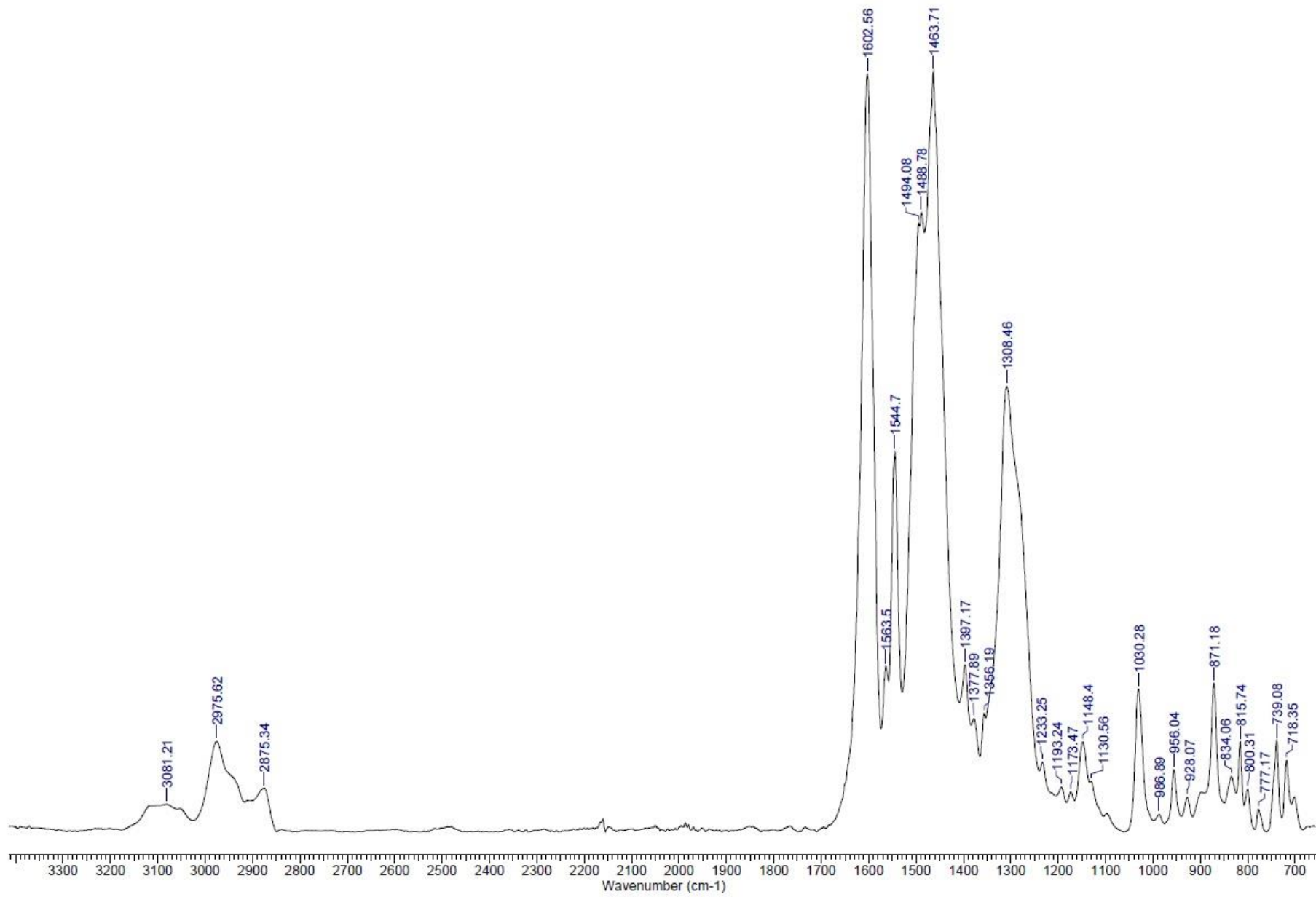


Figure S32. Solid-state IR spectra of complex L4*Eu(NO₃)₃

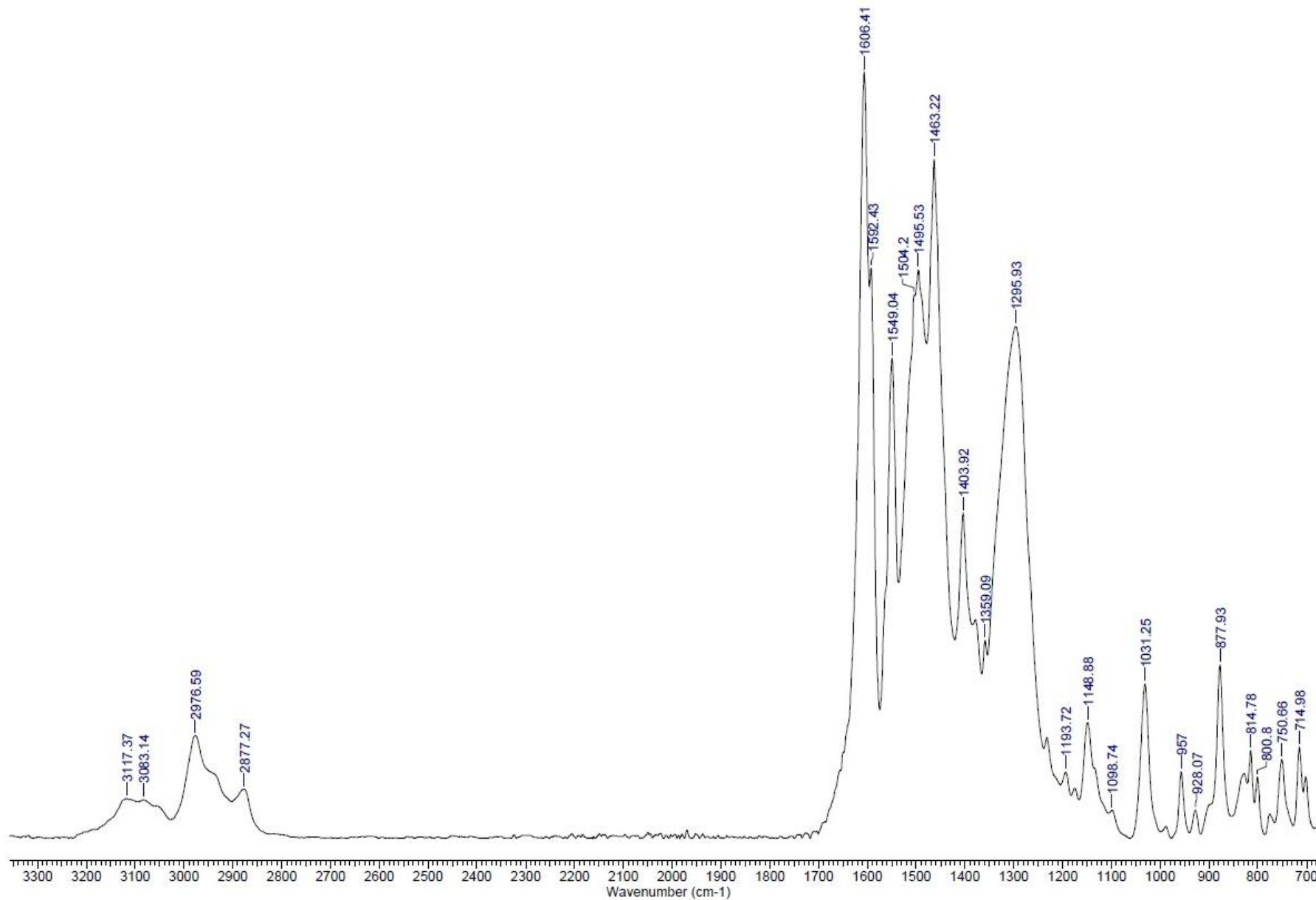


Figure S33. Solid-state IR spectra of complex **L4*Lu(NO₃)₃**

3 X-ray diffraction data

Table S1. Crystal data and structure refinement parameters for **L1**, **L3**, **L4**, **L3*Nd(NO₃)₃** and **L4*Nd(NO₃)₃**

	L1	L3	L4	L3*Nd(NO₃)₃	L4*Nd(NO₃)₃
Empirical formula	C ₂₂ H ₂₂ N ₄ O ₂	C ₂₄ H ₂₆ N ₄ O ₂	C ₂₄ H ₂₄ Cl ₂ N ₄ O ₂	C ₂₄ H ₂₆ N ₇ NdO ₁₁	C ₂₈ H ₃₀ Cl ₂ N ₉ NdO ₁₁
Formula weight	374.3	402.49	471.37	732.76	883.75
T, K	120	120	120	100	100
Crystal system	Monoclinic	Orthorhombic	Orthorhombic	Monoclinic	Monoclinic
Space group	P2 ₁ /c	P2 ₁ 2 ₁ 2 ₁	P2 ₁ 2 ₁ 2 ₁	P2 ₁ /n	P2 ₁ /c
Z	8	4	4	4	8
a, Å	7.5010(9)	8.6426(8)	9.326(3)	9.3150(4)	21.8774(4)
b, Å	22.943(3)	10.6697(10)	10.620(3)	17.7540(7)	17.5953(3)
c, Å	21.104(2)	22.304(2)	22.479(6)	16.6429	19.4525(3)
α/°	90	90	90	90	90
β/°	92.869(3)	90	90	100.3520(10)	113.0550(10)
γ/°	90	90	90	90	90
V, Å ³	3627.3(7)	2056.8(3)	2226.3	2707.58(19)	6890.0(2)
D _{calc} (g cm ⁻³)	1.373	1.300	1.406	1.798	1.704
Linear absorption, μ (cm ⁻¹)	0.90	0.85	3.22	19.92	17.34
F(000)	1584	856	984	1468	3544
2θ _{max} , °	62	56	54	56	56
Reflections measured	49775	23524	14213	29857	84838
Independent reflections	11093	4976	4855	6523	16627
Observed reflections [I > 2σ(I)]	6670	3898	2397	5760	13227
Parameters	512	291	326	420	927
R1	0.0584	0.0538	0.0639	0.0657	0.0409
wR2	0.1428	0.1262	0.1594	0.1403	0.1100
GOF	1.009	1.032	1.003	1.240	0.940
Δρ _{max} / Δρ _{min} (e Å ⁻³)	0.364/-0.365	0.432/-0.249	0.268/-0.344	1.949/-2.344	1.300/-0.911

4 Spectrophotometric titration data

Ligand L1

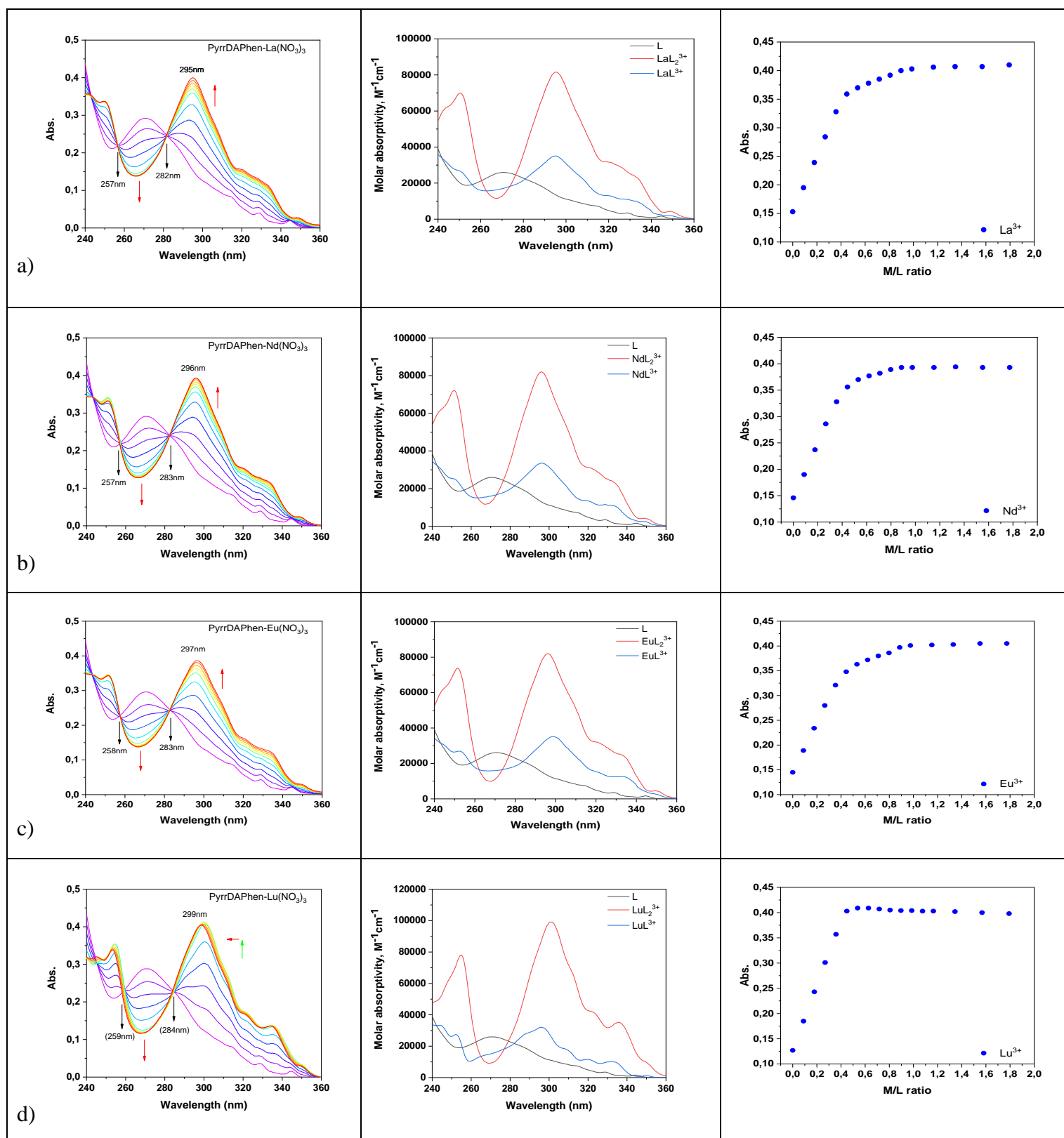


Figure S34. Spectrophotometric titration of **PyrrDAPhen (1)** (ca. 10^{-5} mol/L) with a) La³⁺, b) Nd³⁺, c) Eu³⁺ and d) Lu³⁺ ions (ca. 10^{-3} mol/L) in CH₃CN solution ($T = 25.0 \pm 0.1$ °C, $I = 0$ M, $V_0 = 2.0$ mL). Left: absorption spectra, middle: the molar absorptivities of free ligand **1** and Ln(III) complexes calculated from spectral deconvolution, right: titration curve at maximum absorption wavelength.

Ligand L2

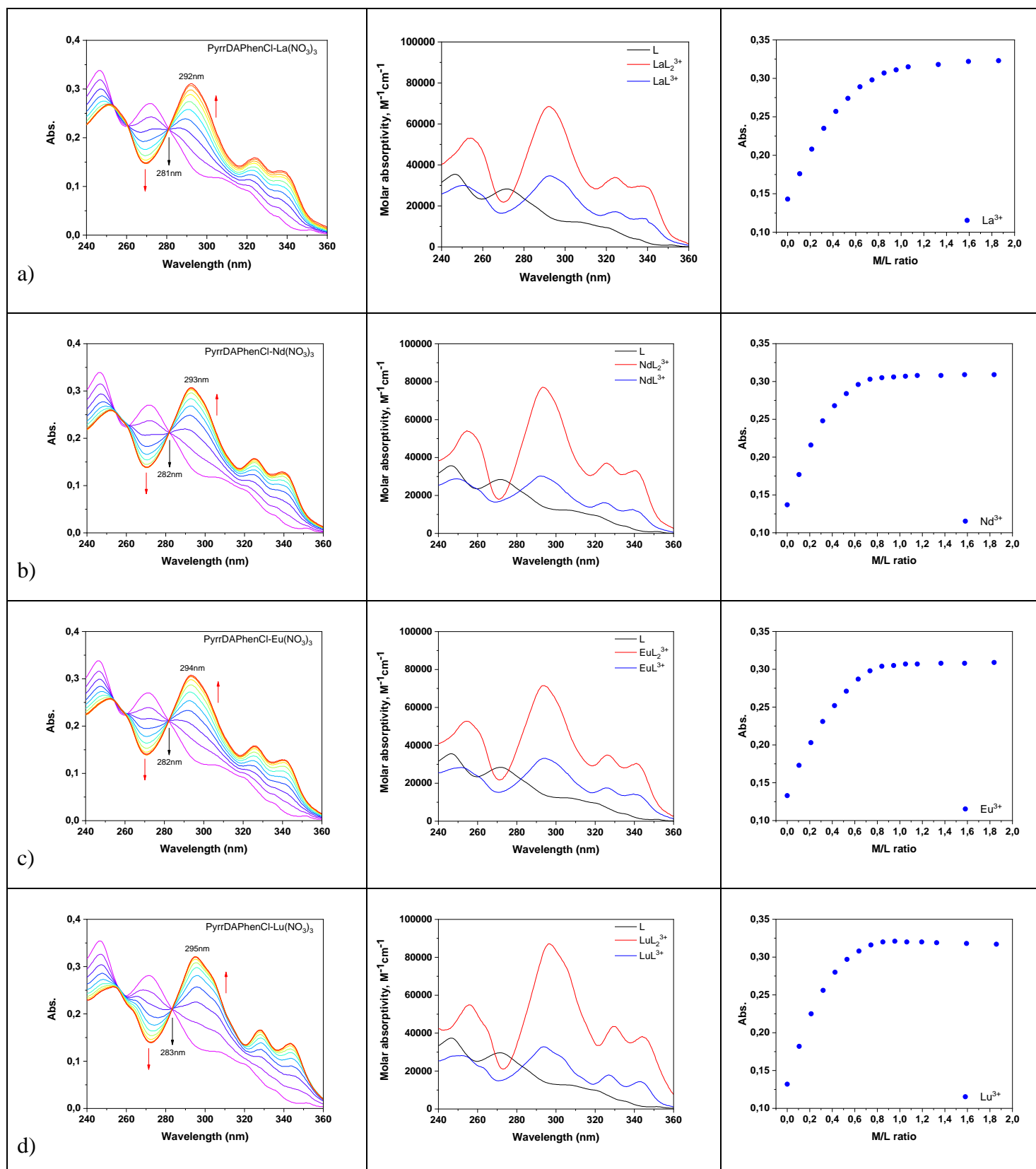


Figure S35. Spectrophotometric titration of **PyrrDAPhenCl (2)** (ca. 10^{-5} mol/L) with a) La^{3+} , b) Nd^{3+} , c) Eu^{3+} and d) Lu^{3+} ions (ca. 10^{-3} mol/L) in CH_3CN solution ($T = 25.0 \pm 0.1$ °C, $I = 0$ M, $V_0 = 2.0$ mL). Left: absorption spectra, middle: the molar absorptivities of free ligand **2** and $\text{Ln}(\text{III})$ complexes calculated from spectral deconvolution, right: titration curve at maximum absorption wavelength.

Ligand L3

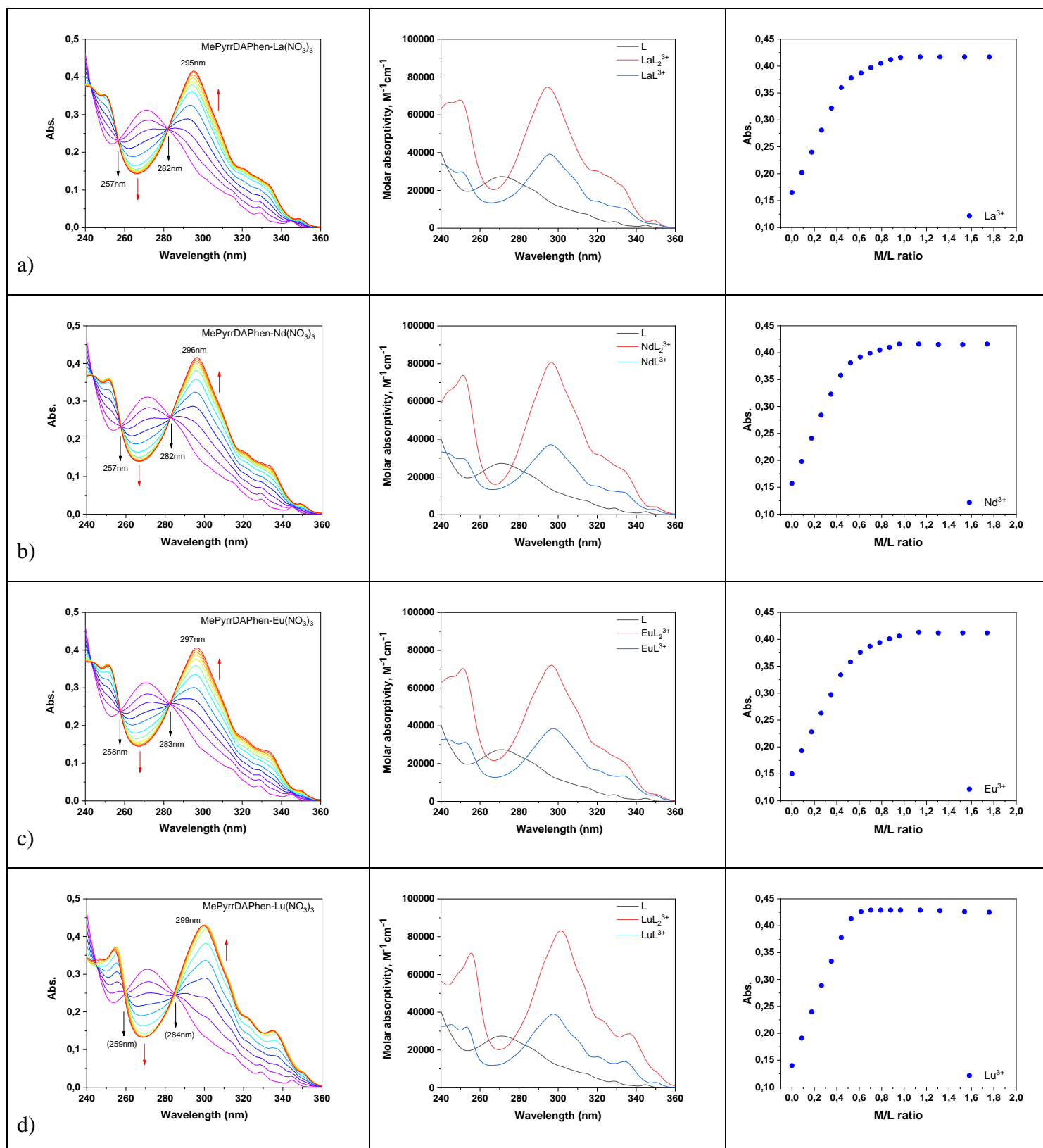


Figure S36. Spectrophotometric titration of L3 (ca. 10^{-5} mol/L) with a) La³⁺, b) Nd³⁺, c) Eu³⁺ and d) Lu³⁺ ions (ca. 10^{-3} mol/L) in CH₃CN solution ($T = 25.0 \pm 0.1$ °C, $I = 0$ M, $V_0 = 2.0$ mL). Left: absorption spectra, middle: the molar absorptivities of free ligand L3 and Ln(III) complexes calculated from spectral deconvolution, right: titration curve at maximum absorption wavelength.

Ligand L4

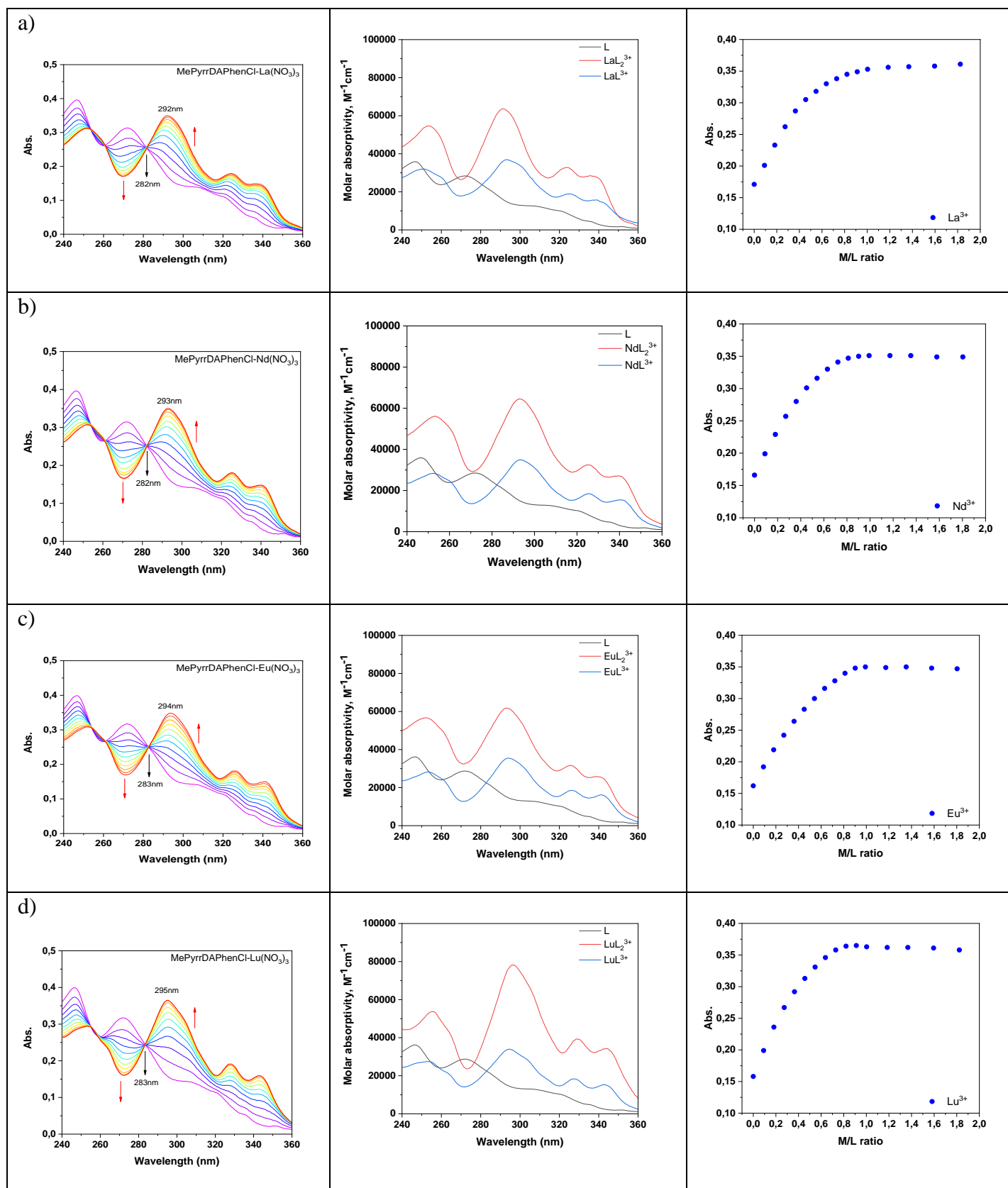


Figure S37. Spectrophotometric titration of **L4** (ca. 10^{-5} mol/L) with a) La^{3+} , b) Nd^{3+} , c) Eu^{3+} and d) Lu^{3+} ions (ca. 10^{-3} mol/L) in CH_3CN solution ($T = 25.0 \pm 0.1$ °C, $I = 0$ M, $V_0 = 2.0$ mL). Left: absorption spectra, middle: the molar absorptivities of free ligand **L4** and Ln(III) complexes calculated from spectral deconvolution, right: titration curve at maximum absorption wavelength.

5 Solvent Extraction Kinetics and Solvation numbers

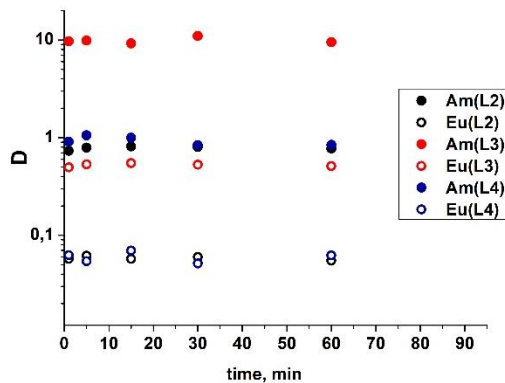


Figure S38. Dependence of the distribution coefficients of Am and Eu on the phase contact time during extraction of 0.012M PyrrDAPhenCl (**L2**), 0.04M MePyrrDAPhen (**L3**), 0.02M MePyrrDAPhenCl (**L4**) from 3M HNO₃

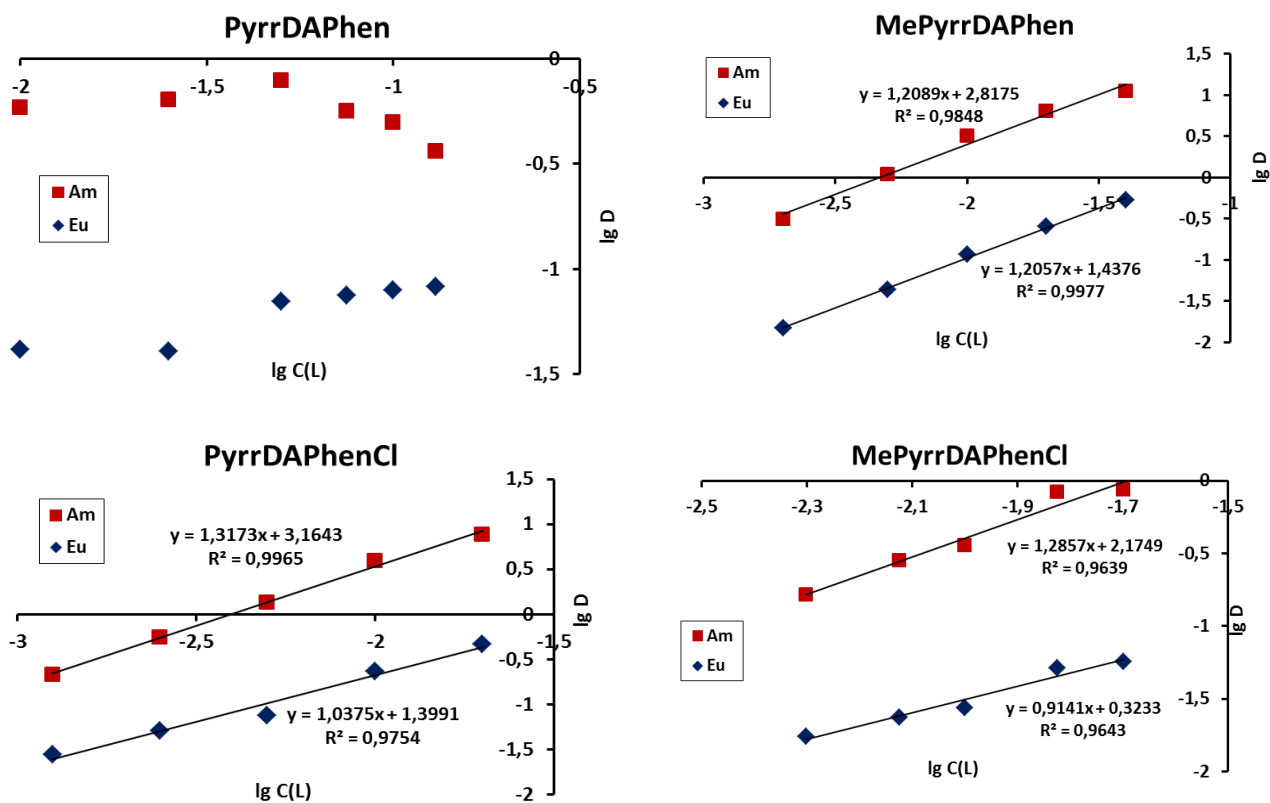


Figure S39. Dependence of the Am/Eu distribution coefficients on the ligand concentration during the extraction of PyrrDAPhen (**L1**), MePyrrDAPhen (**L3**), MePyrrDAPhenCl (**L4**) from 3M HNO₃ and PyrrDAPhenCl (**L2**) from 5M HNO₃.

6. Theoretical computations

All structures were optimized at the DFT level in the gas phase (tolerance on gradient: 10^{-7} au).⁷ We used quantum chemical software PRIODA-19 developed by Laikov⁸ to evaluate quantum chemical calculations. The generalized gradient approximation (GGA) functional PBE was used for the geometry optimization and frequency calculations of all structures as reported in our previous work⁹. All stationary points on the potential energy surface (PES) were checked by vibrational analysis and none of them had imaginary frequencies. For La complexes with ligands **L1-L4**, we used hybrid functional PBE0 containing 25% of exchange HF energy to test the stability of the solution. Full electron relativistic L1 basis set¹⁰ of TZ quality including one polarization function was used for all the atoms to provide the most reliable result. For complexes of NdIII and EuIII the highest spin 4 and 7 respectively were chosen according (2S+1) rule. To make ESP maps for ligand we used Gaussian 1630 at B3LYP/6-31G(d,p) theoretical level. B3LYP is used as an universal, time-saving functional for making ESP maps⁹, 6-31G(d,p) was chosen as a standard basis set.

We used eq. (1) as a model reaction of complex formation.



The energy of complex formation in gas phase was calculated according to eq. (2).

$$\Delta E = E_{4\text{H}_2\text{O}} + E_{\text{L}^*\text{Met}(\text{NO}_3)_3} - E_{\text{Met}(\text{H}_2\text{O})_4(\text{NO}_3)_3} - E_{\text{L}} \quad (2)$$

where $E_{4\text{H}_2\text{O}}$, $E_{\text{L}^*\text{Met}(\text{NO}_3)_3}$, $E_{\text{Met}(\text{H}_2\text{O})_4(\text{NO}_3)_3}$, E_{L} are energies for optimized geometrical structures of $4\text{H}_2\text{O}$, $[\text{Met}(\text{NO}_2)_3]\text{L}$, $\text{Met}_3(\text{NO}_2)_3$, L respectively.

The preorganization energy of a ligand in a complex was calculated as difference between the energy of a ligand in a complex and the energy of the main conformer of the ligand. The energy of a ligand in a complex was calculated by removing $\text{Ln}(\text{NO}_3)_3$ in the structure of the complex and further calculating the energy of obtained geometry of the ligand.

Since **L3** and **L4** ligands possess stereoisomerism, we took these effects into account when modeling their complexes with $\text{La}(\text{NO}_3)_3$. Figure S40 shows the possible positions of Me in the **L3*La(NO₃)₃** complex.

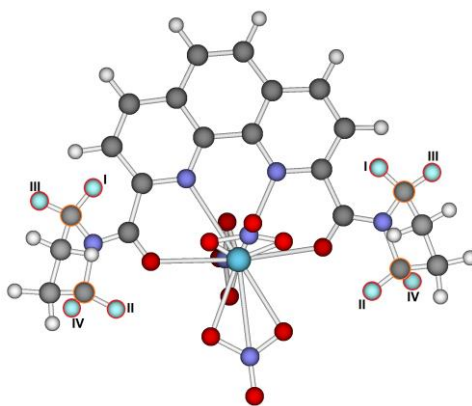


Figure S40. Possible positions of Me in the complex **L3*La(NO₃)₃**.

To describe the rotation of the N-CO amide group we introduced “up” and “down” designators. Figure S41 demonstrates the difference of two isomers on the example of Meso-form.

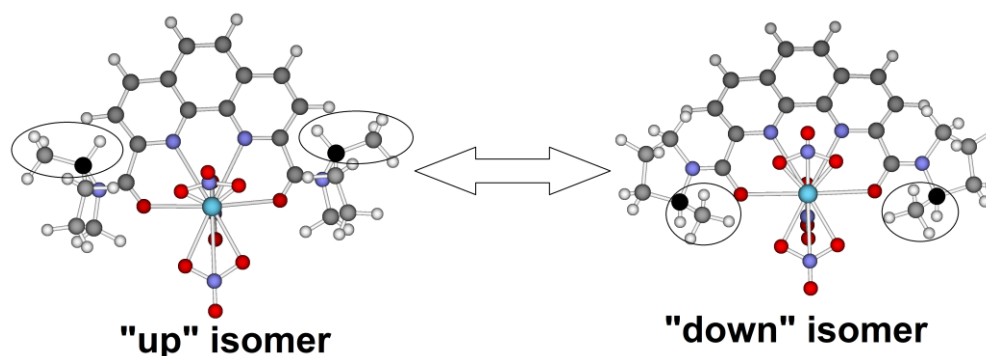


Figure S41. “Up” and “down” isomers of $L3^*[La(NO_3)_3]$ on the example of Meso-form **L3**.

Also “in” and “out” isomers are possible, where the methyls are directed “inside” the complex (“in” geometry) and outside (“out” geometry). Figure S42 demonstrates the difference.

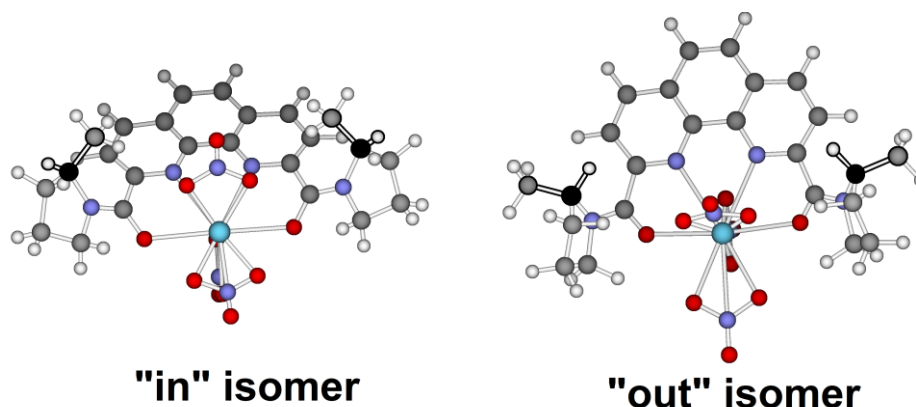


Figure S42. “In” and “out” isomers of $L3^*La(NO_3)_3$ on the example of Meso-form of **L3**.

We compared relative stability of “up”/“down” and “in”/“out” isomers with each other for Meso and Rac-form. For Meso-form of **L3** geometry IV was chosen as zero point (Figure S43).

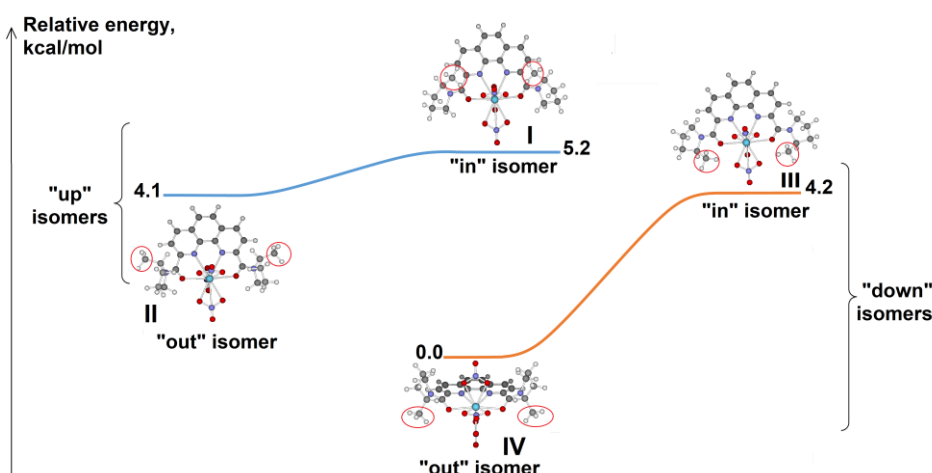


Figure 43. Images of geometries I-IV of $3^*[La(NO_3)_3]$ with corresponding energies of complex formation (E, kcal/mol). Meso-form of of the ligand. Geometry IV chosen as zero point.

In the pair of ligands, where the methyls are directed “inside” the complex (“in” geometry - I, III) and outside (“out” geometry – II, IV), the most stable geometry is “out”. Geometries II, IV (“down” isomers) are more preferable than geometries I, III (“up” methyls). Table S2 shows relative energies of different isomers of $3^*\text{La}(\text{NO}_3)_3$ and preorganization energy of ligand **3** in the corresponding complexes (E, kcal/mol).

Table S2. Relative energies of isomers of $3^*\text{La}(\text{NO}_3)_3$ complex and corresponding energies of ligand preorganization (Meso-form).

Isomer	Relative energy, kcal/mol	Preorganization energy, kcal/mol
I	5.2	23.0
II	4.1	22.7
III	4.2	21.3
IV	0.0	17.8

Figure 44 shows relative energies of $\text{L3}^*\text{La}(\text{NO}_3)_3$ with different configurations of the substituent in the pyrrolidine ring of the Rac-form of **L3** (VIII was chosen as zero point). Table S3 shows relative energy of complex and corresponding preorganization energy of **L3** (E, kcal/mol).

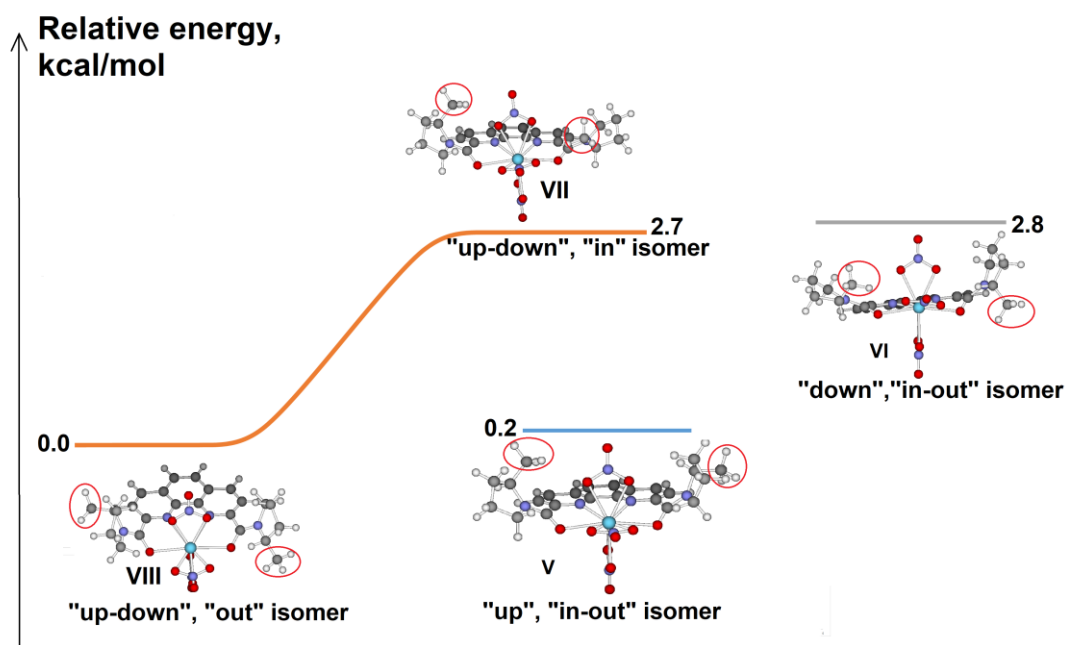


Fig. 44. Images of geometries V-VIII of $\text{L3}^*[\text{La}(\text{NO}_3)_3]$ with corresponding energies of complex formation (E, kcal/mol). Rac-form of the ligand. Geometry VIII chosen as zero point.

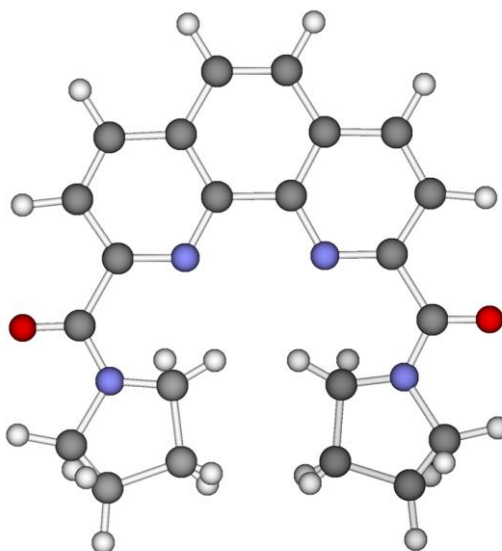
Table S3. Relative energies of **L3*La(NO₃)₃** complex with geometries V-VIII and energies of ligand preorganization (Rac-form).

Isomer	Energy of complex formation, kcal/mol	Preorganization energy, kcal/mol
V	0.2	20.6
VI	2.8	23.0
VII	2.7	22.4
VIII	0.0	19.9

Geometry VIII was used for optimization of complexes of **L3** with Nd(NO₃)₃, Eu(NO₃)₃, Lu(NO₃)₃, Am(NO₃)₃, Cm(NO₃)₃ in case of Rac-isomer.

L1

Major conformer form



PBE/L1 theoretical level

E= -1220.515792

G= 215.1705 kcal/mol, H= 265.5272 kcal/mol, U= 264.9347 kcal/mol, S= 168.8972 cal/mol at T= 298.150 K

C 0.50669205 0.02459001 3.43878412

C 1.65194976 -0.15478058 2.45634866

C 2.94941902 -0.22254448 3.01915288

C 4.02924776 -0.34749103 2.17403865

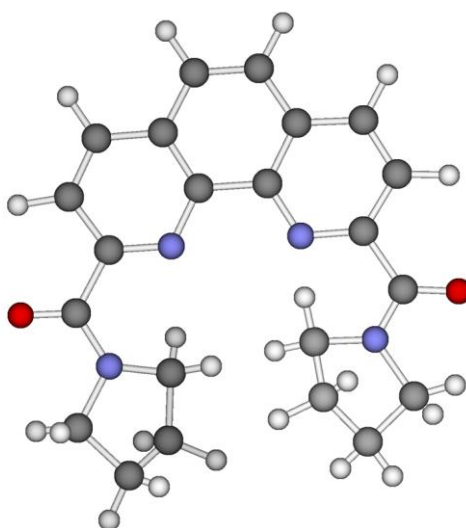
C 3.82200646 -0.36818823 0.77446008

C 2.47820854 -0.25195736 0.30834275
N 1.42391551 -0.16117065 1.14918780
C -0.68469733 0.00051874 -3.41051316
O -0.94687265 -0.54335201 -4.48569393
N -1.62547255 0.67241019 -2.68815398
C -2.98840904 0.77429807 -3.24336934
C -1.44992077 1.54152274 -1.50394046
N -0.73509741 -0.42177150 3.09669256
H 5.04816818 -0.42520496 2.56525731
C 4.89857864 -0.49543497 -0.15820450
O 0.73250860 0.57666463 4.51799297
C -1.82659876 -0.26538542 4.07663679
C -1.13993752 -1.27355349 1.95685780
H 3.04688096 -0.16337749 4.10412169
C -3.62119865 1.93100297 -2.45962405
C -2.89870000 -1.25131309 3.59593415
H -2.19443703 0.77664077 4.06664944
H -2.93743372 0.94305414 -4.33017063
C 2.23036814 -0.23849554 -1.12788475
N 0.96082073 -0.08456746 -1.56525326
C 3.33590221 -0.38020167 -2.01918149
C 0.73348153 -0.09074555 -2.87252092
C 4.66387749 -0.50653398 -1.50386131
H 5.91745186 -0.58595049 0.23012935
C 3.05575061 -0.39294878 -3.40611219
H 3.87853026 -0.50942796 -4.11788321
C 1.75433242 -0.26687273 -3.83769584
H 5.49091721 -0.61078346 -2.21254206
H 1.47054589 -0.30576456 -4.89037704
H -3.53143024 -0.17471781 -3.08313370
H -1.45009196 -0.47031078 5.09075403

C -2.89220858 1.87693322 -1.10746789
H -0.87621468 1.02255476 -0.72698718
H -0.90009797 2.46109080 -1.78134537
C -2.66784883 -1.30512011 2.07721400
H -0.76934236 -0.85583246 1.01328051
H -0.72056228 -2.29136992 2.07093000
H -2.95513272 2.81654596 -0.53849608
H -3.30747581 1.06634068 -0.48479947
H -4.71237135 1.82304430 -2.37133956
H -3.41066813 2.88933539 -2.96303487
H -3.10026789 -2.19737029 1.60025954
H -3.09985852 -0.41123211 1.59600663
H -3.91300201 -0.92677683 3.87157226
H -2.72420502 -2.24599981 4.03898191
PBE0/L1 theoretical level
E= -1220.582278
C -0.18452129 -1.90319395 2.85460877
C 1.02103710 -1.93707776 1.94958055
C 2.03271985 -2.85241151 2.28513932
C 3.13482594 -2.92556190 1.48067784
C 3.20913601 -2.11614394 0.33452967
C 2.11614013 -1.26323462 0.06554813
N 1.05469048 -1.17821229 0.87930983
C -0.03735534 1.99292564 -2.79694676
O 0.16526258 3.02375841 -3.41214418
N -1.26608622 1.63791013 -2.36829805
C -2.37968659 2.53951263 -2.65102124
C -1.72243178 0.34130698 -1.86212742
N -0.91044152 -0.76767385 2.91178560
H 3.95274854 -3.60198164 1.70998228
C 4.33473873 -2.13741422 -0.53872651
O -0.47739634 -2.89637661 3.49488664
C -2.09247708 -0.75026733 3.76933527

C -0.56073713 0.57048339 2.42932868
H 1.90221202 -3.46901703 3.16556120
C -3.57142806 1.84735596 -2.00294995
C -2.66502380 0.64497888 3.55783081
H -1.80405712 -0.91815668 4.81432009
H -2.17626143 3.53356767 -2.24524522
C 2.14658022 -0.44170570 -1.12853026
N 1.08301342 0.32292113 -1.41193008
C 3.29057431 -0.48287809 -1.95557368
C 1.12137496 1.08067715 -2.48283029
C 4.37749577 -1.34635496 -1.63461578
H 5.16138601 -2.80043912 -0.30221495
C 3.30502820 0.35100770 -3.08639646
H 4.17465115 0.35295972 -3.73668242
C 2.22733307 1.14978540 -3.34655809
H 5.24083853 -1.35899377 -2.29292250
H 2.18851328 1.83473122 -4.18424654
H -2.51174283 2.64916301 -3.73447561
H -2.77828884 -1.55300021 3.48749352
C -3.22182631 0.36857787 -2.14412332
H -1.21567011 -0.48024979 -2.37089467
H -1.51261508 0.24207507 -0.79425973
C -1.41866422 1.48625314 3.29751444
H 0.50689936 0.76393402 2.54466987
H -0.79840386 0.67842805 1.36816037
H -3.77747679 -0.27771401 -1.46091676
H -3.41723061 0.03529892 -3.16879630
H -4.51521778 2.11730194 -2.48173404
H -3.63348079 2.11917377 -0.94393104
H -1.63023555 2.43696022 2.80292654
H -0.90627939 1.69621062 4.24228239
H -3.24681091 0.98627228 4.41683578
H -3.31535268 0.65452802 2.67678404

Minor conformer form



PBE/L1 theoretical level

E= -1220.515631

G= 215.1243 kcal/mol, H= 265.4704 kcal/mol, U= 264.8779 kcal/mol, S= 168.8615 cal/mol at T= 298.150 K

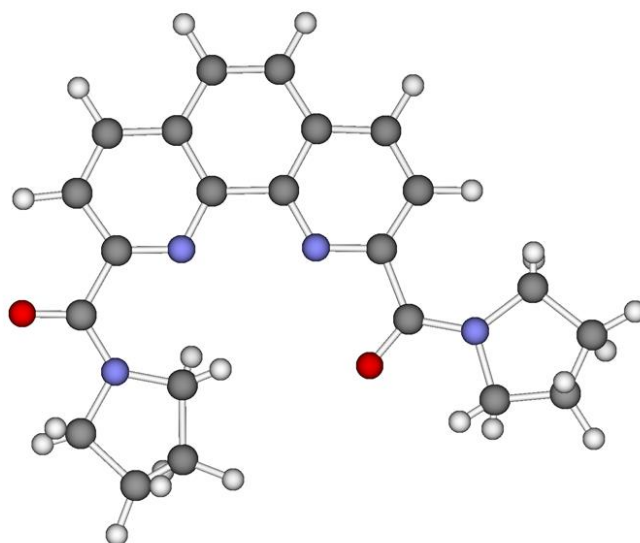
C	-0.15624915	-1.91864336	2.89387560
C	1.05151427	-1.94239974	1.97654676
C	2.07461309	-2.86084795	2.31242728
C	3.18265271	-2.93679523	1.49902654
C	3.25269675	-2.12948465	0.33900470
C	2.14499426	-1.27071202	0.06590890
N	1.07760906	-1.17889571	0.89103365
C	-0.02226211	1.99445093	-2.84622025
O	0.18598066	3.02630067	-3.48717403
N	-1.26539874	1.65943623	-2.39676809
C	-2.37884808	2.57881832	-2.68889642
C	-1.74096560	0.37831354	-1.83636248
N	-0.91733599	-0.78784198	2.93780017
H	4.01038218	-3.61360550	1.73138428
C	4.37964821	-2.15503621	-0.54086554
O	-0.43061602	-2.91757202	3.56163049
C	-2.10257959	-0.78588188	3.81306195

C -0.62046945 0.55883658 2.40930486
H 1.94420445 -3.47795200 3.20278335
C -3.58044028 1.91948688 -2.00204802
C -2.71887112 0.59923655 3.58385634
H -1.79673791 -0.93428832 4.86486864
H -2.14920712 3.58683729 -2.31025290
C 2.17050171 -0.45441958 -1.14262164
N 1.09474266 0.31141907 -1.43347752
C 3.32648206 -0.50087887 -1.97969365
C 1.13580787 1.07017326 -2.52181983
C 4.41909313 -1.36371768 -1.65320325
H 5.21415138 -2.82062435 -0.30055743
C 3.33783579 0.33110127 -3.12428069
H 4.21325922 0.32709587 -3.78064084
C 2.25156713 1.13395977 -3.39012337
H 5.28800869 -1.37969673 -2.31795740
H 2.21017551 1.82142532 -4.23643351
H -2.52338386 2.66430020 -3.78150749
H -2.77280521 -1.61828089 3.54811835
C -3.25341392 0.42125794 -2.10084343
H -1.24678338 -0.47327107 -2.32483006
H -1.51415765 0.31349692 -0.76012081
C -1.49392951 1.47544765 3.27853107
H 0.45136297 0.78712255 2.49072456
H -0.88845611 0.62860394 1.34278190
H -3.81332397 -0.19725122 -1.38357341
H -3.47057676 0.05354926 -3.11770773
H -4.53196716 2.19046021 -2.48287511
H -3.62886453 2.22818136 -0.94428796
H -1.74496806 2.41406488 2.76228547
H -0.96540523 1.72573555 4.21357441

H -3.29540229 0.94467551 4.45467663

H -3.39386463 0.57430989 2.71193695

TS



PBE/L1 theoretical level

E= -1220.500628

G= 216.3676 kcal/mol, H= 264.8377 kcal/mol, U= 264.2452 kcal/mol, S= 162.5694 cal/mol at T= 298.150 K

C -0.66286463 -0.56409121 2.18587375

C 0.74898380 -0.82229871 1.62615013

C 1.84274387 -1.41785109 2.30309772

C 3.04342508 -1.58387339 1.63701236

C 3.17371440 -1.15622294 0.30106142

C 2.01757884 -0.56371444 -0.29127011

N 0.85460532 -0.41550991 0.36319819

C -0.13831694 1.55667448 -4.11031961

O 0.00691081 2.17741299 -5.16764545

N -1.34005249 1.48990047 -3.46940207

C -2.46740055 2.23396420 -4.05727911

C -1.76542640 0.68749338 -2.29571176

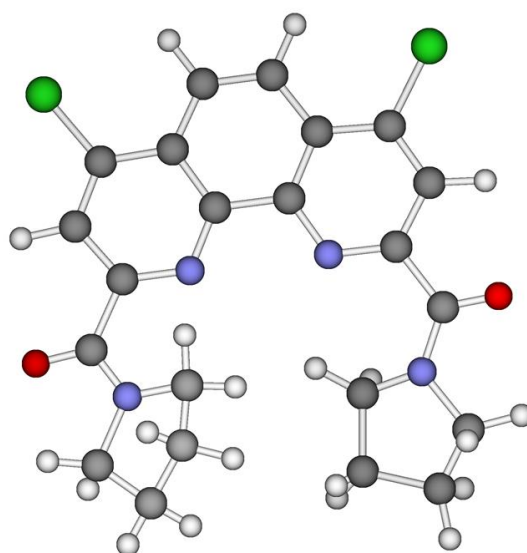
N -0.94595671 -0.74909985 3.52305055

H 3.89706349 -2.04654551 2.14153695
C 4.38268661 -1.29353821 -0.45237002
O -1.53891599 -0.15341127 1.43383193
C -2.28733206 -0.33012763 3.97579646
C -0.15224172 -1.29351556 4.63819504
H 1.76803172 -1.75392938 3.33331609
C -3.55829978 2.14214158 -2.98567724
C -2.14005208 -0.22729287 5.49461794
H -3.04566002 -1.08205688 3.68870902
H -2.15432191 3.26228571 -4.29444027
C 2.09830952 -0.10327463 -1.67409813
N 1.00179768 0.45159006 -2.22509074
C 3.32240796 -0.25967512 -2.38733101
C 1.06107497 0.87431335 -3.47922921
C 4.45281124 -0.86141592 -1.74674046
H 5.25160265 -1.75232768 0.02904502
C 3.35518622 0.20298304 -3.72515416
H 4.27780581 0.10169422 -4.30487156
C 2.22922993 0.77701056 -4.27430868
H 5.38014078 -0.96855074 -2.31790543
H 2.19012642 1.17364502 -5.29024839
H -2.78424335 1.76127124 -5.00575447
H -2.55983424 0.61401755 3.48284173
C -3.29825330 0.76737046 -2.35196352
H -1.39163888 -0.34251699 -2.36663699
H -1.36654091 1.10180724 -1.35819983
C -1.14736474 -1.35293090 5.81178141
H 0.23221838 -2.30040526 4.40878391

H 0.70199037 -0.63494843 4.88114786
H -3.73874426 0.65328664 -1.35080516
H -3.69939065 -0.02824003 -3.00249577
H -4.56720877 2.24323153 -3.41311002
H -3.41822553 2.93850946 -2.23574829
H -0.64158672 -1.23756659 6.78210211
H -1.66733778 -2.32500744 5.80844212
H -3.10171819 -0.34199724 6.01618481
H -1.71151710 0.75133240 5.76803064

L2

Main conformer form



PBE/L1 theoretical level

E= -2142.322484

G= 200.5479 kcal/mol, H= 255.2129 kcal/mol, U= 254.6205 kcal/mol, S= 183.3474 cal/mol at T= 298.150 K

Cl -4.29350901 4.24362421 -1.86920726
Cl -3.94397187 -3.05972767 -3.86619782
N -1.08451378 1.43870521 -0.26835915
N 0.54019773 2.46715355 1.88851488
N -0.88402522 -1.15145838 -1.09416842
N 1.48223913 -2.76844192 -0.53604239

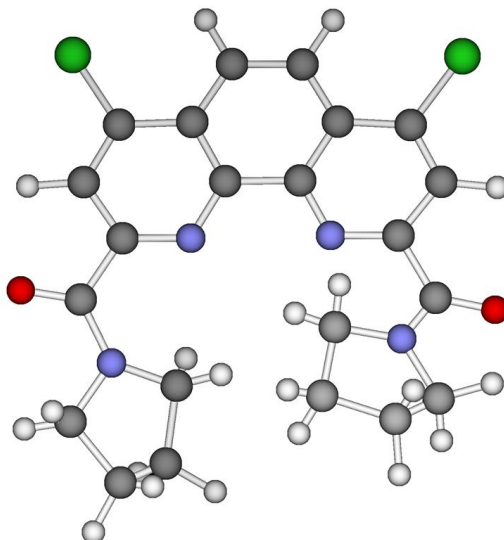
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C -1.14608943 2.71318078 0.09241261
C -2.10713673 3.62439418 -0.40015197
H -2.05478072 4.66638899 -0.08432339
C -3.06205678 3.15179205 -1.26991141
C -3.05010962 1.79257214 -1.68318915
C -4.00587988 1.22781658 -2.57836962
H -4.79711485 1.87160027 -2.96612859
C -3.94037819 -0.08718046 -2.94340634
H -4.68125439 -0.51113194 -3.62329936
C -2.90473986 -0.93609041 -2.45347595
C -2.77910948 -2.30944681 -2.79465795
C -1.74720883 -3.06404519 -2.28653336
H -1.63538694 -4.12876415 -2.49084997
C -0.80262834 -2.42498541 -1.45161843
C -1.91310060 -0.41611612 -1.56449711
C -2.00131297 0.98083198 -1.14813602
C -0.09712393 3.30125308 1.02010071
C 0.29057896 -3.32326198 -0.89231282
C 0.19841297 1.08367074 2.27855682
H 0.62242717 0.35975578 1.56454074
H -0.89016187 0.93469542 2.28998518
C 0.83542401 0.94673055 3.66919088
H 0.15078458 1.33920228 4.43953896
H 1.06585991 -0.10095011 3.91354680
C 2.08188963 1.83948481 3.56731844
H 2.87782502 1.31789291 3.00954843
H 2.48622322 2.13647437 4.54617548
C 1.57727671 3.04359579 2.76367164
H 1.13304043 3.81880212 3.41405749

H 2.35707927 3.53166080 2.15889931
C 2.53469825 -3.65920091 -0.00964912
H 2.56347394 -4.59202337 -0.59385419
H 2.30421400 -3.93320513 1.03554296
C 3.81491804 -2.81997609 -0.11176435
C 3.30087280 -1.37673473 0.01500098
C 1.99499595 -1.40357172 -0.78669721
H 4.00627279 -0.62641662 -0.37221035
H 3.08790421 -1.13999677 1.07148516
H 4.28570032 -2.96610856 -1.09809244
H 4.54921293 -3.09085417 0.66108602
H 1.25678587 -0.65336692 -0.47860202
H 2.19963098 -1.26370025 -1.86528623
PBE0/L1 theoretical level
E= -2142.446397
Cl -4.61403799 3.95509982 -1.46872211
Cl -3.42003655 -2.87574625 -4.38296556
N -1.13852799 1.37555456 -0.21634842
N 0.88480210 2.69225144 1.38010347
N -0.77720344 -1.12957084 -1.17318702
N 1.09476006 -2.92737484 0.03918375
O -0.84128475 3.91193700 2.15462112
O 1.10480988 -3.95840979 -1.96020770
C -1.32108533 2.57225132 0.28504363
C -2.40227175 3.39894962 -0.05703879
H -2.51153803 4.35612392 0.43461958
C -3.28337598 2.94682503 -0.99633658
C -3.11898112 1.67124379 -1.57484150
C -3.98786116 1.13400197 -2.56273866
H -4.82486582 1.73420513 -2.89741778
C -3.77623701 -0.09742694 -3.08136344

H -4.43949556 -0.49494454 -3.83955622
C -2.68643165 -0.89893454 -2.64554834
C -2.41127896 -2.18630385 -3.15128517
C -1.34691083 -2.89950943 -2.68106723
H -1.08065212 -3.87581301 -3.06334448
C -0.56669909 -2.32616830 -1.66600883
C -1.80344081 -0.41537246 -1.65290701
C -2.01450109 0.91698366 -1.11794853
C -0.39545348 3.11268568 1.35178578
C 0.61445940 -3.14339805 -1.20118535
C 1.62555134 1.91463947 0.38065293
H 1.75602317 2.50074124 -0.53877139
H 1.09475935 0.99969524 0.12660155
C 2.96924376 1.68243575 1.05897653
H 2.90248728 0.81743485 1.72780073
H 3.76606202 1.49712908 0.33523953
C 3.17012215 2.95828295 1.87179303
H 3.50346923 3.76946139 1.21632361
H 3.89941382 2.84927988 2.67737961
C 1.77162743 3.25504279 2.39913034
H 1.58950126 2.76669431 3.36383224
H 1.56505883 4.32013226 2.52724814
C 2.25392389 -3.70687294 0.46935335
H 3.09131145 -3.55211592 -0.21541397
H 2.01304626 -4.77668428 0.45607525
C 2.51884961 -3.20246387 1.88170207
C 1.12307775 -2.83714032 2.37866020
C 0.47909263 -2.19943166 1.15145993
H 1.12870979 -2.15942216 3.23520851
H 0.57736886 -3.74380255 2.66017509
H 3.15206695 -2.30955720 1.84912312

H 3.01649261 -3.95274663 2.49979424
 H -0.60620117 -2.30865788 1.14161587
 H 0.70228136 -1.13121390 1.09070051

Minor conformer form



PBE/L1 theoretical level

E= -2142.322322

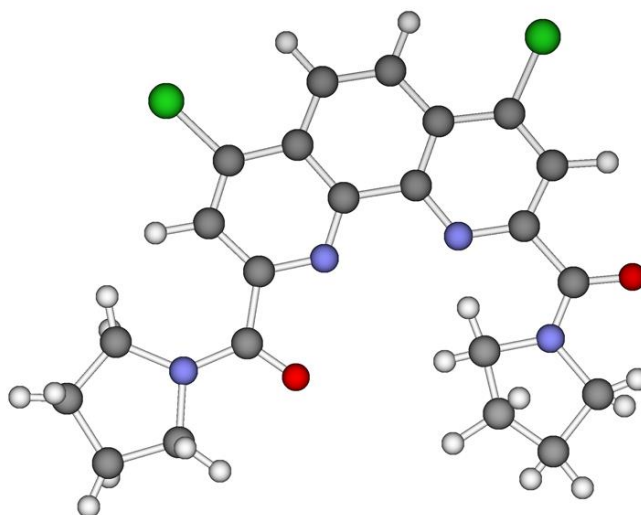
G= 200.5423 kcal/mol, H= 255.2157 kcal/mol, U= 254.6232 kcal/mol, S= 183.3755 cal/mol at T= 298.150 K

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 Cl -3.53411746 -2.57139349 -4.56343985
 N -1.50298703 0.91586417 0.44106477
 N 0.42048100 2.36072779 2.09331298
 N -0.71935260 -0.97167420 -1.36251295
 N 1.84781384 -2.28223038 -1.15776730
 O -1.34076762 2.63996148 3.50532007
 O 1.60989428 -2.68687749 -3.38161731
 C -1.88364220 1.79829717 1.35361540
 C -3.21203589 2.26259828 1.48544729
 H -3.45274806 2.94995713 2.29630303
 C -4.14927053 1.81085789 0.58543181
 C -3.79064703 0.87421888 -0.42075109
 C -4.70123243 0.36388993 -1.39215767

H -5.73516750 0.71216023 -1.36823559
C -4.29393816 -0.53616548 -2.33597374
H -4.99641180 -0.91400820 -3.08071256
C -2.94853592 -1.00770819 -2.37248898
C -2.46386719 -1.93921828 -3.32946563
C -1.15183556 -2.35069346 -3.29940200
H -0.72664887 -3.03503895 -4.03365707
C -0.32031226 -1.84929204 -2.27284884
C -1.99871075 -0.54146487 -1.41040838
C -2.42681718 0.44523734 -0.42263901
C -0.90481418 2.30458522 2.40242386
C 1.12519884 -2.31364059 -2.31236815
C 1.08401716 2.19508314 0.78116930
H 0.82932192 3.04060721 0.11421576
H 0.75431669 1.26731563 0.29814592
C 2.57283497 2.22688365 1.14387667
H 2.90129852 1.22529626 1.47013426
H 3.19725919 2.53488851 0.29199517
C 2.62189031 3.21107626 2.32373905
H 2.56910515 4.24782467 1.95189762
H 3.53049326 3.11295199 2.93587470
C 1.35329652 2.87150097 3.11652541
H 1.53974855 2.09101748 3.87601399
H 0.90481985 3.73288846 3.63521934
C 3.25736451 -2.71101642 -1.21495914
H 3.80999899 -2.10525417 -1.94964564
H 3.31731796 -3.76357937 -1.54624045
C 3.74855208 -2.53289986 0.22644217
C 2.48227882 -2.79319000 1.05695784
C 1.38273931 -2.10680699 0.23354658
H 2.53971934 -2.39206004 2.07981014

H	2.28676271	-3.87662506	1.12044775
H	4.09897614	-1.49875653	0.38273552
H	4.57598257	-3.21619058	0.46791553
H	0.39263457	-2.56042218	0.37856415
H	1.29558265	-1.03778017	0.48540643

TS



PBE/L1 theoretical level

E= -2142.308103

G= 202.0217 kcal/mol, H= 254.5708 kcal/mol, U= 253.9783 kcal/mol, S= 176.2505 cal/mol at T= 298.150 K

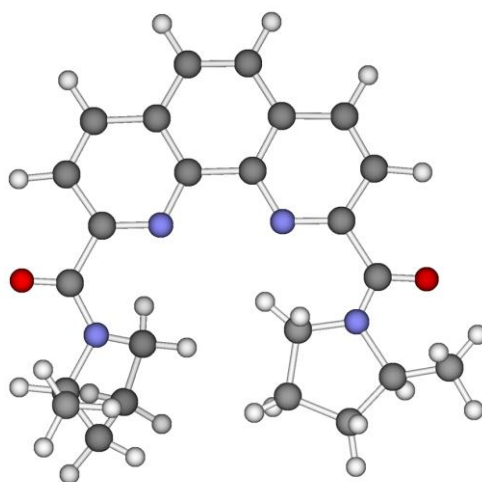
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Cl	-4.04154348	-3.10402417	-4.36550474
N	-0.78990543	0.59731156	-0.24904518
N	0.60899365	2.89512157	2.22231627
N	-0.65067792	-1.68808031	-1.68822122
N	1.67576838	-3.32358956	-1.44545138
O	1.41683960	1.12038827	1.09254956
O	0.85866147	-4.54525042	-3.18120837
C	-0.81338423	1.71194363	0.47574839
C	-1.92933977	2.58111906	0.46147841
H	-1.96933508	3.49784541	1.04045045
C	-3.01854634	2.25705242	-0.32577321

C -3.03045654 1.07755113 -1.10384631
C -4.11349678 0.66474569 -1.93644381
H -5.00317049 1.29492700 -1.98632312
C -4.04294682 -0.49445754 -2.65680861
H -4.87616634 -0.80300975 -3.29084301
C -2.88561201 -1.32922542 -2.60469747
C -2.74217486 -2.54225254 -3.33118629
C -1.58641791 -3.28289104 -3.23509526
H -1.41523075 -4.20703077 -3.78795552
C -0.55932051 -2.80849409 -2.38649654
C -1.77563703 -0.95772159 -1.78698969
C -1.84730411 0.27932891 -1.01022232
C 0.48921287 1.89880502 1.27939248
C 0.71483916 -3.63601804 -2.35923338
C -0.28571928 3.99697518 2.61990690
H -1.21136594 3.61224055 3.08588743
H -0.55762565 4.62919474 1.75922322
C 0.54331338 4.80373049 3.63617039
H 1.12942469 5.57395029 3.10862231
H -0.09679489 5.30646467 4.37633753
C 1.48323846 3.75449133 4.24321318
H 0.95046550 3.15079045 4.99664927
H 2.37123966 4.19634962 4.71862602
C 1.84245002 2.88860750 3.03502178
H 2.68494153 3.31668043 2.46108055
H 2.10851479 1.85156429 3.28454661
C 2.94032335 -4.07865095 -1.50427532
H 3.30210090 -4.12020969 -2.54293680
H 2.77741027 -5.12069321 -1.17170894
C 3.86163521 -3.31469131 -0.54834718
C 2.88770008 -2.79030800 0.51721406

C	1.65443289	-2.37926364	-0.30044422
H	3.28182888	-1.94076753	1.09365022
H	2.62814403	-3.59957242	1.22056282
H	4.33722639	-2.47140837	-1.07625401
H	4.65471172	-3.95728374	-0.13763843
H	0.71876252	-2.46916294	0.26658735
H	1.71708369	-1.33448648	-0.63888144

L3 (meso-form)

Major conformer form



PBE/L1 theoretical level

E= -1299.088466

G= 247.8562 kcal/mol, H= 301.4012 kcal/mol, U= 300.8088 kcal/mol, S= 179.5911 cal/mol at T= 298.150 K

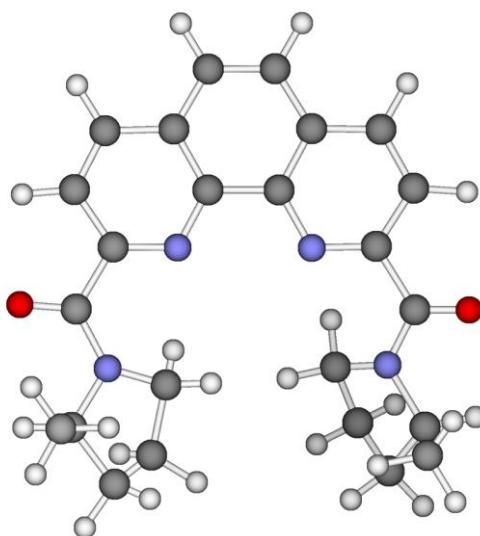
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N	0.34175634	2.66875148	1.55578172
N	-1.29380679	-1.37179327	-0.74728328
N	1.40638399	-2.53051925	-1.17062330
O	-0.72449744	4.52292013	0.75930125
O	0.31477761	-4.50516987	-0.89276832
C	-1.88787138	2.46830201	0.50204033
C	-3.13634753	3.12872362	0.41342810
H	-3.18914628	4.18056011	0.69888294
C	-4.22592402	2.41875553	-0.03917619
C	-4.06280279	1.07121682	-0.43889642

C -5.15154839 0.27924079 -0.92136228
H -6.14518690 0.73445326 -0.97238570
C -4.96004105 -1.01679277 -1.30823493
H -5.79814816 -1.61984718 -1.67025435
C -3.66246486 -1.61507320 -1.25311089
C -3.42438889 -2.95279384 -1.64796793
C -2.14933014 -3.46726584 -1.57651627
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C -1.09840894 -2.62437081 -1.13722908
C -2.54457283 -0.86210549 -0.78602815
C -2.75211382 0.51247263 -0.34791222
C -0.70898169 3.30686975 0.96224838
C 0.27471945 -3.28092980 -1.04985344
C 0.32918185 1.34232080 2.20108080
H 0.74586689 0.57378602 1.52860630
C 1.22114289 1.55118418 3.43160820
H 0.63911027 2.01733637 4.24412537
H 1.64060068 0.60460508 3.80463815
C 2.28736091 2.52242780 2.90930128
H 3.03958631 1.97182631 2.31735492
H 2.81450272 3.06677723 3.70695496
C 1.51013017 3.47946715 1.98568702
C 2.32878327 3.99778247 0.80333376
C 2.72310281 -3.20980620 -1.02787983
C 3.04471183 -4.13482475 -2.20339775
C 3.72194862 -2.04050088 -0.87868983
C 2.86312556 -0.83783644 -0.46076179
C 1.56691229 -1.06586194 -1.24347794
H 3.33026814 0.12970939 -0.70033085
H 2.65356874 -0.86655229 0.62200302
H 4.19609499 -1.83778250 -1.85460782
H 4.51972771 -2.27983475 -0.15984203
H 1.69554961 -0.74891031 -2.29666066
H 0.68297940 -0.56794554 -0.82754177
H -0.69481772 1.04001451 2.45435333

H 4.03711796 -4.59169292 -2.05636191
H 3.06066918 -3.56794357 -3.14843869
H 2.29373026 -4.93377066 -2.26961994
H 1.70988131 4.65095091 0.17286631
H 2.70556474 3.15733671 0.19811307
H 3.19088960 4.57728767 1.17198873
H 1.12452900 4.34658670 2.55430365
H 2.67876482 -3.81601882 -0.10529969
H -5.21619701 2.87995791 -0.10080498
H -4.26038456 -3.56394720 -2.00129962
PBE0/L1 theoretical level
E= -1299.169662
N -1.68689263 1.20631182 0.12307533
N 0.33680353 2.64305234 1.53576756
N -1.28655279 -1.36326110 -0.72488070
N 1.39776528 -2.50427699 -1.13380003
O -0.71838039 4.48467064 0.76527417
O 0.32132542 -4.46001387 -0.87069023
C -1.87390280 2.45383501 0.48696706
C -3.11235523 3.11113000 0.39915964
H -3.16741157 4.15409660 0.68471360
C -4.19227362 2.40599728 -0.05264061
C -4.02858829 1.06643486 -0.44339558
C -5.11245155 0.27670503 -0.92494988
H -6.09764767 0.72945273 -0.98202628
C -4.92149925 -1.00794196 -1.30211461
H -5.75090170 -1.60740733 -1.66481268
C -3.62887049 -1.60336804 -1.23782432
C -3.39190102 -2.93361902 -1.62307131
C -2.12697077 -3.44383407 -1.54385650
H -1.88904846 -4.46838856 -1.79842234
C -1.08848107 -2.60341644 -1.10251665
C -2.52539253 -0.85618585 -0.77462524
C -2.73264146 0.51326805 -0.34871557
C -0.70086241 3.28160167 0.95295179

C 0.28000182 -3.24973440 -1.01744044
C 0.30835521 1.32819283 2.17777061
H 0.70186347 0.55761939 1.50832367
C 1.20833302 1.52246392 3.39204836
H 0.64313018 1.99196041 4.20397282
H 1.61719406 0.57755160 3.75782180
C 2.27212453 2.47717619 2.86567640
H 3.00283003 1.92513907 2.26288843
H 2.81332207 3.00628543 3.65331721
C 1.49625599 3.44055963 1.96643591
C 2.30785537 3.96667361 0.79588062
C 2.70253825 -3.17984271 -1.01497316
C 3.00954366 -4.08444023 -2.19728994
C 3.69924760 -2.02157307 -0.87308657
C 2.85248351 -0.82839423 -0.44349214
C 1.55626202 -1.05227792 -1.20770359
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H 2.65535498 -0.86419731 0.63330621
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H 4.49949217 -2.26324606 -0.16989645
H 1.67439437 -0.73650163 -2.25359058
H 0.69007719 -0.54901314 -0.78539538
H -0.70886260 1.04402852 2.44486308
H 4.00194073 -4.52952385 -2.07359934
H 3.00502682 -3.50916529 -3.12854719
H 2.27102494 -4.88416672 -2.26302791
H 1.69803619 4.62906456 0.17986335
H 2.67137194 3.13664556 0.18220359
H 3.17093372 4.52879763 1.16615999
H 1.12222278 4.29396582 2.54688644
H 2.67531943 -3.78941083 -0.10424390
H -5.17350912 2.86590886 -0.12137170
H -4.21911860 -3.54241467 -1.97554350

Minor conformer form



PBE/L1 theoretical level

E= -1299.087579

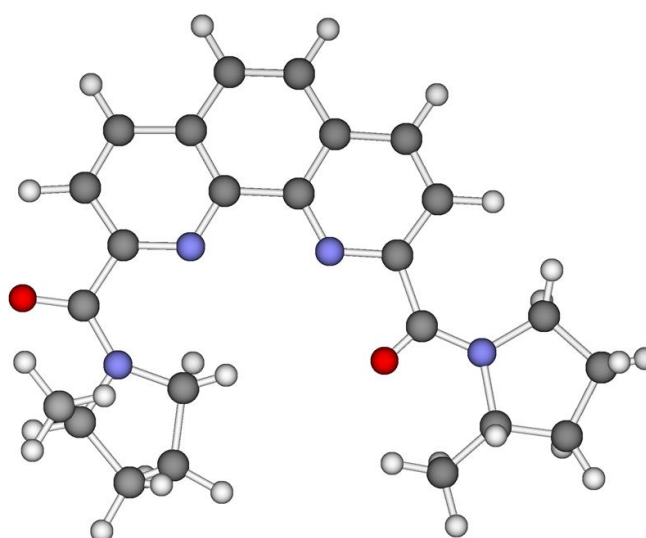
G= 247.5977 kcal/mol, H= 301.3502 kcal/mol, U= 300.7577 kcal/mol, S= 180.2865 cal/mol at T= 298.150 K

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N	1.59155428	-1.96527886	-1.74129796
O	-1.59994888	3.26888132	3.19446707
O	1.50219822	-1.58721864	-3.99076581
C	-2.19244885	1.84503496	1.38692653
C	-3.53457975	2.27167058	1.53557503
H	-3.78119946	2.88862610	2.40079451
C	-4.44966650	1.91786373	0.57108825
C	-4.03027821	1.15039730	-0.54072785
C	-4.92408276	0.79516423	-1.59826696
H	-5.96659851	1.12066293	-1.53218007
C	-4.48403978	0.08198099	-2.67589498
H	-5.16580677	-0.17200339	-3.49313045
C	-3.12400079	-0.35032752	-2.76398683
C	-2.63931513	-1.07366765	-3.87884879

C -1.32021379 -1.46526027 -3.91018891
H -0.87697023 -1.98603392 -4.76053858
C -0.50490111 -1.17853558 -2.79015446
C -2.20077920 -0.05534205 -1.71412396
C -2.66002846 0.74941856 -0.58568162
C -1.22237062 2.37122750 2.43615079
C 0.94892722 -1.60419536 -2.88988686
C 0.55886620 0.61273146 1.91498160
H 1.02664948 0.78090930 0.92927510
C 1.58702338 0.16218401 2.96026254
H 1.07652724 -0.34841135 3.79399443
H 2.33452415 -0.52656525 2.53707576
C 2.19137192 1.48978806 3.43259335
H 2.93641496 1.84549451 2.69958949
H 2.68433952 1.42385721 4.41395569
C 0.99837059 2.46357155 3.46145010
C 1.38038373 3.90626407 3.12855053
C 3.01338816 -2.38679338 -1.82605684
C 3.95443845 -1.21454072 -2.10207868
C 3.25871706 -3.08180690 -0.47329167
C 1.86945271 -3.56849098 -0.04020175
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H 1.79378283 -3.76082134 1.04086637
H 1.59987926 -4.49290466 -0.57768267
H 3.64281058 -2.34431815 0.25361916
H 3.99992633 -3.89019656 -0.55999362
H 0.94580418 -1.60541606 0.25701129
H -0.07799070 -2.72812748 -0.66485548
H -0.25949135 -0.10050450 1.76539993
H 4.99605894 -1.57287228 -2.14228392
H 3.87463713 -0.45885500 -1.30416763

H 3.70543170 -0.75083804 -3.06661916
 H 0.48806062 4.54655027 3.14282560
 H 1.85313225 3.95984650 2.13468146
 H 2.09713364 4.28196716 3.87700438
 H 0.50240099 2.44897890 4.44995403
 H 3.09822464 -3.10970378 -2.65930820
 H -5.49545050 2.23244786 0.64078981
 H -3.31853580 -1.30326247 -4.70538807

TS



PBE/L1 theoretical level

E= -1299.071038

G= 248.7280 kcal/mol, H= 300.6613 kcal/mol, U= 300.0688 kcal/mol, S= 174.1851 cal/mol at T= 298.150 K

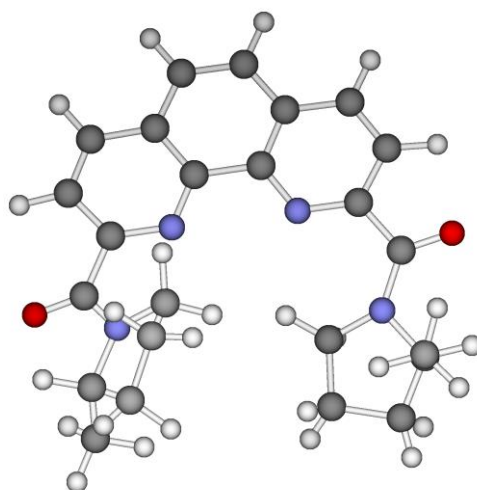
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 N 1.72109401 -2.63805580 -1.99655354
 O -1.75453269 4.14749002 3.05946326
 O 1.75459075 -0.51644397 -1.19800651
 C -2.31339097 2.40202522 1.54727304
 C -3.67959118 2.76402044 1.63700402
 H -3.96222496 3.51575279 2.37582588

C -4.57720852 2.17239022 0.77502358
C -4.11665964 1.22810125 -0.17384705
C -4.98604918 0.58727831 -1.11370277
H -6.05060720 0.84031850 -1.09623528
C -4.50334787 -0.31738314 -2.01665115
H -5.17410278 -0.80000395 -2.73394513
C -3.11386824 -0.65925688 -2.03984118
C -2.56491852 -1.59408140 -2.93984866
C -1.21654820 -1.89613163 -2.88687086
H -0.81590617 -2.62276769 -3.58906984
C -0.39647534 -1.24360323 -1.93297195
C -2.20561242 -0.05181603 -1.12119603
C -2.72267985 0.92875451 -0.17143203
C -1.35077417 3.14754701 2.45738769
C 1.12118530 -1.42416060 -1.72239208
C 0.49290386 1.38585830 2.18384600
H 0.87112039 1.36158001 1.14888299
C 1.61798489 1.20432556 3.21015525
H 1.20584297 0.83395422 4.16403913
H 2.37795281 0.49046275 2.85824227
C 2.15927410 2.62812996 3.37854409
H 2.81999302 2.88125825 2.53095317
H 2.72613263 2.77796507 4.30979919
C 0.90509176 3.51966190 3.32981777
C 1.16648316 4.90273714 2.73155093
C 3.11070323 -2.84806371 -1.49834490
C 3.21753860 -2.77571774 0.02516067
C 3.47408056 -4.23274040 -2.05462050
C 2.68277168 -4.32748461 -3.35972929
C 1.35180616 -3.64198780 -3.01131105
H 2.53373981 -5.35963440 -3.71069360

H 3.19200563 -3.76179552 -4.15713406
H 3.13763809 -5.01093006 -1.34724343
H 4.55983067 -4.34285975 -2.19329405
H 0.61660349 -4.36844110 -2.61758375
H 0.92960888 -3.16644263 -3.90788221
H -0.28333047 0.61561882 2.25659132
H 4.25704193 -2.98178077 0.32793999
H 2.56224608 -3.52931499 0.49113658
H 2.93507957 -1.77716398 0.38259408
H 0.23623993 5.48586941 2.70221353
H 1.57150662 4.80791521 1.71123672
H 1.90274239 5.44024277 3.35145283
H 0.47528741 3.64772153 4.34144068
H 3.76097274 -2.06869316 -1.93911958
H -5.64147472 2.42520881 0.80660617
H -3.21289897 -2.07955194 -3.67591500

L3 (rac-form)

Major conformer form



PBE/L1 theoretical level

E= -1299.089322

G= 247.8562 kcal/mol, H= 301.3675 kcal/mol, U= 300.7750 kcal/mol, S= 180.6215 cal/mol at T= 298.150 K

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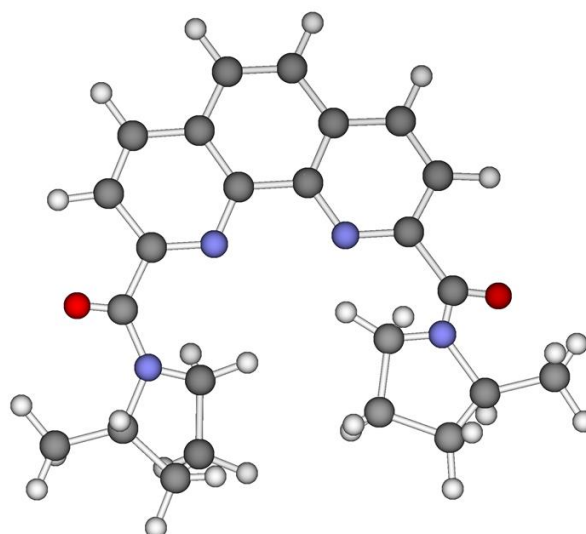
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N -1.28650415 -1.33457685 -0.88830990
N 0.99880058 -2.81767440 0.04051958
O -0.94803435 4.33189821 1.43631327
O 0.55023032 -4.22240734 -1.70061779
C -1.75267816 2.61279464 0.01357835
C -2.95572567 3.32573032 -0.20907135
H -3.00831318 4.36601067 0.11549281
C -4.00783157 2.67183542 -0.81113827
C -3.87394333 1.30763304 -1.16324103
C -4.92456341 0.56794792 -1.79114795
H -5.86730146 1.07963789 -2.00677824
C -4.75769806 -0.74795002 -2.11859965
H -5.56328249 -1.30678332 -2.60433292
C -3.53099442 -1.42714810 -1.83611631
C -3.32070851 -2.78544784 -2.17270613
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H -1.87532032 -4.40900469 -2.14646602
C -1.12587941 -2.61115932 -1.21514404
C -2.45821571 -0.73510176 -1.19770646
C -2.63072419 0.67360133 -0.86572063
C -0.64321184 3.37060595 0.72501272
C 0.20804100 -3.29246831 -0.96667230
C 1.19233489 2.00566387 -0.42843279
H 1.04983819 2.40401268 -1.45088124
C 2.68241477 1.94868338 -0.07744909
H 2.85572743 1.20749760 0.72052938
H 3.29710841 1.66558230 -0.94501287
C 2.97445917 3.36709213 0.43649733

H	3.08182502	4.05992699	-0.41474658
H	3.88781762	3.43014193	1.04730093
C	1.71777976	3.72468567	1.25122321
C	1.81479347	3.35134053	2.73488379
H	1.46649837	4.79607010	1.17662644
C	2.31789041	-3.46450543	0.26348636
C	3.32202935	-3.13964963	-0.84253883
H	2.15510058	-4.55846357	0.28069869
C	2.73690557	-2.95248795	1.65470314
C	1.41142118	-2.61654043	2.34963942
C	0.57875389	-2.01928067	1.20833933
H	1.52611327	-1.91455770	3.18941808
H	0.92998189	-3.53419447	2.72688699
H	3.34034348	-3.69653392	2.19575930
H	-0.50304139	-2.10104585	1.37060416
H	0.81076127	-0.95114940	1.05917752
H	3.34522700	-2.03777385	1.54141939
H	4.28634357	-3.62765908	-0.62590504
H	3.48719192	-2.05183339	-0.90578628
H	2.95116568	-3.50810552	-1.80892265
H	0.67469984	1.04076123	-0.36840284
H	0.84727699	3.52898192	3.22586060
H	2.57512927	3.97728562	3.22979403
H	2.09349990	2.29331946	2.86361718
PBE0/L1 theoretical level			
E= -1299.171027			
H	-5.10137606	1.28590834	2.71428299
H	-4.37017298	-3.29692602	-2.17720747
N	-1.67026913	0.65423101	1.05370021
N	0.44115311	2.51560736	1.66070497
N	-1.35402071	-1.25552630	-0.87234473
N	1.24158108	-2.05304551	-1.74309254

O -0.63160962 2.76725245 3.62749147
O 0.18990660 -2.71847987 -3.62687945
C -1.80894005 1.55843425 1.99302506
C -3.02944684 1.81414795 2.64224911
H -3.04913592 2.55068588 3.43537164
C -4.13481045 1.11186171 2.25101352
C -4.01870108 0.14445046 1.23835480
C -5.12976313 -0.62102258 0.78032941
H -6.10194921 -0.44568804 1.23169720
C -4.98079300 -1.54382145 -0.19734554
H -5.83145237 -2.12087011 -0.54701662
C -3.70766997 -1.78184485 -0.79178709
C -3.52048635 -2.72546172 -1.81588733
C -2.27379513 -2.90248346 -2.34736156
H -2.07130861 -3.59039116 -3.15863705
C -1.21035540 -2.14824700 -1.82386339
C -2.57644463 -1.05491829 -0.36118558
C -2.74051261 -0.05476298 0.67423719
C -0.61065775 2.33502793 2.48804975
C 0.13997829 -2.34096074 -2.47010899
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H -0.21661355 2.94353318 -0.30367783
C 1.92917597 2.69413543 -0.14034088
H 2.60494089 1.84636855 0.01157503
H 2.01709962 3.01522756 -1.18070579
C 2.23506832 3.80293870 0.86187094
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C 1.57534623 3.31300282 2.15113354
C 2.49830651 2.48275948 3.03205585
H 1.17780077 4.14050388 2.74656129

C 2.55855203 -2.20703197 -2.38184452
C 2.82227612 -1.14332104 -3.43304372
H 2.58642054 -3.19281387 -2.86387420
C 3.53137994 -2.15644455 -1.20275331
C 2.70445609 -2.63733673 -0.01739087
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H 2.61583328 -3.72866988 -0.03240126
H 4.42285824 -2.75997496 -1.38787174
H 0.52433103 -2.54210806 0.18658531
H 1.31015956 -0.97003949 0.07702852
H 3.85090280 -1.12053800 -1.03874171
H 3.82187462 -1.28109753 -3.85711932
H 2.76956749 -0.14587431 -2.98566484
H 2.08880305 -1.21598995 -4.23738003
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H 1.93665028 2.07370615 3.87435579
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H 2.94510627 1.65769720 2.46934319

Minor conformer form



PBE/L1 theoretical level

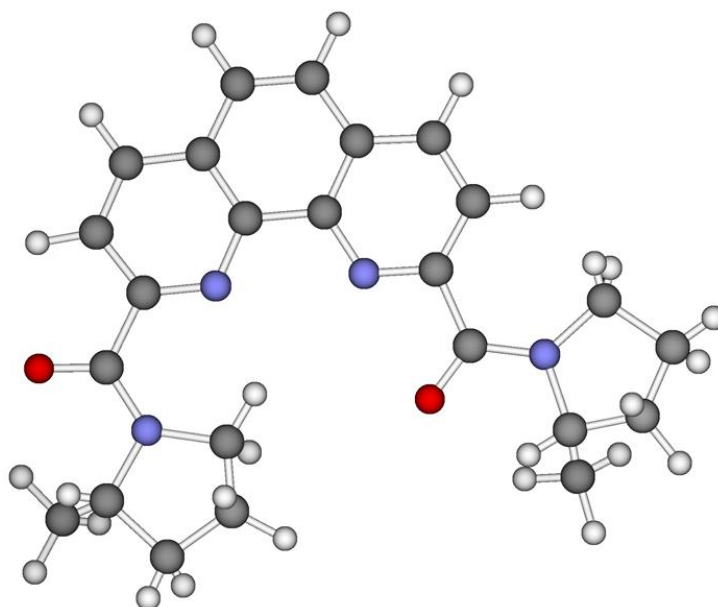
E= -1299.087480

G= 247.7569 kcal/mol, H= 301.4334 kcal/mol, U= 300.8409 kcal/mol, S= 180.0320 cal/mol at T= 298.150 K

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H	-4.69886923	-2.91718698	-2.04866815
N	-1.52963018	1.30465138	0.40752789
N	0.73390883	2.41782284	1.87364864
N	-1.43725765	-1.14430010	-0.86070716
N	1.07847488	-2.43997884	-1.79628038
O	-0.22122470	4.41969728	1.34955943
O	-0.13203956	-4.34091091	-1.49152267
C	-1.57196939	2.50979757	0.96133316
C	-2.75993705	3.27005410	1.08569753
H	-2.69327092	4.27237844	1.51138139
C	-3.94474506	2.71514630	0.65742332
C	-3.94010949	1.42779970	0.06985374
C	-5.13558674	0.79533279	-0.39444286
H	-6.08504534	1.32717001	-0.28122607
C	-5.09703684	-0.44535160	-0.96434051
H	-6.01554060	-0.92812091	-1.31130898
C	-3.85801148	-1.14035439	-1.12636423
C	-3.78092146	-2.42562962	-1.71266687
C	-2.55644488	-3.04052544	-1.84555173
H	-2.43965554	-4.04496336	-2.25425649
C	-1.39632463	-2.34454608	-1.42532468
C	-2.63709307	-0.54400700	-0.69086766
C	-2.68145990	0.76562029	-0.05245718
C	-0.29084423	3.18942142	1.41407228
C	-0.08583107	-3.10953045	-1.56751525
C	0.77267826	0.95197284	2.06394362
H	0.75297534	0.43658605	1.09253037
C	2.09542227	0.72445041	2.81003332

H 1.94410729 0.80544323 3.89854240
H 2.51446056 -0.27098721 2.59943390
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H 3.36435056 1.64183164 1.29786491
H 3.84242225 2.07851267 2.96274328
C 2.01530743 3.06790495 2.24095058
C 1.91390526 3.84691596 3.55833292
H 2.28034377 3.77297854 1.43556762
C 2.34546065 -3.21698785 -1.86887455
C 2.43838167 -4.08659172 -3.12430811
H 2.37551761 -3.87508535 -0.98198086
C 3.44207096 -2.13051820 -1.79458821
C 2.73900175 -0.89668560 -1.20885456
C 1.33823895 -0.98932767 -1.82093096
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H 2.66901469 -0.97264582 -0.11065595
H 4.30419922 -2.46617270 -1.19918931
H 0.55789471 -0.45946953 -1.26158583
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H 3.40286756 -4.62028170 -3.13665342
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H 1.62484658 -4.82470417 -3.13137531
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H 1.12481022 4.60733080 3.47660613
H 2.86968732 4.35572290 3.76429009
H 1.68480945 3.17852187 4.40349674

TS



PBE/L1 theoretical level

E= -1299.072438

G= 248.5127 kcal/mol, H= 300.7382 kcal/mol, U= 300.1457 kcal/mol, S= 175.1651 cal/mol at T= 298.150 K

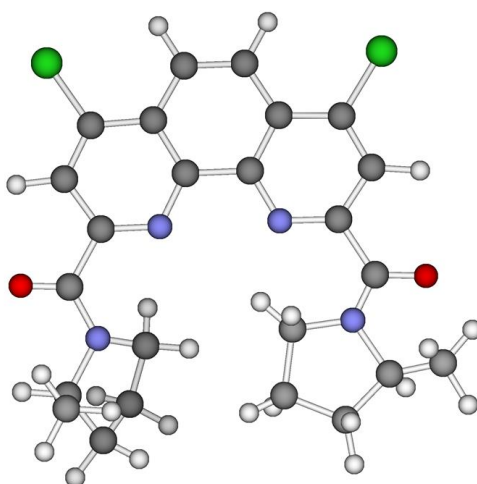
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N	0.42612353	3.09589767	2.15483689
N	-1.23474753	-1.88351119	-1.13491285
N	1.31409347	-3.03149438	-1.98126042
O	1.10392749	1.29997921	0.96801269
O	0.09056699	-4.81836271	-2.67127037
C	-1.27008045	1.53819871	1.05863452
C	-2.47363448	2.18983388	1.42783439
H	-2.47669721	3.10803747	2.00765920
C	-3.68602204	1.64599955	1.04382825
C	-3.71872640	0.45525563	0.29219100
C	-4.93285513	-0.17097387	-0.13445356
H	-5.88576603	0.29653919	0.13136014
C	-4.90510845	-1.33137894	-0.85531819

H -5.83659601 -1.80896759 -1.17449772
C -3.66396213 -1.95128906 -1.20940721
C -3.58931732 -3.15793443 -1.94548416
C -2.35799789 -3.69890904 -2.24459219
H -2.22807574 -4.63415861 -2.79093075
C -1.19018245 -3.01512122 -1.82155561
C -2.43141794 -1.35524797 -0.81572586
C -2.45476651 -0.12220485 -0.03499721
C 0.17219353 1.97468221 1.39183497
C 0.13262308 -3.68361115 -2.18123889
C -0.48006585 4.03231144 2.84165668
H -1.10138297 3.50706077 3.59028339
C 0.46151942 5.03402233 3.53164935
H 0.67230785 5.87857771 2.85656929
H 0.01828748 5.43906975 4.45362520
C 1.73469365 4.21373463 3.77420855
H 1.60838270 3.56655955 4.65810013
H 2.62641525 4.83959246 3.92918229
C 1.84825385 3.35347867 2.50661230
C 2.60751843 4.03179312 1.36060429
H 2.31892300 2.37798381 2.70680666
C 2.56560588 -3.76061559 -2.32914186
C 2.75307059 -3.92138648 -3.83933854
H 2.49203014 -4.76572180 -1.87642014
C 3.67927909 -2.92630267 -1.65880156
C 2.95662642 -2.08884740 -0.59492069
C 1.62170315 -1.77061296 -1.27004254
H 3.49973083 -1.17451429 -0.31382829
H 2.77913570 -2.68241310 0.31738466
H 4.47213268 -3.56997418 -1.24878347
H 0.81397307 -1.48483407 -0.59067738

H 1.74716413 -0.94963759 -2.00142860
H 4.13912439 -2.26010966 -2.40952420
H 3.70049691 -4.44746161 -4.04233360
H 2.79244256 -2.93529487 -4.33011961
H 1.92561150 -4.50772953 -4.26174498
H -1.14519012 4.54976702 2.13153529
H 2.55190325 3.40198755 0.46158564
H 3.66822934 4.15336657 1.63459253
H 2.19106293 5.02514601 1.12954569

L4 (meso-form)

Major conformer form



PBE/L1 theoretical level

E= -2220.895107

G= 233.1652 kcal/mol, H= 291.0904 kcal/mol, U= 290.4979 kcal/mol, S= 194.2819 cal/mol at T= 298.150 K

N -1.68222964 1.19140697 0.12522300
N 0.36680117 2.64804387 1.54559672
N -1.28667235 -1.36126566 -0.74221671
N 1.42162895 -2.50645471 -1.15295625
O -0.68017685 4.50255966 0.72132540
O 0.34081659 -4.49176216 -0.90728408
C -1.85979140 2.45458055 0.48864168
C -3.09575200 3.13286138 0.39979583

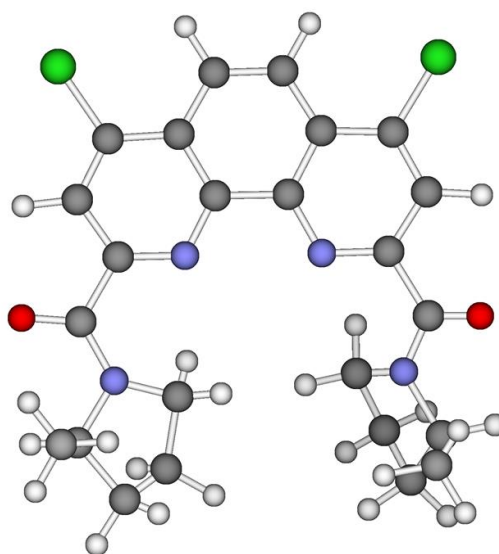
H -3.14234734 4.18658209 0.67506033
C -4.19050980 2.42900062 -0.04593609
C -4.06047964 1.07118392 -0.44292381
C -5.14549446 0.27641574 -0.91724563
H -6.13616896 0.73077363 -0.97229922
C -4.95670271 -1.02339101 -1.29381537
H -5.79489374 -1.62493312 -1.64955890
C -3.66495657 -1.62468290 -1.23926365
C -3.39779949 -2.96649885 -1.62100279
C -2.12110925 -3.47316957 -1.54994142
H -1.87900436 -4.50614977 -1.79825509
C -1.08199978 -2.61389494 -1.12216914
C -2.54209781 -0.86836112 -0.78194147
C -2.74806333 0.51065516 -0.34872717
C -0.67403048 3.29034472 0.94225085
C 0.29624921 -3.26584053 -1.04446518
C 0.33344966 1.33299220 2.21458149
H 0.74580848 0.54876965 1.55800033
C 1.21917808 1.55297816 3.44749093
H 0.63661772 2.03947544 4.24745893
H 1.62491417 0.60813475 3.83947134
C 2.30049539 2.50287104 2.91682386
H 3.05127931 1.93410778 2.34049368
H 2.82709312 3.05454803 3.70964456
C 1.54183137 3.45314169 1.97138822
C 2.37403655 3.94259524 0.78641802
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C 3.06184912 -4.08315897 -2.22503304
C 3.73719931 -2.01109934 -0.86515421
C 2.87479162 -0.81796026 -0.42796624
C 1.57663584 -1.04025340 -1.20908391

H 3.33679199 0.15468705 -0.65640646
H 2.66932583 -0.86214143 0.65504092
H 4.20921946 -1.79220152 -1.83847976
H 4.53681421 -2.25778580 -0.15098555
H 1.70086896 -0.71161753 -2.25904894
H 0.69287878 -0.54845852 -0.78617066
H -0.69579154 1.04807281 2.46693707
H 4.05743933 -4.53715658 -2.09190583
H 3.07029772 -3.49811172 -3.15900111
H 2.31537676 -4.88517570 -2.30316067
H 1.76732063 4.59166145 0.14000200
H 2.74684644 3.08830643 0.19840118
H 3.23912001 4.51959324 1.15174556
H 1.16060185 4.33341694 2.52219272
H 2.70614982 -3.80594254 -0.11911415
Cl -5.74820185 3.22545052 -0.12750359
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PBE0/L1 theoretical level
E= -2221.033897
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N 0.35832262 2.62424707 1.53430736
N -1.27857172 -1.35059536 -0.71823096
N 1.41441977 -2.48073697 -1.12165868
O -0.67891222 4.46593523 0.73646057
O 0.34489664 -4.44162941 -0.86019999
C -1.84771013 2.44129777 0.47854879
C -3.07459283 3.11490560 0.39058542
H -3.12584186 4.15951490 0.66705543
C -4.15862846 2.41618466 -0.05641447
C -4.02576637 1.06806207 -0.44797421
C -5.10570574 0.27592626 -0.92359775

H -6.08922338 0.72522348 -0.98353672
C -4.91638899 -1.01151359 -1.29336262
H -5.74673891 -1.60822594 -1.65011466
C -3.62869453 -1.60912251 -1.22946501
C -3.36284018 -2.94237781 -1.60352445
C -2.09651804 -3.44460392 -1.52348506
H -1.85809672 -4.46988440 -1.77057612
C -1.07019436 -2.58966112 -1.08906627
C -2.52224779 -0.85956877 -0.77170068
C -2.72874594 0.51336902 -0.34973374
C -0.66901487 3.26612639 0.94043136
C 0.30213934 -3.23179317 -1.00531507
C 0.31270334 1.31769872 2.19283366
H 0.70086229 0.53493142 1.53453720
C 1.20990038 1.51753533 3.40821099
H 0.64638358 2.00237298 4.21211767
H 1.60703993 0.57264364 3.78649092
C 2.28598857 2.45453644 2.87489915
H 3.01396227 1.88793874 2.28252101
H 2.82856178 2.98750234 3.65885115
C 1.52481782 3.41526151 1.96056199
C 2.34614801 3.91859436 0.78701091
C 2.72337675 -3.15148878 -1.01018441
C 3.02733207 -4.05469704 -2.19415355
C 3.71554685 -1.98888445 -0.87432861
C 2.86672068 -0.79964739 -0.43843782
C 1.56655407 -1.02761292 -1.19474411
H 3.32240963 0.16404654 -0.67853910
H 2.67671704 -0.83697850 0.63954765
H 4.16739941 -1.78127766 -1.85073733
H 4.52119255 -2.22743130 -0.17639531

H 1.67656612 -0.71091741 -2.24104190
 H 0.70171058 -0.52699769 -0.76683003
 H -0.70866185 1.04843557 2.45999503
 H 4.02265167 -4.49440145 -2.07557869
 H 3.01482630 -3.47970080 -3.12544560
 H 2.29333520 -4.85881042 -2.25625682
 H 1.74660766 4.58025312 0.16020101
 H 2.70373368 3.07754993 0.18500096
 H 3.21339607 4.47598553 1.15439212
 H 1.15633118 4.27896214 2.52900290
 H 2.70324516 -3.76037598 -0.09890726
 Cl -5.70113945 3.20508432 -0.14596324
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Minor conformer form



PBE/L1 theoretical level

E= -2220.894257

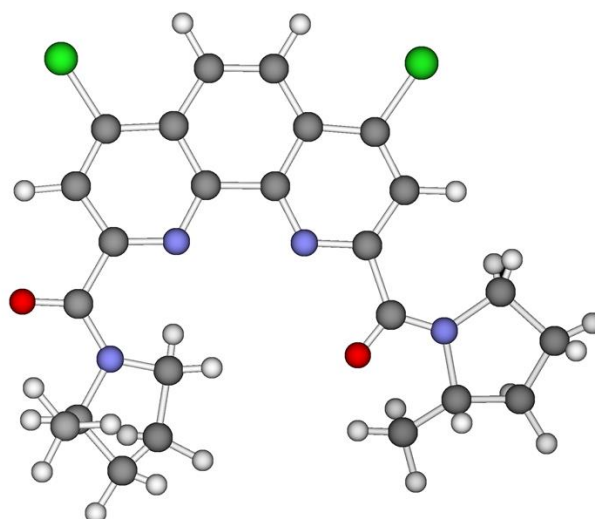
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 N 0.08126734 1.86845720 2.45949030
 N -0.91803122 -0.49026221 -1.70883787
 N 1.59674275 -1.95862830 -1.71314836

O -1.56395316 3.26438618 3.18371844
O 1.53811979 -1.51982486 -3.95470357
C -2.16666126 1.83265114 1.38573778
C -3.50241423 2.26383710 1.55429065
H -3.74213147 2.88286591 2.41887093
C -4.42445803 1.90900636 0.59917164
C -4.03270626 1.14320695 -0.53103757
C -4.92053080 0.78690863 -1.58770359
H -5.96170568 1.10680640 -1.52102017
C -4.47932529 0.07945841 -2.66909242
H -5.16126299 -0.17089754 -3.48276353
C -3.12270451 -0.34909540 -2.76422763
C -2.60480380 -1.06961513 -3.87326717
C -1.28398991 -1.45225155 -3.89902759
H -0.83655465 -1.96269143 -4.75197983
C -0.48776606 -1.16252315 -2.76921082
C -2.19841981 -0.05674856 -1.71108973
C -2.65887713 0.74604887 -0.57875055
C -1.18958402 2.36314106 2.42919755
C 0.97237927 -1.57413983 -2.86233497
C 0.58072102 0.59675020 1.90305042
H 1.03889835 0.75718421 0.91170895
C 1.61791301 0.15129536 2.94151711
H 1.11458838 -0.35277638 3.78343606
H 2.35978675 -0.54165906 2.51545477
C 2.22980332 1.48059928 3.39911366
H 2.96842527 1.83026314 2.65685296
H 2.73204470 1.41951382 4.37596750
C 1.03951120 2.45727634 3.43412161
C 1.42047405 3.89714766 3.08894205
C 3.02730083 -2.35545778 -1.77796662

C 3.95347834 -1.16239810 -2.01045680
C 3.25506878 -3.07387090 -0.43470487
C 1.86685324 -3.59974265 -0.04697176
C 0.94364429 -2.45659471 -0.48870313
H 1.76951587 -3.82013726 1.02686870
H 1.63002563 -4.51594925 -0.61298364
H 3.60490346 -2.34391117 0.31669173
H 4.01595974 -3.86379218 -0.52009243
H 0.89193130 -1.66518128 0.27644557
H -0.08197879 -2.78782392 -0.70046490
H -0.24086364 -0.11588620 1.76808667
H 5.00131607 -1.50310075 -2.03671622
H 3.84532642 -0.42550051 -1.19842172
H 3.71719122 -0.68170589 -2.96984673
H 0.53039151 4.54035568 3.10868239
H 1.88355696 3.94422269 2.09026313
H 2.14546037 4.27512503 3.82811069
H 0.55231684 2.44842958 4.42694902
H 3.14071274 -3.06055045 -2.62294245
Cl -6.08883619 2.42695642 0.77806920
Cl -3.64085865 -1.47091854 -5.22745848

TS



PBE/L1 theoretical level

E= -2220.878515

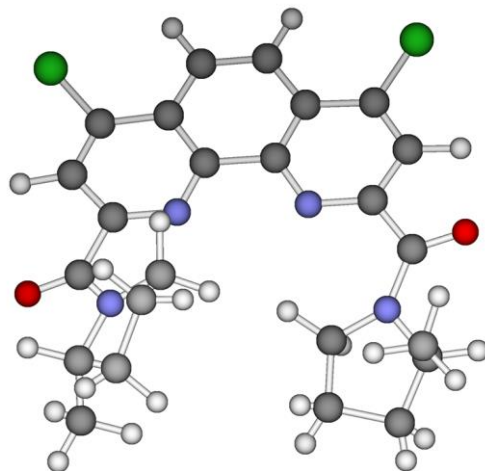
G= 234.3500 kcal/mol, H= 290.3729 kcal/mol, U= 289.7804 kcal/mol, S= 187.9019 cal/mol at T= 298.150 K

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N	-0.89647794	-0.33031118	-1.07796609
N	1.73782229	-2.60859275	-1.97596586
O	-1.72483873	4.13628435	3.05437279
O	1.75278544	-0.48464817	-1.17930853
C	-2.29295278	2.38992143	1.54686844
C	-3.65203977	2.76564026	1.65035832
H	-3.92807341	3.51976371	2.38789320
C	-4.55446148	2.17851067	0.79306692
C	-4.12229061	1.22849441	-0.17120174
C	-4.98672104	0.58980596	-1.11115205
H	-6.04850245	0.84226054	-1.09341550
C	-4.50454617	-0.31318820	-2.01644301
H	-5.17486334	-0.79177457	-2.73255849
C	-3.11966348	-0.65683889	-2.04341793
C	-2.54026723	-1.58761871	-2.93532443
C	-1.19167876	-1.88571405	-2.87760806
H	-0.79359877	-2.61027956	-3.58136392
C	-0.38794252	-1.22727644	-1.91818666
C	-2.20833206	-0.05210707	-1.12200856
C	-2.72598338	0.92833525	-0.16827513
C	-1.32486558	3.13344789	2.45596957
C	1.13171434	-1.40009689	-1.70431852
C	0.50611806	1.35962677	2.17686272
H	0.88007927	1.33492100	1.14034426
C	1.63464427	1.17320693	3.19843006
H	1.22472012	0.80550188	4.15419960

H 2.38927221 0.45520821 2.84356713
C 2.18464851 2.59410048 3.36310601
H 2.84388852 2.84223938 2.51314235
H 2.75537992 2.74123383 4.29228783
C 0.93630213 3.49386406 3.31795883
C 1.20236659 4.87254667 2.71206975
C 3.12761688 -2.81329441 -1.47348011
C 3.23260593 -2.72919917 0.04943538
C 3.49219966 -4.20203161 -2.01849461
C 2.70361400 -4.30793905 -3.32432342
C 1.37142897 -3.62015462 -2.98538017
H 2.55499744 -5.34300423 -3.66630530
H 3.21425772 -3.74945545 -4.12576628
H 3.15533400 -4.97460032 -1.30530977
H 4.57816792 -4.31233978 -2.15478754
H 0.63478607 -4.34295273 -2.58842254
H 0.95403779 -3.15088558 -3.88762498
H -0.27322772 0.59284914 2.25357318
H 4.27153683 -2.93496585 0.35402918
H 2.57611036 -3.47851992 0.52047694
H 2.95196700 -1.72781670 0.40023100
H 0.27631843 5.46242714 2.68555641
H 1.60133576 4.77117348 1.69004548
H 1.94547570 5.40754938 3.32573509
H 0.51244336 3.62797141 4.33117819
H 3.77709103 -2.03696680 -1.92051935
Cl -6.24862862 2.61841822 0.89357179
Cl -3.52999902 -2.39177036 -4.13945341

L4 (rac-form)

Major conformer form



PBE/L1 theoretical level

E= -2220.896082

G= 233.0034 kcal/mol, H= 291.1060 kcal/mol, U= 290.5136 kcal/mol, S= 194.8772 cal/mol at T= 298.150 K

Cl -5.45170927 3.56670976 -1.11302674

Cl -4.53442144 -3.73248506 -2.95739841

N -1.58054936 1.32147682 -0.30457449

N 0.68018275 2.92892408 0.55662441

N -1.28157794 -1.32147396 -0.87586540

N 0.99699110 -2.80276632 0.08071533

O -0.90486568 4.31713676 1.42781866

O 0.56525958 -4.21083403 -1.66365933

C -1.72142029 2.60071635 0.00862123

C -2.91415167 3.32936859 -0.20293280

H -2.96268010 4.36718750 0.12655167

C -3.97020626 2.68436813 -0.80444098

C -3.86654592 1.31533122 -1.17008376

C -4.91205454 0.57678026 -1.79862273

H -5.85104465 1.08844972 -2.01647496

C -4.74712896 -0.73956603 -2.12662911

H -5.55123329 -1.29361761 -2.61383438

C -3.52806163 -1.42332590 -1.84258127
C -3.29165936 -2.78675914 -2.16442990
C -2.08570290 -3.37581086 -1.86197448
H -1.84735262 -4.40645361 -2.12506557
C -1.11352885 -2.59755683 -1.19464409
C -2.45293283 -0.73332000 -1.20030785
C -2.62202477 0.67898721 -0.87110782
C -0.60513008 3.35459042 0.71729457
C 0.21959510 -3.27997327 -0.93364310
C 1.21417189 1.98180377 -0.44954205
H 1.05458772 2.38132906 -1.46865439
C 2.70949793 1.92915845 -0.12012754
H 2.89790654 1.18329751 0.66989315
H 3.31182861 1.65442121 -0.99884701
C 3.00485587 3.34531426 0.39801905
H 3.09906435 4.04331875 -0.45042232
H 3.92618346 3.40703344 0.99664760
C 1.75873065 3.69536185 1.23128068
C 1.87329805 3.31254387 2.71104932
H 1.50329387 4.76624775 1.16635692
C 2.31858444 -3.44214702 0.31589049
H 2.15993547 -4.53648996 0.34150693
C 2.72612953 -2.91681242 1.70506954
C 1.39445770 -2.58841419 2.39163351
C 0.56147462 -2.00455832 1.24362195
H 1.49914420 -1.88043666 3.22751760
H 0.91925204 -3.50777078 2.77224278
H 3.33363104 -3.65139937 2.25417566
H -0.52001768 -2.10041666 1.40150881
H 0.78082001 -0.93436551 1.09173167
H 3.32673717 -1.99751770 1.58809435

H 0.70252424 1.01414728 -0.38378796
C 3.32718349 -3.12100530 -0.78668237
H 4.29273033 -3.60114145 -0.55869418
H 3.48631883 -2.03293967 -0.85897452
H 2.96668077 -3.50135565 -1.75233042
H 2.14880729 2.25260997 2.83006477
H 0.91334713 3.49168158 3.21630740
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PBE0/L1 theoretical level

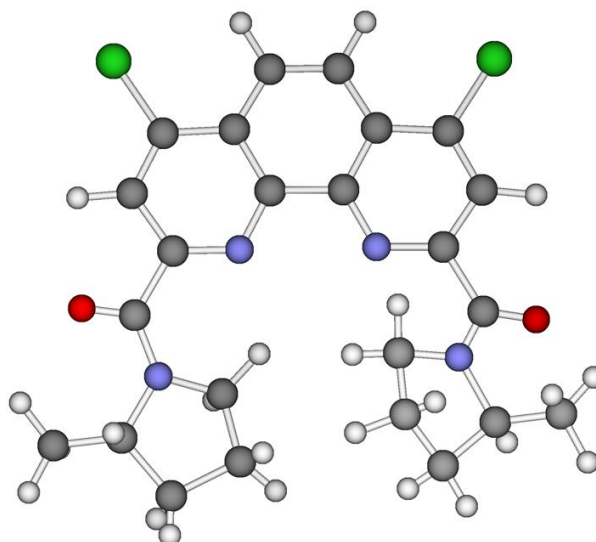
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N 0.46316168 2.50281620 1.64189887
N -1.34632182 -1.24336028 -0.86268091
N 1.25822496 -2.03391933 -1.72391570
O -0.59763700 2.74630952 3.61756396
O 0.21440171 -2.68725348 -3.61781073
C -1.78412783 1.54687285 1.98419225
C -2.99269700 1.81009316 2.64751506
H -3.00826883 2.54090858 3.44473720
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C -4.01658535 0.14182436 1.24299037
C -5.12345266 -0.62071401 0.78111416
H -6.09359312 -0.44960421 1.23107171
C -4.97588491 -1.53903663 -0.20162863
H -5.82712793 -2.11031508 -0.55074316
C -3.70791292 -1.77773809 -0.79817194
C -3.49115491 -2.71353841 -1.83064580
C -2.24299002 -2.88466692 -2.35655713
H -2.04045868 -3.56610990 -3.17196822

C -1.19170690 -2.12926483 -1.81679571
C -2.57409835 -1.05368948 -0.36383435
C -2.73737049 -0.05500160 0.67582166
C -0.58110124 2.32098579 2.47612929
C 0.16284987 -2.31793380 -2.45915413
C 0.51265448 2.28799725 0.18995708
H -0.21109080 2.94156790 -0.31417331
C 1.93598330 2.69054151 -0.17090154
H 2.61258030 1.84156191 -0.03019827
H 2.01470327 3.01790071 -1.20992529
C 2.25122428 3.79322672 0.83511734
H 1.78182685 4.73033524 0.51843202
H 3.32176375 3.97253132 0.96025425
C 1.60342956 3.29600573 2.12748170
C 2.53256941 2.45848060 2.99457884
H 1.21172857 4.12001133 2.73142028
C 2.57990646 -2.17982602 -2.35680938
C 2.84532905 -1.10892379 -3.39996767
H 2.61281109 -3.16269517 -2.84423137
C 3.54526305 -2.13419747 -1.17158651
C 2.71350145 -2.62781334 0.00510168
C 1.35334873 -1.99581110 -0.26335883
H 3.11910534 -2.33426189 0.97609866
H 2.62896156 -3.71921921 -0.01913430
H 4.43992710 -2.73301458 -1.35606885
H 0.53235304 -2.54321718 0.19794530
H 1.31262612 -0.96646911 0.10587833
H 3.86000991 -1.09843314 -0.99789453
H 3.84657812 -1.24278569 -3.82116079
H 2.78976727 -0.11431795 -2.94670248
H 2.11570239 -1.17743301 -4.20815182

H 0.26870465 1.25872612 -0.06418513
H 1.97860873 2.04429698 3.83948350
H 3.34112740 3.08308506 3.38656926
H 2.97388482 1.63694835 2.42250323

Minor conformer form



E= -2220.894088

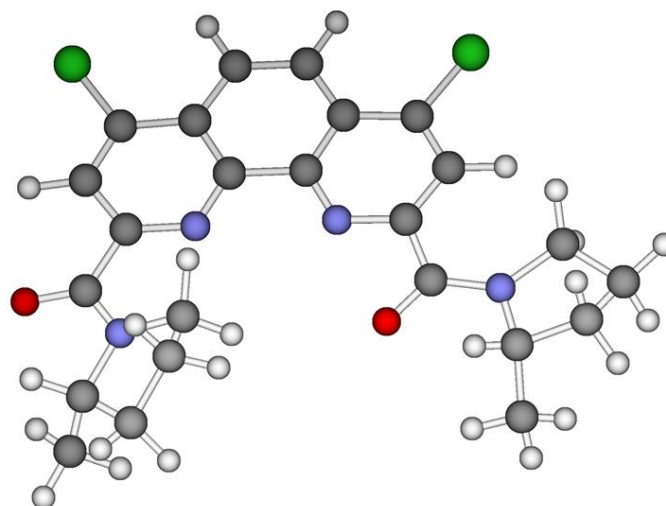
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Cl -5.18540668 -3.27782488 -2.24985647
N -1.51676524 1.29036009 0.39953786
N 0.75557607 2.39699435 1.86616766
N -1.42682183 -1.13336730 -0.85242194
N 1.09755623 -2.42172050 -1.78426301
O -0.18413778 4.40142107 1.31934750
O -0.10481817 -4.32725096 -1.46890891
C -1.54618192 2.49631667 0.94908994
C -2.72037482 3.27299500 1.07484436
H -2.64877892 4.27751732 1.49157560
C -3.90848613 2.72488213 0.65114599
C -3.93652892 1.43141448 0.06417760
C -5.12720966 0.79592359 -0.39577258

H -6.07441425 1.32660127 -0.28598449
C -5.09018183 -0.44858593 -0.95817673
H -6.00788784 -0.93035990 -1.29959285
C -3.85728955 -1.14624822 -1.11962414
C -3.75021863 -2.43907261 -1.69805026
C -2.52350783 -3.04728937 -1.82797611
H -2.40458775 -4.05401850 -2.22741485
C -1.37547719 -2.33465171 -1.41074479
C -2.63277221 -0.54760051 -0.68919492
C -2.67603040 0.76650321 -0.05423302
C -0.25982466 3.17298794 1.39777839
C -0.06100222 -3.09680986 -1.55109680
C 0.77773559 0.93310577 2.07625890
H 0.75487596 0.40555227 1.11145687
C 2.09638286 0.70108783 2.82822084
H 1.94285619 0.79528213 3.91524482
H 2.50577545 -0.30074975 2.62976670
C 2.99721885 1.83528340 2.31475282
H 3.38005638 1.58897567 1.31026399
H 3.85598636 2.03904819 2.97199750
C 2.04233336 3.03894091 2.23242307
C 1.94246900 3.83260870 3.54090476
H 2.31740642 3.73214841 1.42025721
C 2.36927247 -3.19252276 -1.85862684
C 2.46126103 -4.06859207 -3.10937166
H 2.40699792 -3.84442711 -0.96766031
C 3.45953679 -2.09907913 -1.79654884
C 2.75245762 -0.86531949 -1.21586072
C 1.34929001 -0.96953464 -1.82040596
H 3.25078487 0.08022261 -1.47855020
H 2.68804741 -0.93371528 -0.11683956

H 4.32613277 -2.42580056 -1.20284271
H 0.56987792 -0.43828905 -1.26134217
H 1.35446739 -0.60902590 -2.86714745
H 3.81406665 -1.87839401 -2.81816077
H 3.43069887 -4.59302187 -3.12392378
H 2.38794661 -3.45154047 -4.01961470
H 1.65527630 -4.81492424 -3.10870457
H -0.10098964 0.60349554 2.65117145
H 1.16207242 4.60071135 3.44859219
H 2.90261054 4.33353233 3.74534273
H 1.70309126 3.17575073 4.39199162

TS



PBE/L1 theoretical level

E= -2220.880462

G= 234.6186 kcal/mol, H= 290.4846 kcal/mol, U= 289.8921 kcal/mol, S= 187.3754 cal/mol at T= 298.150 K

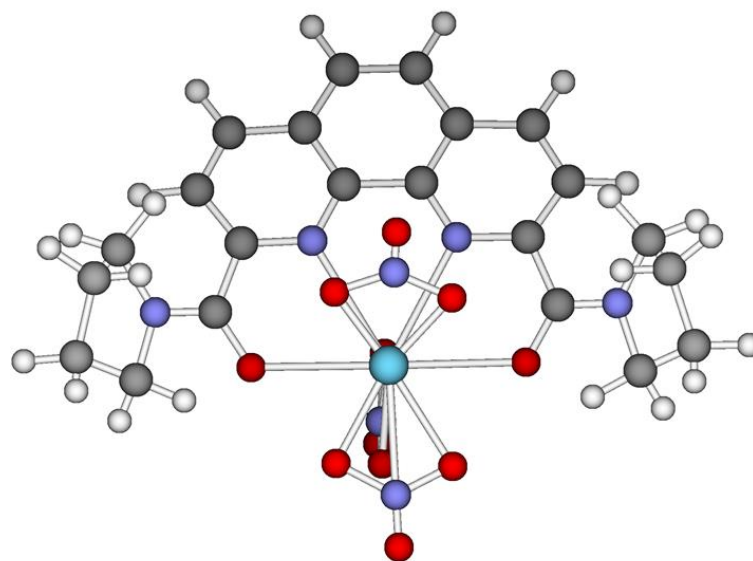
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N 0.49775940 3.10674095 1.97679257
N -1.22646952 -1.88627470 -1.19424844
N 1.28617561 -3.05650520 -1.83911824

O 1.14468193 1.31529737 0.76440358
O 0.13595940 -4.43139982 -3.25617456
C -1.22389936 1.53635097 0.94150865
C -2.41082788 2.19236064 1.34455776
H -2.40995789 3.12109208 1.90513933
C -3.63024831 1.63140452 1.01323402
C -3.70349503 0.42425457 0.28268403
C -4.91706705 -0.22879855 -0.08790895
H -5.86505508 0.22576065 0.20516859
C -4.89724588 -1.40050471 -0.79099667
H -5.83006573 -1.89566875 -1.06698930
C -3.66590667 -2.00632405 -1.18568313
C -3.57238197 -3.21983171 -1.91904306
C -2.34429884 -3.72955418 -2.27468681
H -2.22047782 -4.64040565 -2.86113071
C -1.18826985 -3.01776910 -1.88034797
C -2.42525959 -1.38507652 -0.84737766
C -2.44018769 -0.13918696 -0.08101075
C 0.22677712 1.98637784 1.22273922
C 0.14124691 -3.57525134 -2.36686802
C -0.39276156 4.03450441 2.69694304
H -0.98782462 3.50062394 3.46027684
C 0.56382322 5.03808117 3.36340594
H 0.74367279 5.89052343 2.68948126
H 0.14854771 5.43063927 4.30342770
C 1.85188675 4.22773409 3.55559707
H 1.76270306 3.57367086 4.43886757
H 2.74253583 4.86104965 3.68350744
C 1.92962468 3.37690449 2.27913332
C 2.63951111 4.06970882 1.11064231
H 2.41621709 2.40486240 2.45638990

C 2.58691478 -3.51952672 -2.39193773
C 2.80032229 -3.08217764 -3.84161615
H 2.59615064 -4.62529945 -2.35072517
C 3.61900496 -2.92895341 -1.41464806
C 2.85267019 -2.78559399 -0.09527064
C 1.46093869 -2.33453941 -0.55538392
H 3.30603266 -2.05672121 0.59277815
H 2.78657818 -3.75915504 0.41911221
H 4.51364946 -3.56512117 -1.33861935
H 0.66926008 -2.60593843 0.15288088
H 1.40649867 -1.24322510 -0.69520319
H 3.93502498 -1.93451607 -1.77511752
H 3.78611279 -3.43055987 -4.19066381
H 2.77086544 -1.98341572 -3.91840553
H 2.02445650 -3.51407576 -4.48803234
H -1.08086920 4.55334473 2.01008201
H 2.55846763 3.44583201 0.20938830
H 3.70803094 4.20038748 1.34714055
H 2.20517254 5.06031084 0.90157181

Complexes

L1*La(NO₃)₃



PBE/L1 theoretical level

E= -10556.886345

G= 230.8106 kcal/mol, H= 304.9870 kcal/mol, U= 304.3945 kcal/mol, S= 248.7887 cal/mol at T= 298.150 K

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H -3.50268483 -2.97827387 -3.28968263
N -1.47856951 1.08658290 0.30045471
N -0.09366491 3.89596319 1.94958937
N -1.07944095 -1.37790608 -0.70982087
N 1.19820797 -4.01222277 -1.26134396
O -0.12904730 1.71322906 2.53076386
O 0.53269392 -3.03243709 0.66759455
C -1.62093258 2.31493306 0.79196364
C -2.71388578 3.13975191 0.45021725
H -2.82580471 4.12592649 0.90344417
C -3.65971041 2.66287255 -0.44035134
C -3.50651670 1.37853110 -1.00618947
C -4.42143106 0.80737954 -1.94949973
H -5.29259348 1.39412987 -2.25376987
C -4.21711206 -0.44282344 -2.46414804
H -4.92285490 -0.86542672 -3.18464994
C -3.08114195 -1.22636688 -2.07821369
C -2.81223440 -2.51993394 -2.57629704
C -1.68336511 -3.19966817 -2.15315914
H -1.46688008 -4.20463085 -2.51974487
C -0.83188897 -2.58589005 -1.21068501
C -2.15833735 -0.69797117 -1.13352609
C -2.37382770 0.62610191 -0.58916259
C -0.56019324 2.64100885 1.81921852
C 0.36009955 -3.24029756 -0.54925495
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H -1.03639483 5.69682217 1.30262291
C 1.13614762 5.70734262 1.08515859

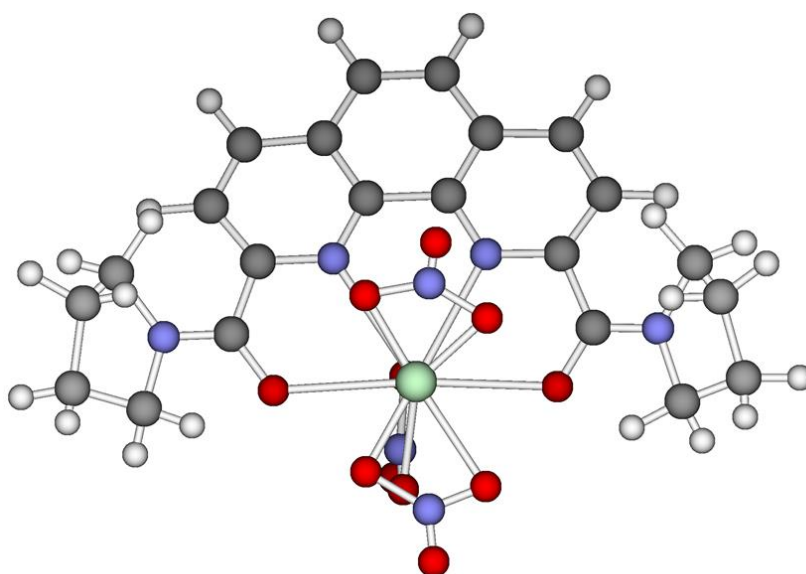
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H 2.56166410 5.68503189 2.77602172
C 1.02790463 4.12573433 2.89630842
H 1.80914855 3.36962700 2.70648909
H 0.68314916 3.99076056 3.93308640
C 2.42460465 -4.51393747 -0.58797944
H 2.16551018 -5.30457926 0.13315034
H 2.87730002 -3.68224955 -0.02132681
C 3.30622387 -4.99460316 -1.74775875
C 2.85963655 -4.11032343 -2.92267060
C 1.33916855 -4.04470015 -2.73119307
H 3.13644481 -4.51389790 -3.90781784
H 3.27982426 -3.09639168 -2.81910706
H 3.10917091 -6.05643559 -1.97225523
H 4.37489796 -4.88683462 -1.51177883
H 0.88793933 -3.15030503 -3.18356919
La 0.55687028 -0.54815400 1.45456898
N -1.43108499 -1.54435408 3.44929218
O -0.17494348 -1.44090831 3.73142600
O -1.76759434 -1.19087648 2.23628426
O -2.25597286 -1.94175220 4.25006580
N 3.20336342 -0.73231447 2.81889963
O 2.48524618 0.35161147 2.83371592
O 2.68211341 -1.73351550 2.17585111
O 4.28763008 -0.80197847 3.36563444
N 1.96410143 0.57403320 -0.99773806
O 2.46891284 1.02194226 -2.01469922
O 1.88594496 -0.70144236 -0.77274525

O 1.46768785 1.34006739 -0.07905519
H 0.85301238 -4.94699287 -3.14674330
H -0.44639614 4.63105822 -0.01830472
PBE0/L1 theoretical level
E= -10556.761402
H -4.50731087 3.24989724 -0.71083337
H -3.46190643 -2.96149230 -3.26079583
N -1.49956954 1.07727027 0.31923148
N -0.09229148 3.83641148 1.93340480
N -1.09010231 -1.36547375 -0.68106097
N 1.21024525 -3.93163037 -1.24399614
O -0.21535704 1.69166577 2.56332183
O 0.55529588 -2.96132946 0.66465604
C -1.64252484 2.29117393 0.80508751
C -2.71902990 3.11632156 0.45641845
H -2.82584333 4.09745884 0.90250069
C -3.65081859 2.64312983 -0.43479204
C -3.49663115 1.36511767 -0.99091095
C -4.40049171 0.79514480 -1.93808150
H -5.26277256 1.37692714 -2.24761081
C -4.19226789 -0.44249591 -2.44596910
H -4.88585377 -0.86316788 -3.16693020
C -3.06179333 -1.22070265 -2.05176044
C -2.78521442 -2.50330353 -2.54657388
C -1.66256452 -3.17098475 -2.12198830
H -1.43708050 -4.16560698 -2.48663068
C -0.82988882 -2.55448532 -1.17977166
C -2.15975475 -0.69622570 -1.10800612
C -2.38068986 0.61958092 -0.56865048
C -0.59385872 2.61027288 1.83529818
C 0.37441909 -3.18278193 -0.53341162
C -0.17239182 4.90413761 0.93413758

H -0.94197661 5.63521290 1.21240187
C 1.21388113 5.53346205 1.00351810
H 1.91180277 4.93030405 0.41444400
H 1.22051430 6.55708981 0.62297094
C 1.55098188 5.43017340 2.48840737
H 1.02677858 6.21065044 3.05007291
H 2.61969018 5.52189827 2.69179726
C 1.02537131 4.05174208 2.86911201
H 1.76756084 3.26121521 2.71588421
H 0.67385042 3.98132396 3.90110469
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H 2.20105267 -5.16886091 0.15863106
H 2.90516162 -3.56422877 -0.06321718
C 3.29004526 -4.91835022 -1.74290156
C 2.83250356 -4.05864954 -2.91799951
C 1.32578015 -3.97942424 -2.70324349
H 3.08762407 -4.47831392 -3.89342380
H 3.25945973 -3.05385685 -2.83977580
H 3.07543540 -5.97394228 -1.94060969
H 4.35650587 -4.82019424 -1.53086472
H 0.88004726 -3.09285998 -3.15735531
La 0.51794839 -0.52735049 1.49316382
N -1.46797037 -1.62853479 3.39965630
O -0.23757119 -1.54166281 3.69028330
O -1.79207051 -1.21201479 2.23455119
O -2.28205204 -2.07035065 4.15954685
N 3.15771198 -0.63921475 2.83673811
O 2.39055824 0.37294418 2.92704058
O 2.70854998 -1.60426569 2.13840318
O 4.23076868 -0.67858309 3.36831355
N 1.89353228 0.67819297 -0.91496646

O 2.38161325 1.15921569 -1.90269518
 O 1.78606176 -0.57798684 -0.76071090
 O 1.44751811 1.39544082 0.03334945
 H 0.83208835 -4.87567711 -3.09968829
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L1*Nd(NO₃)₃



PBE/L1 theoretical level

E= -11688.280784

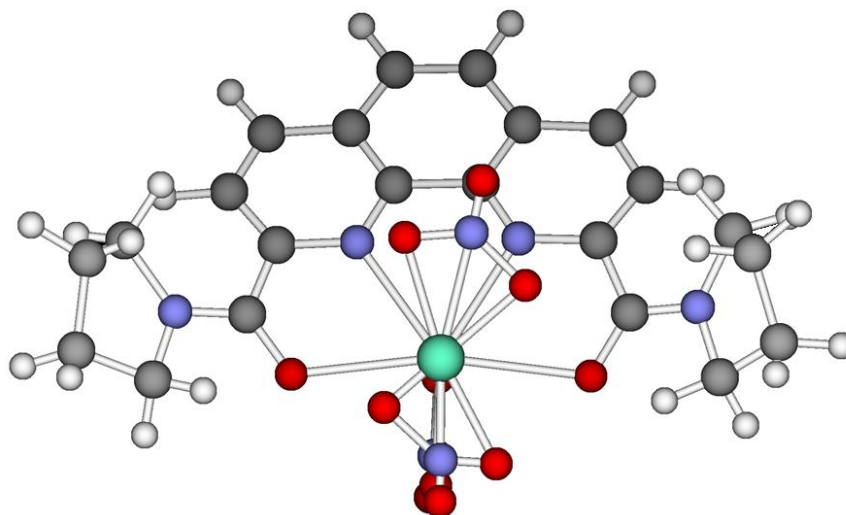
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 H -3.46296883 -2.93699884 -3.34870839
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 N -0.10647288 3.91030550 2.01392865
 N -1.04427326 -1.36418104 -0.74703217
 N 1.16663122 -4.08239746 -1.19836283
 O 0.05246217 1.69004607 2.37779999
 O 0.49634355 -3.00909114 0.67906213
 C -1.56385636 2.32015705 0.76759195
 C -2.66697574 3.14053321 0.44793436
 H -2.78803015 4.11638689 0.91924137

C -3.61468983 2.67595863 -0.44755721
C -3.45721149 1.40307546 -1.03610456
C -4.36885262 0.84503686 -1.99011254
H -5.23730469 1.43748403 -2.29116511
C -4.16436481 -0.39945155 -2.51858592
H -4.86742449 -0.81317192 -3.24686790
C -3.03451371 -1.19142950 -2.13218522
C -2.77480030 -2.48654723 -2.62831783
C -1.66146302 -3.18242049 -2.18867135
H -1.47616637 -4.19536781 -2.54728699
C -0.81411022 -2.58324027 -1.23509240
C -2.11322832 -0.67252910 -1.18062377
C -2.32422137 0.64625371 -0.62835336
C -0.48253894 2.63810515 1.77254200
C 0.34252694 -3.25559855 -0.53276688
C -0.35441166 5.10574055 1.18384719
H -1.21759021 5.67793846 1.57255447
C 0.93968254 5.91413212 1.34807158
H 1.70540547 5.52510071 0.65698969
H 0.78690183 6.98346043 1.14005637
C 1.33738959 5.62038469 2.80270100
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H 1.85894859 3.47796297 2.66636515
H 0.71729445 3.84052992 3.97806859
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H 2.05267978 -5.34680319 0.27341518
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H 3.32097793 -3.32704949 -2.74910045
H 2.99296618 -6.23579502 -1.78098154
H 4.30505371 -5.10807562 -1.34555352
H 0.93904483 -3.27889824 -3.15642571
Nd 0.59163088 -0.51438659 1.26162875
N -1.22815120 -1.37509978 3.36670852
O 0.04768837 -1.26018405 3.54520321
O -1.64762032 -1.06987047 2.17181563
O -1.98594320 -1.73954666 4.24467659
N 3.26579833 -0.70425910 2.40704799
O 2.61615038 0.41821823 2.30857372
O 2.62426591 -1.74253583 1.97387254
O 4.38883162 -0.76971948 2.86816740
N 1.93616426 0.45895538 -1.19546294
O 2.47861719 0.83873916 -2.21935463
O 1.92613173 -0.79302788 -0.84377909
O 1.32887053 1.26369250 -0.38947767
H 0.81279373 -5.06918955 -3.05592966
H -0.55238175 4.82093000 0.14054143

L1*Eu(NO₃)₃



PBE/L1 theoretical level

E= -12909.277954

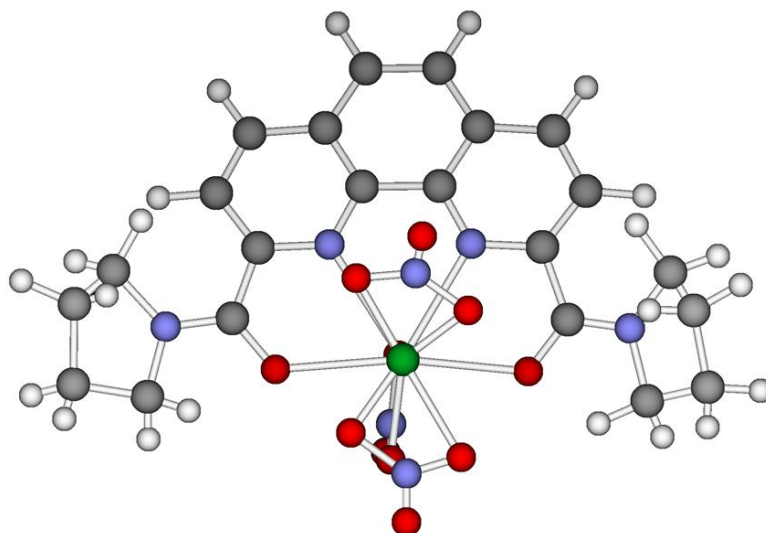
G= 232.5764 kcal/mol, H= 304.7929 kcal/mol, U= 304.2004 kcal/mol, S= 242.2152 cal/mol at T= 298.150 K

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H	-3.47777200	-2.93646646	-3.32435012
N	-1.43908632	1.10169768	0.28113699
N	-0.09651148	3.87951303	2.05691862
N	-1.04306889	-1.34770739	-0.74998987
N	1.14012742	-4.09135866	-1.15178239
O	0.00474465	1.65450573	2.42379069
O	0.45450643	-3.00597119	0.72052002
C	-1.57537961	2.32275724	0.79217076
C	-2.66493487	3.15514207	0.45539644
H	-2.78638363	4.13066244	0.92747664
C	-3.60137677	2.69935250	-0.45642841
C	-3.44572496	1.42707205	-1.04806089
C	-4.35266447	0.87243551	-2.00892830
H	-5.21439075	1.46940374	-2.32000923
C	-4.15618086	-0.37824497	-2.52655125
H	-4.86018515	-0.79058945	-3.25470877
C	-3.03545403	-1.17832196	-2.12908316
C	-2.78728628	-2.48377657	-2.60739779
C	-1.68441975	-3.18630314	-2.15259719
H	-1.49161768	-4.20509481	-2.49367356
C	-0.82680196	-2.57773733	-1.21232629
C	-2.11075902	-0.65626663	-1.18405664
C	-2.32205319	0.66253537	-0.63045710
C	-0.50147909	2.61691833	1.81507170
C	0.31842276	-3.25502968	-0.49092472
C	-0.32318369	5.08302116	1.23179710
H	-1.17905378	5.66545773	1.62102389

C 0.98265141 5.87068892 1.40443599
H 1.74423826 5.47596550 0.71204609
H 0.84606218 6.94355392 1.20380008
C 1.37364972 5.56131411 2.85769820
H 0.76911783 6.16803026 3.55247116
H 2.43543386 5.75470686 3.06763482
C 1.03089523 4.07467985 3.00404787
H 1.86190414 3.41274118 2.70464277
H 0.72535068 3.78362036 4.02072620
C 2.33286715 -4.60076857 -0.42656657
H 2.03907943 -5.38820791 0.28486159
H 2.76637888 -3.76819158 0.15326577
C 3.26154923 -5.09045839 -1.54572880
C 2.87176800 -4.20515823 -2.73983335
C 1.34482014 -4.13359213 -2.61431026
H 3.19026375 -4.61072016 -3.71152997
H 3.28748059 -3.19185615 -2.61602426
H 3.06846285 -6.15170765 -1.77656448
H 4.31932974 -4.98734331 -1.26308525
H 0.91987622 -3.23890662 -3.09081101
Eu 0.53357255 -0.48613361 1.22236919
N -1.28251946 -1.44405508 3.28205419
O -0.00619730 -1.34024012 3.45067334
O -1.71440721 -1.11681283 2.10575938
O -2.02984881 -1.82220221 4.16698837
N 3.27523971 -0.45313212 2.19890356
O 2.65627742 0.61963916 1.81135619
O 2.58467698 -1.53761828 2.13545275
O 4.42875528 -0.42766666 2.59214926
N 1.91109276 0.15764186 -1.31937385
O 2.48145866 0.44676176 -2.36070538

O 2.01010513 -1.01043797 -0.77776301
O 1.15511322 1.00084960 -0.69458401
H 0.87114209 -5.03514814 -3.04580545
H -0.52217209 4.80689049 0.18630683

L1*Lu(NO₃)₃



PBE/L1 theoretical level

E= -16631.682739

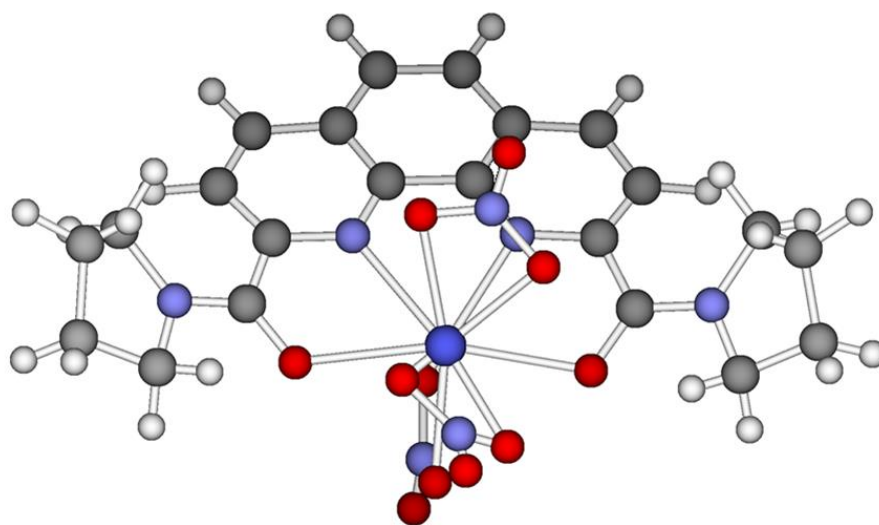
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H -4.46818399 3.32488418 -0.76679200
H -3.42177510 -2.92817831 -3.39439750
N -1.40889060 1.13183939 0.17493676
N -0.11702256 3.86151862 2.07804322
N -1.00112820 -1.29095471 -0.83221257
N 1.13799679 -4.10696745 -1.09413922
O 0.12378850 1.62765980 2.20838356
O 0.51210564 -2.82285810 0.66071099
C -1.55220699 2.34188509 0.70574301
C -2.65815639 3.16378379 0.39345291
H -2.79318976 4.12876177 0.88238508
C -3.59642959 2.71270299 -0.52052903
C -3.43218350 1.45019448 -1.13091683
C -4.33388996 0.88665509 -2.09229875

H -5.20400620 1.47254920 -2.40124774
C -4.12383842 -0.36170545 -2.61246872
H -4.82534122 -0.78006762 -3.33959484
C -2.99561810 -1.15336108 -2.21674466
C -2.73662400 -2.46060681 -2.68194461
C -1.63026989 -3.15028620 -2.21385002
H -1.43583417 -4.17328024 -2.53979993
C -0.77836657 -2.52606320 -1.27898097
C -2.07445526 -0.61818606 -1.27653873
C -2.29811716 0.69730443 -0.72609574
C -0.45946312 2.61092782 1.71342051
C 0.35337260 -3.17891598 -0.52284694
C -0.43980837 5.13370371 1.40397334
H -1.32631075 5.60619879 1.86700821
C 0.81275326 5.98552942 1.65403903
H 1.58299720 5.73488283 0.90646428
H 0.59702420 7.06224775 1.58992815
C 1.25975418 5.52988291 3.05159092
H 0.63377547 6.00476503 3.82542562
H 2.31105018 5.76987886 3.26583719
C 1.02022874 4.01666498 3.02068639
H 1.88379014 3.45113277 2.62993598
H 0.76068205 3.58355379 3.99870682
C 2.30061221 -4.60632324 -0.31321049
H 1.95612323 -5.26600885 0.49801645
H 2.80470705 -3.74127126 0.15171392
C 3.16573834 -5.31522179 -1.36308527
C 2.82780671 -4.56917381 -2.66361189
C 1.31456220 -4.34727097 -2.53974986
H 3.09092951 -5.12860775 -3.57349348
H 3.33538055 -3.59103417 -2.68506265
H 2.88281345 -6.37786818 -1.44845974
H 4.23343325 -5.26393080 -1.10539830
H 0.96082389 -3.48411679 -3.12138271
Lu 0.61865473 -0.42394879 1.05481398

N -0.93413794 -1.23308909 3.21904159
 O 0.34618238 -1.07856965 3.28894711
 O -1.44318175 -0.98533642 2.04274702
 O -1.61660850 -1.57863235 4.16271210
 N 3.27214193 -0.51751155 1.98444581
 O 2.58864760 0.58083290 1.81948209
 O 2.62188220 -1.59115672 1.68889284
 O 4.42225504 -0.51778507 2.38027263
 N 1.83278871 0.41160598 -1.37471247
 O 2.35476947 0.75126529 -2.42123485
 O 1.88103545 -0.81130838 -0.93549335
 O 1.18082571 1.22816718 -0.61614418
 H 0.75980514 -5.25115442 -2.85396099
 H -0.63619989 4.96977234 0.33464190

L1*Am(NO₃)₃



PBE/L1 theoretical level

E= -32481.788647

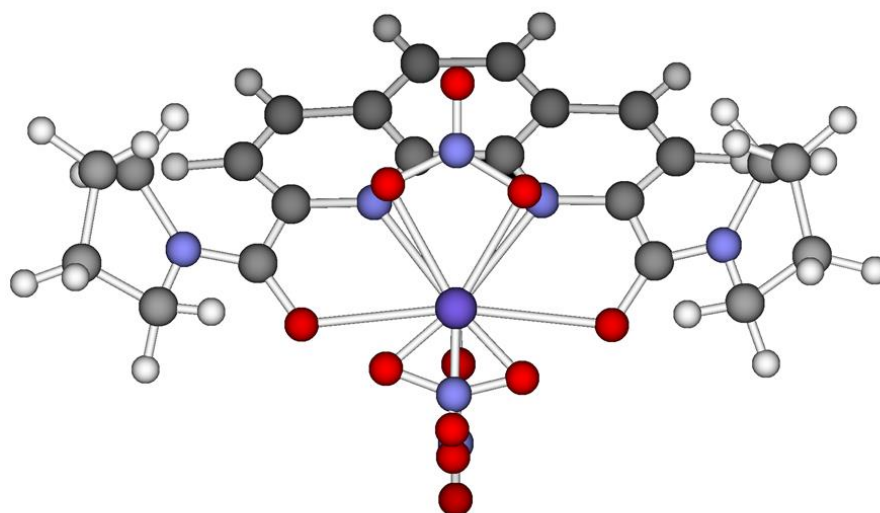
G= 232.9302 kcal/mol, H= 304.5881 kcal/mol, U= 303.9956 kcal/mol, S= 240.3419 cal/mol at T= 298.150 K

H -4.44610596 3.32322645 -0.72309446
 H -3.40981102 -2.90548658 -3.36085081
 N -1.37977099 1.14430630 0.24257338

N -0.14140336 3.92860246 2.12169194
N -0.96395510 -1.29950476 -0.80222005
N 1.14971483 -4.13849592 -1.14916861
O 0.12296699 1.69694734 2.31690454
O 0.60346550 -2.86508393 0.64157468
C -1.53754401 2.36144400 0.77549374
C -2.64605784 3.17416096 0.45018980
H -2.79032159 4.13697290 0.94039327
C -3.57141018 2.71839762 -0.46986246
C -3.39559579 1.45562863 -1.08135223
C -4.29363823 0.90222633 -2.04456782
H -5.16216516 1.49205792 -2.35011601
C -4.08693266 -0.34714606 -2.57060075
H -4.79011822 -0.76272684 -3.29759145
C -2.96450949 -1.13904762 -2.17636251
C -2.71675086 -2.44899821 -2.64920592
C -1.61725354 -3.15123558 -2.18838358
H -1.43687892 -4.17572069 -2.51757717
C -0.75144637 -2.54098701 -1.25805354
C -2.03860974 -0.61303419 -1.23197734
C -2.26013231 0.70051706 -0.67096853
C -0.47117805 2.66393185 1.78540635
C 0.39091083 -3.20569587 -0.54305398
C -0.44852942 5.17535686 1.39370859
H -1.34948719 5.66046572 1.81361461
C 0.79233092 6.04191256 1.64928353
H 1.58569849 5.76985455 0.93392634
H 0.57434249 7.11465359 1.54140329
C 1.19946945 5.63691425 3.07409525
H 0.54529238 6.13029718 3.81226087
H 2.24165559 5.89283609 3.31329179

C 0.97266394 4.12158060 3.08347392
H 1.85230935 3.55775976 2.72726393
H 0.69626051 3.71615553 4.06893682
C 2.32167101 -4.66854906 -0.40778261
H 1.98865497 -5.30425882 0.42705137
H 2.87899137 -3.81808043 0.02110865
C 3.12121677 -5.41683388 -1.48097003
C 2.78143334 -4.64964867 -2.76828480
C 1.28294337 -4.36510277 -2.60193181
H 2.99601269 -5.21429205 -3.68763494
H 3.33093333 -3.69459939 -2.79883218
H 2.78183031 -6.46342659 -1.55926275
H 4.19711494 -5.42045593 -1.25386322
H 0.94980806 -3.48048091 -3.16361117
Am 0.60585040 -0.39851704 1.10938442
N -1.12435460 -1.40793300 3.22696352
O 0.16473480 -1.31127656 3.33064103
O -1.60602355 -1.02678120 2.08344245
O -1.82609224 -1.82282650 4.12781334
N 3.36850762 -0.28606406 2.01527429
O 2.72840023 0.76551145 1.59971035
O 2.66850090 -1.37507355 2.01573420
O 4.52949047 -0.24815817 2.37182140
N 1.95858049 0.24688917 -1.43975043
O 2.51538944 0.55200541 -2.47904563
O 2.11278319 -0.90326196 -0.87220722
O 1.14871573 1.05661190 -0.82610369
H 0.68336755 -5.23992348 -2.91627169
H -0.61593562 4.97148275 0.32612649

L1*Cm(NO₃)₃



PBE/L1 theoretical level

E= -33318.106718

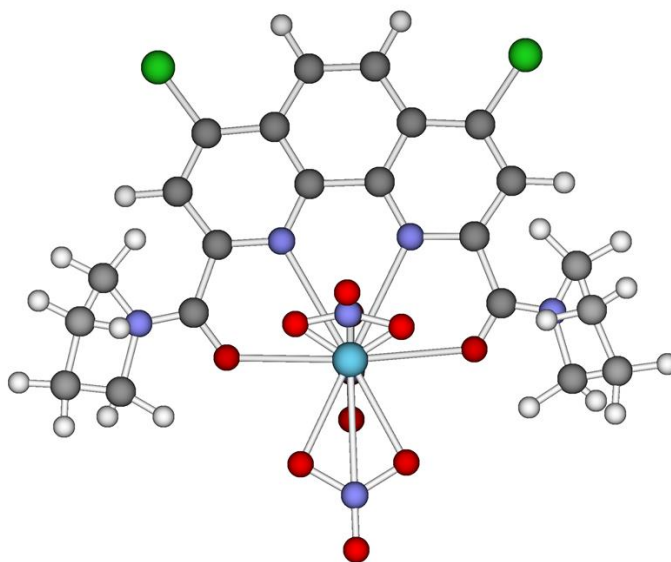
G= 233.3266 kcal/mol, H= 304.4248 kcal/mol, U= 303.8323 kcal/mol, S= 238.4645 cal/mol at T= 298.150 K

H	-4.50152969	3.30145550	-0.76869041
H	-3.45823789	-2.95980263	-3.34764433
N	-1.45464444	1.11159778	0.23404010
N	-0.12447076	3.87733126	2.01321769
N	-1.05024970	-1.33677483	-0.76707661
N	1.18418097	-4.04390478	-1.19862199
O	-0.10957855	1.66224098	2.45064282
O	0.54706460	-2.91522956	0.65503889
C	-1.60802853	2.32916689	0.74944991
C	-2.70243573	3.15335488	0.41053081
H	-2.82740355	4.12998533	0.88056445
C	-3.63522434	2.69006419	-0.50187445
C	-3.47307706	1.41476643	-1.08544707
C	-4.37597561	0.84635311	-2.04225063
H	-5.24404383	1.43319321	-2.35514784
C	-4.16765881	-0.40441042	-2.55608582

H -4.86793137 -0.82518274 -3.28300762
C -3.03950381 -1.19271648 -2.15609980
C -2.77372456 -2.49492431 -2.63288736
C -1.65647674 -3.17797327 -2.18289661
H -1.44919205 -4.19213486 -2.52860737
C -0.80798239 -2.55678010 -1.24246740
C -2.12296295 -0.66035056 -1.20863855
C -2.34251118 0.66166633 -0.66622853
C -0.55991304 2.62337017 1.79586148
C 0.36697358 -3.20016408 -0.54582769
C -0.28330564 5.05215597 1.13352644
H -1.11874783 5.68798304 1.48126662
C 1.05504632 5.78500509 1.29720628
H 1.80883741 5.31897402 0.64178884
H 0.97486693 6.85211182 1.04255962
C 1.40140426 5.52898121 2.77236199
H 0.81430280 6.19819164 3.42338920
H 2.46715212 5.68096066 2.99594951
C 0.98418850 4.06883287 2.98341393
H 1.78930688 3.35295463 2.74330521
H 0.63731593 3.84523082 4.00383282
C 2.39092588 -4.53552437 -0.48382238
H 2.10083413 -5.24752760 0.30402839
H 2.88035893 -3.67689610 0.00763600
C 3.24540973 -5.15395784 -1.59730804
C 2.83958077 -4.34954071 -2.84261966
C 1.32420385 -4.19361925 -2.66090274
H 3.09428596 -4.84764194 -3.78976011
H 3.31147456 -3.35364628 -2.82342315
H 2.99557257 -6.21965933 -1.73306680
H 4.31855297 -5.07939100 -1.36957002

H 0.91840780 -3.31410098 -3.18071175
 Cm 0.55561316 -0.47382635 1.29950523
 N -1.22789490 -1.49580479 3.34853244
 O 0.04490770 -1.36646724 3.53608465
 O -1.65115941 -1.13552368 2.16671062
 O -1.98216677 -1.91960049 4.20189381
 N 3.19126964 -0.59109998 2.54270053
 O 2.44421172 0.47224477 2.57153797
 O 2.67226577 -1.60094619 1.91548204
 O 4.29072142 -0.63292015 3.06072164
 N 1.93142283 0.62412322 -1.08342624
 O 2.45465016 1.07269692 -2.08955431
 O 1.84145749 -0.65060514 -0.85867774
 O 1.42160225 1.38463712 -0.16765098
 H 0.79425097 -5.09921503 -3.01058316
 H -0.47658923 4.73823214 0.09779645

L2*La(NO₃)₃



PBE/L1 theoretical level

E= -11478.690625

G= 216.3096 kcal/mol, H= 294.6496 kcal/mol, U= 294.0571 kcal/mol, S= 262.7537 cal/mol at T= 298.150 K

H -4.52806473 3.27118492 -0.70783961
H -3.50268483 -2.97827387 -3.28968263
N -1.47856951 1.08658290 0.30045471
N -0.09366491 3.89596319 1.94958937
N -1.07944095 -1.37790608 -0.70982087
N 1.19820797 -4.01222277 -1.26134396
O -0.12904730 1.71322906 2.53076386
O 0.53269392 -3.03243709 0.66759455
C -1.62093258 2.31493306 0.79196364
C -2.71388578 3.13975191 0.45021725
H -2.82580471 4.12592649 0.90344417
C -3.65971041 2.66287255 -0.44035134
C -3.50651670 1.37853110 -1.00618947
C -4.42143106 0.80737954 -1.94949973
H -5.29259348 1.39412987 -2.25376987
C -4.21711206 -0.44282344 -2.46414804
H -4.92285490 -0.86542672 -3.18464994
C -3.08114195 -1.22636688 -2.07821369
C -2.81223440 -2.51993394 -2.57629704
C -1.68336511 -3.19966817 -2.15315914
H -1.46688008 -4.20463085 -2.51974487
C -0.83188897 -2.58589005 -1.21068501
C -2.15833735 -0.69797117 -1.13352609
C -2.37382770 0.62610191 -0.58916259
C -0.56019324 2.64100885 1.81921852
C 0.36009955 -3.24029756 -0.54925495
C -0.22750410 5.01040459 0.99001980
H -1.03639483 5.69682217 1.30262291
C 1.13614762 5.70734262 1.08515859
H 1.86601686 5.16614485 0.46088079
H 1.08957326 6.75415945 0.75052357

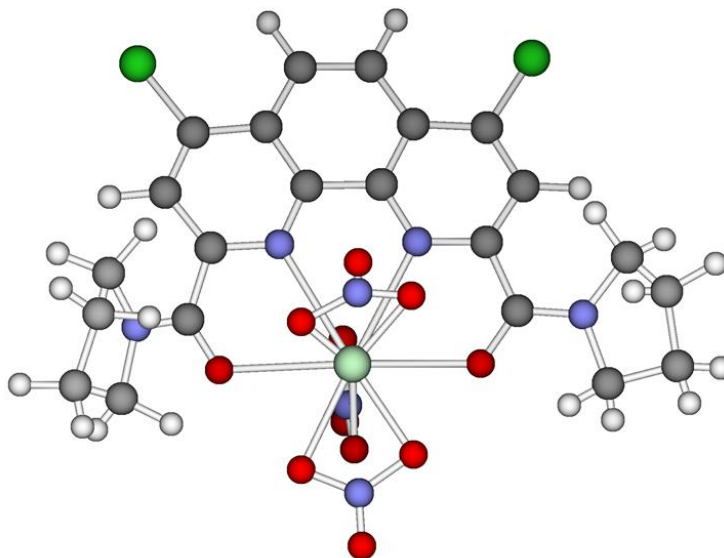
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H 2.56166410 5.68503189 2.77602172
C 1.02790463 4.12573433 2.89630842
H 1.80914855 3.36962700 2.70648909
H 0.68314916 3.99076056 3.93308640
C 2.42460465 -4.51393747 -0.58797944
H 2.16551018 -5.30457926 0.13315034
H 2.87730002 -3.68224955 -0.02132681
C 3.30622387 -4.99460316 -1.74775875
C 2.85963655 -4.11032343 -2.92267060
C 1.33916855 -4.04470015 -2.73119307
H 3.13644481 -4.51389790 -3.90781784
H 3.27982426 -3.09639168 -2.81910706
H 3.10917091 -6.05643559 -1.97225523
H 4.37489796 -4.88683462 -1.51177883
H 0.88793933 -3.15030503 -3.18356919
La 0.55687028 -0.54815400 1.45456898
N -1.43108499 -1.54435408 3.44929218
O -0.17494348 -1.44090831 3.73142600
O -1.76759434 -1.19087648 2.23628426
O -2.25597286 -1.94175220 4.25006580
N 3.20336342 -0.73231447 2.81889963
O 2.48524618 0.35161147 2.83371592
O 2.68211341 -1.73351550 2.17585111
O 4.28763008 -0.80197847 3.36563444
N 1.96410143 0.57403320 -0.99773806
O 2.46891284 1.02194226 -2.01469922
O 1.88594496 -0.70144236 -0.77274525
O 1.46768785 1.34006739 -0.07905519
H 0.85301238 -4.94699287 -3.14674330

H -0.44639614 4.63105822 -0.01830472
PBE0/L1 theoretical level
E= -11478.622988
Cl -4.96386528 3.65538692 -0.86824650
Cl -3.79013586 -3.26458740 -3.70398712
N -1.49596488 1.06776083 0.31849381
N -0.07792855 3.81932139 1.93347430
N -1.08463609 -1.35743392 -0.67522907
N 1.23179662 -3.91055465 -1.23108184
O -0.23838735 1.68164647 2.58485889
O 0.54931742 -2.96440792 0.68148839
C -1.63341033 2.28152013 0.80432516
C -2.69648242 3.11800528 0.45508754
H -2.80679560 4.10044241 0.89491570
C -3.62557983 2.65008330 -0.44165596
C -3.49037457 1.36831546 -1.00768733
C -4.38489771 0.80067986 -1.95936179
H -5.24186325 1.38245547 -2.27556348
C -4.17492867 -0.43703991 -2.46659875
H -4.86253405 -0.85387212 -3.19204354
C -3.05194044 -1.21627355 -2.06683922
C -2.75157261 -2.50271463 -2.55309963
C -1.63050854 -3.16772604 -2.12030292
H -1.40631270 -4.15983772 -2.48943901
C -0.81510860 -2.54407048 -1.17267025
C -2.15416384 -0.69679534 -1.11414552
C -2.37782574 0.62164068 -0.57386339
C -0.59254450 2.59943843 1.84427333
C 0.38618293 -3.17486954 -0.52073985
C -0.13304920 4.87596226 0.91980165
H -0.89773673 5.61869907 1.17961907

C 1.25951755 5.48981953 0.99999863
H 1.95807576 4.87111664 0.42803302
H 1.28266323 6.50831223 0.60680586
C 1.57557881 5.40162802 2.49048233
H 1.05250645 6.19453192 3.03543305
H 2.64241910 5.48430634 2.70696831
C 1.03033412 4.03374052 2.88116503
H 1.76543009 3.23333025 2.74608564
H 0.66448075 3.97929430 3.90908146
C 2.45653796 -4.39030266 -0.56612933
H 2.21026635 -5.15866232 0.17038196
H 2.91565704 -3.55165386 -0.03210652
C 3.31664276 -4.89180183 -1.71923041
C 2.86989808 -4.02192593 -2.89094853
C 1.36114764 -3.94466686 -2.69022441
H 3.13372612 -4.43327284 -3.86750293
H 3.29595184 -3.01783156 -2.80042839
H 3.10413861 -5.94564390 -1.92784369
H 4.38103485 -4.79519081 -1.49654758
H 0.92026597 -3.05373645 -3.14050341
La 0.50878137 -0.53753483 1.52559733
N -1.50732303 -1.64481461 3.39347744
O -0.28094628 -1.56325018 3.70281482
O -1.81224144 -1.21832788 2.22602892
O -2.33377242 -2.08976316 4.13698006
N 3.13163352 -0.65423256 2.89490104
O 2.35942650 0.35424703 2.98775864
O 2.69207525 -1.61395121 2.18240547
O 4.19931698 -0.69509858 3.43576193
N 1.90227091 0.67915243 -0.86613357
O 2.39756608 1.16520071 -1.84723735

O 1.78833747 -0.57768834 -0.72132969
O 1.45395708 1.39140320 0.08535604
H 0.87124187 -4.83722734 -3.09913111
H -0.35534516 4.45932007 -0.06400257

L2*Nd(NO₃)₃



PBE/L1 theoretical level

E= -12610.085242

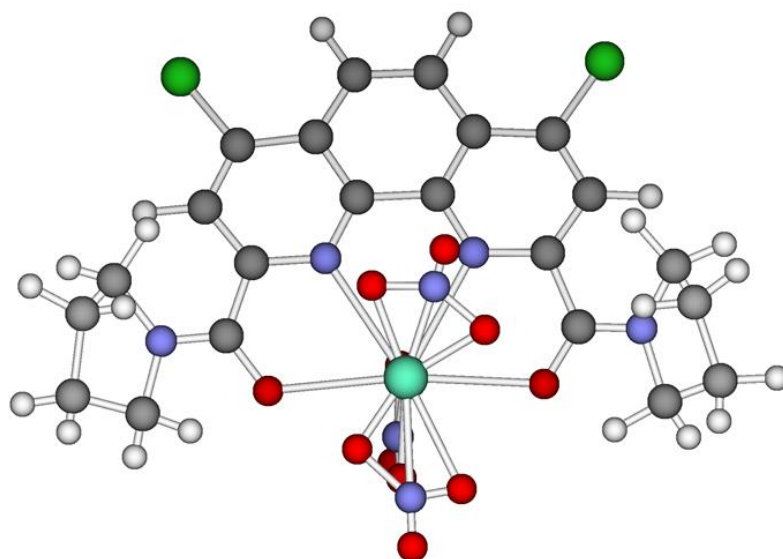
G= 217.2371 kcal/mol, H= 294.5433 kcal/mol, U= 293.9508 kcal/mol, S= 259.2863 cal/mol at T= 298.150 K

Cl -4.99604464 3.69126296 -0.93883449
Cl -3.77347350 -3.31733513 -3.70130157
N -1.47018707 1.12109780 0.27965912
N -0.14713034 3.86973071 2.04644084
N -1.02503312 -1.31188345 -0.71092403
N 1.25980496 -3.99714184 -1.22559321
O -0.33631992 1.68931139 2.63623738
O 0.76770771 -2.76354289 0.59906882
C -1.64474404 2.33942556 0.78911680
C -2.72180557 3.16689467 0.42555252
H -2.85491705 4.15043879 0.87678951
C -3.63993430 2.68956804 -0.49559432

C -3.48583198 1.40104222 -1.06619716
C -4.37520552 0.81575382 -2.01882052
H -5.24215031 1.39352405 -2.34338260
C -4.15393734 -0.43830088 -2.51825166
H -4.84293127 -0.87193960 -3.24491763
C -3.02303219 -1.20888829 -2.10890841
C -2.71699834 -2.51338720 -2.57043314
C -1.57787919 -3.16674423 -2.13096547
H -1.36125672 -4.17510748 -2.48189783
C -0.74261802 -2.51648474 -1.20277870
C -2.11311913 -0.66435438 -1.15840244
C -2.35089231 0.66155553 -0.62614238
C -0.65516597 2.63718534 1.89260435
C 0.48851541 -3.11431551 -0.56317669
C -0.14817993 4.95982122 1.04977298
H -0.92290491 5.70948601 1.29670668
C 1.25638187 5.55721617 1.20354581
H 1.97472894 4.93490076 0.64507991
H 1.30995870 6.59034443 0.82985455
C 1.50846446 5.43574667 2.71481085
H 0.97581893 6.23541689 3.25650263
H 2.57471991 5.49480534 2.97742391
C 0.92071366 4.06219101 3.06247902
H 1.65210927 3.24231791 2.95793486
H 0.49515793 4.00157022 4.07604790
C 2.49828386 -4.47146034 -0.55637091
H 2.24291372 -5.07948828 0.32502896
H 3.06471300 -3.59398198 -0.19932374
C 3.23108125 -5.24456978 -1.65816891
C 2.77812958 -4.53675413 -2.94439816
C 1.29053819 -4.27144241 -2.67648339

H 2.93237686 -5.13512421 -3.85436392
H 3.30713630 -3.57630539 -3.05820775
H 2.90908599 -6.29930115 -1.67009866
H 4.32086325 -5.21991444 -1.51418197
H 0.89883846 -3.41456437 -3.24324417
Nd 0.53074694 -0.37173703 1.37562680
N -1.26735687 -1.72081232 3.22478390
O -0.00224403 -1.57383370 3.45247173
O -1.68334699 -1.22556913 2.09372997
O -2.01657915 -2.27811909 4.00191545
N 3.13441706 -0.29800323 2.68013024
O 2.18000317 0.52109337 2.99105811
O 2.82872438 -1.16474080 1.75980604
O 4.23054314 -0.26000693 3.20308828
N 1.86457014 1.02364695 -0.87538946
O 2.40255451 1.61732507 -1.79386580
O 1.59168172 -0.23656048 -0.92398500
O 1.51671278 1.62483251 0.22481938
H 0.68964761 -5.16872597 -2.91555190
H -0.33642393 4.56293488 0.04206917

L2*Eu(NO₃)₃



PBE/L1 theoretical level

E= -13831.082768

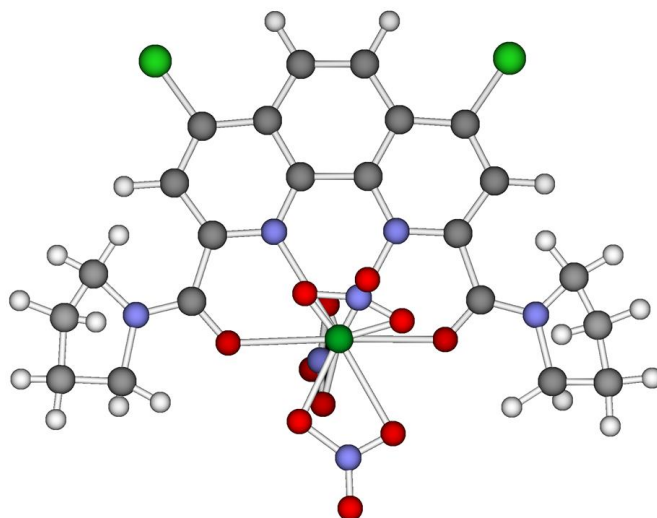
G= 217.9382 kcal/mol, H= 294.4433 kcal/mol, U= 293.8508 kcal/mol, S= 256.5994 cal/mol at T= 298.150 K

Cl	-4.93080473	3.72583795	-0.86443150
Cl	-3.81243610	-3.23828149	-3.77598262
N	-1.43359625	1.09178293	0.27913573
N	-0.08063873	3.86602616	2.05261898
N	-1.03434992	-1.33986056	-0.74665576
N	1.15956533	-4.07837343	-1.14180255
O	-0.01144298	1.64244437	2.44175935
O	0.44867781	-3.01051903	0.73237377
C	-1.56468642	2.31306815	0.78938538
C	-2.64149141	3.15636063	0.45422700
H	-2.76673341	4.13297129	0.92038441
C	-3.57615757	2.70440173	-0.46202239
C	-3.43925381	1.42868900	-1.06473756
C	-4.33631134	0.87669647	-2.02999902
H	-5.19247341	1.47483909	-2.34608769
C	-4.13757467	-0.37360942	-2.54759359
H	-4.83407450	-0.78370124	-3.28076839
C	-3.02442670	-1.17420495	-2.14528251
C	-2.75166249	-2.48386550	-2.61633062
C	-1.65038741	-3.18476701	-2.15396118
H	-1.45869589	-4.20099354	-2.49958825
C	-0.80995512	-2.56807423	-1.20893610
C	-2.10304451	-0.65771484	-1.19115627
C	-2.31769395	0.66387928	-0.63587517
C	-0.49721870	2.60689688	1.82070184
C	0.33038294	-3.25032735	-0.48230755
C	-0.29381347	5.06747866	1.22013390
H	-1.15156138	5.65431643	1.59834254

C 1.01308715 5.85045481 1.40485132
H 1.78072548 5.45101452 0.72203726
H 0.88214302 6.92301941 1.19927502
C 1.38711154 5.54479074 2.86335397
H 0.77757746 6.15609741 3.54960823
H 2.44729567 5.73497200 3.08388233
C 1.03733468 4.06009674 3.01167035
H 1.86879706 3.39370990 2.72333956
H 0.71900994 3.77356720 4.02570438
C 2.34468937 -4.59447432 -0.40783656
H 2.04185104 -5.38579655 0.29540366
H 2.77338743 -3.76608396 0.18157056
C 3.28310275 -5.07854748 -1.52104735
C 2.90653110 -4.18557215 -2.71363521
C 1.37865567 -4.11085320 -2.60306168
H 3.23286557 -4.58673191 -3.68448353
H 3.32359719 -3.17398190 -2.58079720
H 3.09079313 -6.13811493 -1.75985622
H 4.33824205 -4.97864532 -1.22764444
H 0.96089387 -3.21182609 -3.07776499
Eu 0.53196633 -0.49620482 1.24868178
N -1.31116557 -1.45120049 3.28352714
O -0.03613247 -1.35615885 3.46602058
O -1.72749102 -1.12036598 2.10228825
O -2.07051969 -1.82551515 4.15926218
N 3.25877833 -0.48032799 2.26033187
O 2.64487123 0.59929109 1.88378596
O 2.56753707 -1.56286955 2.16987038
O 4.40730190 -0.46357048 2.66687942
N 1.93034196 0.16886137 -1.27388644
O 2.50537300 0.46378407 -2.31040335

O 2.01754713 -1.00628543 -0.74439043
 O 1.18100131 1.01188147 -0.64080709
 H 0.90682316 -5.00833988 -3.04471803
 H -0.48206571 4.78852892 0.17344499

L2*Lu(NO₃)₃



PBE/L1 theoretical level

E= -17553.487293

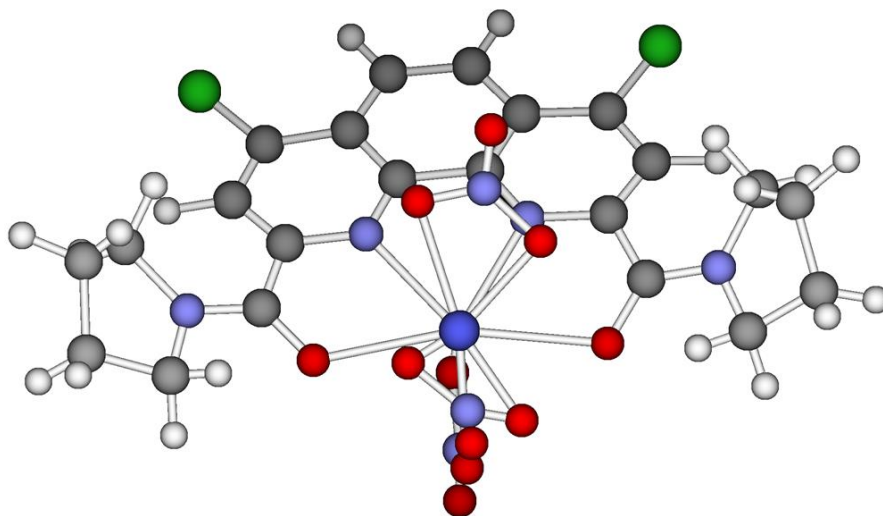
G= 220.1956 kcal/mol, H= 295.1782 kcal/mol, U= 294.5857 kcal/mol, S= 251.4928 cal/mol at T= 298.150 K

Cl -4.95321989 3.72104454 -0.87271386
 Cl -3.77729845 -3.24286866 -3.81366348
 N -1.40895307 1.11782789 0.18855096
 N -0.09820830 3.85047722 2.07489967
 N -1.00051820 -1.28758657 -0.81671029
 N 1.15819263 -4.08816910 -1.09052122
 O 0.11793174 1.61408234 2.23058105
 O 0.51092571 -2.82797718 0.67550707
 C -1.54470778 2.32891417 0.71773076
 C -2.64056015 3.16046333 0.41241270
 H -2.77698970 4.12794685 0.89358848
 C -3.58214736 2.71020985 -0.49946380
 C -3.43982720 1.44373214 -1.11937523
 C -4.33739328 0.88176143 -2.07913017

H -5.20448208 1.46822298 -2.38763022
C -4.12636280 -0.36583531 -2.60076857
H -4.82409000 -0.78298730 -3.32883430
C -3.00171924 -1.15605044 -2.20715213
C -2.71865106 -2.46627998 -2.66750979
C -1.60962081 -3.15318179 -2.19971347
H -1.41809106 -4.17361164 -2.53166080
C -0.76953566 -2.51985979 -1.26579070
C -2.07853532 -0.62557560 -1.26358581
C -2.30420923 0.69223392 -0.70963138
C -0.45139703 2.60003614 1.72586501
C 0.36482552 -3.17418504 -0.51225758
C -0.40619418 5.11784410 1.38316822
H -1.28781676 5.60556507 1.83945107
C 0.85568821 5.95786476 1.62563610
H 1.62564600 5.68543530 0.88540924
H 0.65356737 7.03588438 1.54340112
C 1.29090166 5.51778316 3.03171730
H 0.66421968 6.00789309 3.79539847
H 2.34292245 5.75144768 3.24915385
C 1.03834641 4.00659657 3.01932263
H 1.89741158 3.42883301 2.63651347
H 0.77193266 3.58706427 4.00131750
C 2.31957769 -4.59168673 -0.30971193
H 1.97331083 -5.25977516 0.49374986
H 2.81907582 -3.72930551 0.16500399
C 3.19047141 -5.28809834 -1.36320782
C 2.85302901 -4.53349066 -2.65896344
C 1.33870697 -4.31755877 -2.53776908
H 3.11964679 -5.08571625 -3.57212448
H 3.35755682 -3.55367684 -2.67276311
H 2.91291380 -6.35130024 -1.45747578
H 4.25715446 -5.23361778 -1.10216439
H 0.98373139 -3.45153284 -3.11428547
Lu 0.62473065 -0.43405655 1.08431816

N	-0.93570405	-1.24836624	3.23876357
O	0.34415352	-1.09019613	3.31482434
O	-1.43940258	-0.99873585	2.06006813
O	-1.62144125	-1.59826958	4.17769480
N	3.27095509	-0.53387046	2.02405071
O	2.58746672	0.56575447	1.86297381
O	2.62240124	-1.60544312	1.71560931
O	4.41797590	-0.53667080	2.42659807
N	1.84243453	0.41713357	-1.33672225
O	2.36944222	0.76419461	-2.37761378
O	1.88293147	-0.81082040	-0.90913099
O	1.19140172	1.22902310	-0.57207644
H	0.78779459	-5.22127151	-2.85881329
H	-0.60229719	4.94235897	0.31565481

L2*Am(NO₃)₃



PBE/L1 theoretical level

E= -33403.593584

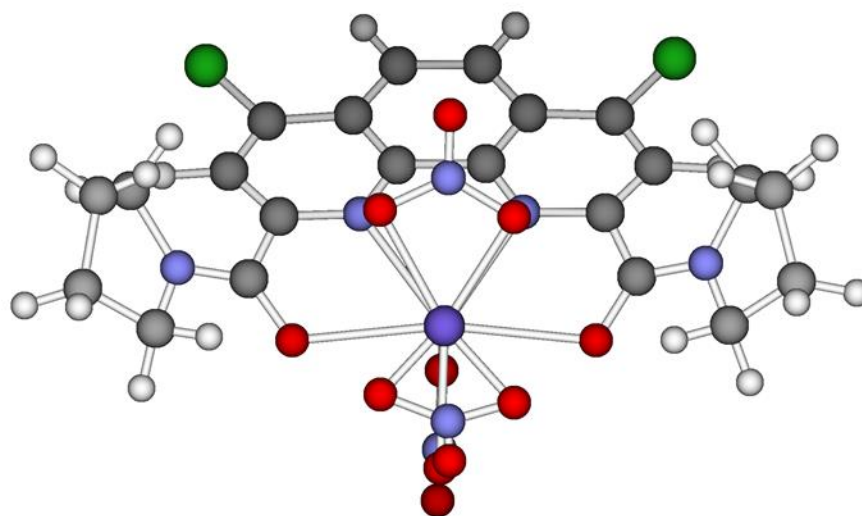
G= 218.5290 kcal/mol, H= 294.2819 kcal/mol, U= 293.6894 kcal/mol, S= 254.0765 cal/mol at T= 298.150 K

Cl	-4.99025249	3.68193388	-0.86140257
Cl	-3.84908080	-3.29197359	-3.72857165
N	-1.47340620	1.07433367	0.29461485
N	-0.07207524	3.87620068	1.94335961

N -1.08135593 -1.37634170 -0.69966781
N 1.21461034 -3.99234438 -1.24314868
O -0.15003774 1.69898283 2.54635215
O 0.51172435 -3.04631805 0.69195622
C -1.60723412 2.30403185 0.78381664
C -2.68598413 3.14155412 0.44321853
H -2.79906774 4.12983131 0.88875711
C -3.63259339 2.66926169 -0.44998515
C -3.50235510 1.37949061 -1.02421999
C -4.40930223 0.81026876 -1.96995842
H -5.27386808 1.39909446 -2.28057361
C -4.20530272 -0.44096071 -2.48246551
H -4.90525293 -0.86087137 -3.20663500
C -3.07854843 -1.22705317 -2.09037733
C -2.78749251 -2.52684760 -2.57743311
C -1.66063797 -3.20531607 -2.14500928
H -1.44577515 -4.20852184 -2.51400518
C -0.82685953 -2.58338881 -1.19746113
C -2.15826106 -0.70373172 -1.13787663
C -2.37291002 0.62518293 -0.59561676
C -0.55275524 2.62774944 1.81993580
C 0.36172345 -3.24060678 -0.52968001
C -0.18249519 4.98397303 0.97158051
H -0.98732585 5.68115616 1.26954889
C 1.18891919 5.66400671 1.07552040
H 1.91740096 5.10779381 0.46301553
H 1.15867853 6.70795202 0.73042578
C 1.52535927 5.51811075 2.56768441
H 0.97372514 6.26775026 3.15929508
H 2.59797931 5.63645554 2.77893853
C 1.03994596 4.10274172 2.90253663

H 1.81250584 3.33305407 2.73290515
H 0.67860925 3.98559713 3.93585372
C 2.43915963 -4.49104595 -0.56298470
H 2.18056297 -5.29517221 0.14314049
H 2.87552595 -3.66257668 0.02112184
C 3.33955431 -4.94176054 -1.71986985
C 2.90080619 -4.03752375 -2.88221145
C 1.37696373 -3.99208021 -2.71257472
H 3.19579792 -4.41683245 -3.87163401
H 3.30718112 -3.02121401 -2.75094819
H 3.15397334 -6.00036383 -1.96794379
H 4.40404797 -4.83007669 -1.46746314
H 0.92371249 -3.09223914 -3.15166783
La 0.54075778 -0.56361133 1.48560572
N -1.48182309 -1.57339489 3.43639469
O -0.22732911 -1.49386775 3.73346519
O -1.80007648 -1.18559599 2.22823930
O -2.32035136 -1.97913349 4.21764231
N 3.17151093 -0.74826908 2.87606764
O 2.44498587 0.33022791 2.89851761
O 2.66264367 -1.74486196 2.21527457
O 4.25156450 -0.81702518 3.43009377
N 1.98283184 0.55249655 -0.95051062
O 2.50978851 0.99965984 -1.95603263
O 1.87848926 -0.72338581 -0.73784733
O 1.48757160 1.31955886 -0.03166909
H 0.90557724 -4.89034939 -3.15245461
H -0.39437768 4.59620667 -0.03497869

L2*Cm(NO₃)₃



PBE/L1 theoretical level

E= -34239.911197

G= 216.4264 kcal/mol, H= 294.6924 kcal/mol, U= 294.0999 kcal/mol, S= 262.5054 cal/mol at T= 298.150 K

Cl	-4.98590899	3.69758964	-0.87716216
Cl	-3.81569624	-3.27557278	-3.76647115
N	-1.45093322	1.09965909	0.24165782
N	-0.10156716	3.86424208	2.00851154
N	-1.04964995	-1.33204007	-0.75361097
N	1.20016849	-4.02689075	-1.18988037
O	-0.10802089	1.65155339	2.46417904
O	0.54082555	-2.92052078	0.67114061
C	-1.59744966	2.31696749	0.75822753
C	-2.68456721	3.14939213	0.43121412
H	-2.81217074	4.12618065	0.89755571
C	-3.62173963	2.68799019	-0.47845381
C	-3.48045325	1.40961885	-1.07509696
C	-4.38058662	0.84166437	-2.02836895
H	-5.24764872	1.42736816	-2.33817077
C	-4.17129517	-0.40816566	-2.54427910
H	-4.86978054	-0.82857710	-3.26967621

C -3.04556298 -1.19452083 -2.14888597
C -2.75617790 -2.50044775 -2.61971617
C -1.63607717 -3.18009353 -2.16987753
H -1.43044519 -4.19147062 -2.52110672
C -0.80002844 -2.54963207 -1.22994220
C -2.12617564 -0.66592515 -1.19940376
C -2.34663129 0.65889829 -0.65429574
C -0.54652315 2.61322284 1.80272114
C 0.37526944 -3.19529796 -0.53388238
C -0.25162670 5.03426886 1.11979771
H -1.08311677 5.67758846 1.46300626
C 1.09149408 5.75902414 1.28020155
H 1.84283602 5.28313732 0.62909353
H 1.01844513 6.82458925 1.01746285
C 1.43378198 5.51175928 2.75780249
H 0.85060620 6.18983936 3.40303683
H 2.50030136 5.65791130 2.98132443
C 1.00648773 4.05624676 2.97993779
H 1.80690670 3.33287978 2.74674368
H 0.65526032 3.84280610 4.00099421
C 2.40147257 -4.52601576 -0.46995375
H 2.10426044 -5.24733734 0.30661985
H 2.88524842 -3.67245197 0.03586535
C 3.26695514 -5.12954855 -1.58286667
C 2.87334228 -4.30790901 -2.82056904
C 1.35567522 -4.15531254 -2.65340304
H 3.13708448 -4.79178905 -3.77247190
H 3.34375787 -3.31184411 -2.78321695
H 3.01812291 -6.19303751 -1.73560238
H 4.33768415 -5.05790758 -1.34339356
H 0.95597869 -3.26787615 -3.16439533

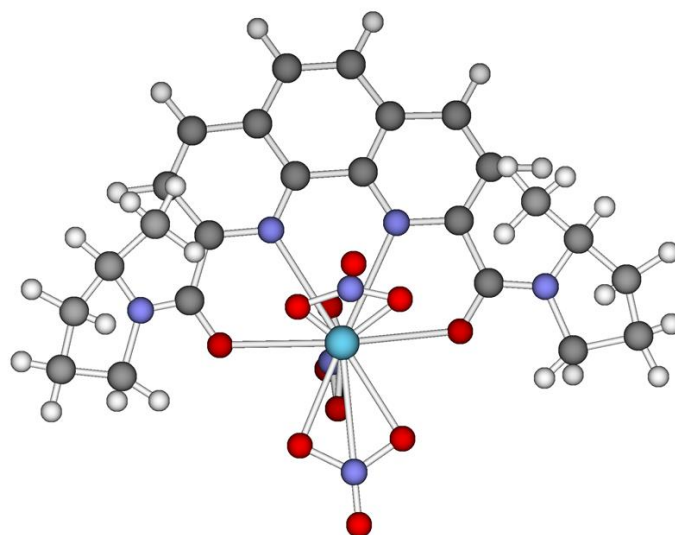
Cm 0.56096154 -0.48223004 1.31962037
N -1.22655690 -1.50511062 3.36241746
O 0.04598800 -1.37942708 3.55272341
O -1.64603996 -1.14034605 2.17962790
O -1.98414707 -1.92887473 4.21209526
N 3.19567823 -0.60509259 2.55859780
O 2.44702959 0.45724371 2.59579682
O 2.67402530 -1.61304367 1.92980814
O 4.29766989 -0.64764512 3.07000518
N 1.93140638 0.61717063 -1.06375742
O 2.44871855 1.06726646 -2.07148910
O 1.84321070 -0.65817010 -0.83958364
O 1.42540300 1.37593484 -0.14373136
H 0.82987392 -5.05600071 -3.02114940
H -0.44535422 4.71411228 0.08607770

L3*La(NO₃)₃

Searching the most stable geometry

Meso-form

isomer I



PBE/L1 theoretical level

E= -10635.454491

G= 263.6789 kcal/mol, H= 340.6639 kcal/mol, U= 340.0714 kcal/mol, S= 258.2090 cal/mol at T= 298.150 K

N	-1.44597805	1.09205532	0.39710894
N	-0.02985763	3.90292931	2.02853322
N	-1.08161914	-1.39246380	-0.57429272
N	1.14159739	-4.10608864	-1.10950625
O	-0.14541648	1.73291910	2.65400338
O	0.56630665	-3.01339126	0.78466856
C	-1.58548427	2.32124472	0.88543332
C	-2.70205116	3.12989545	0.58487165
H	-2.79899263	4.12162066	1.03031349
C	-3.68096137	2.63281584	-0.25656229
C	-3.53975439	1.34175706	-0.81165200
C	-4.49688578	0.74382842	-1.69418299
H	-5.38779020	1.31730878	-1.96483290
C	-4.31126165	-0.51770014	-2.18835497
H	-5.05208731	-0.96280265	-2.85835862
C	-3.15316772	-1.28607607	-1.84078729
C	-2.91055655	-2.59751987	-2.30585146
C	-1.76010013	-3.26157999	-1.92006934
H	-1.56014061	-4.27833414	-2.26289535
C	-0.85813004	-2.61437726	-1.04898429
C	-2.18277335	-0.72707599	-0.96410954
C	-2.37866020	0.60834062	-0.44192448
C	-0.52157944	2.65815067	1.90510535
C	0.35390976	-3.26233149	-0.41998419
C	-0.05558782	5.03112841	1.04589629
H	-1.02675045	5.55522394	1.12826657
C	1.05800784	5.95678663	1.58365881
H	2.01295471	5.67319822	1.10873473
H	0.85154617	7.00972462	1.34016216
C	1.11809456	5.66662025	3.08595920

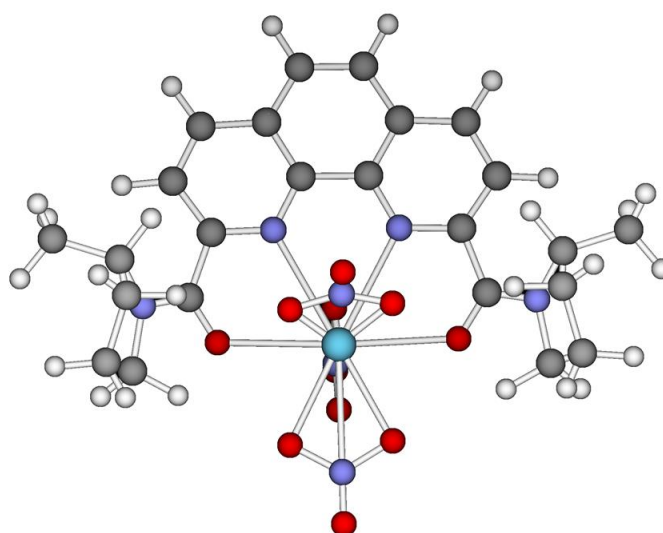
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O -1.77316833 -1.17816627 2.32790828
O -2.28196096 -2.05723381 4.28404379
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O -0.13621764 1.71061003 2.62483287
O 0.55704588 -2.98616409 0.78272402
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H -2.78074980 4.08188248 1.03877878
C -3.65124869 2.61068034 -0.25021821
C -3.50792122 1.33037543 -0.80530882
C -4.45805407 0.73911631 -1.69142294
H -5.33920002 1.31095040 -1.96417487
C -4.27377987 -0.50960797 -2.18111372
H -5.00556040 -0.94990814 -2.85076904
C -3.12313724 -1.27690411 -1.82782376
C -2.88513780 -2.58114815 -2.28623509
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C -0.06230564 4.97710037 1.03836739
H -1.02412915 5.49869967 1.12795913
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H 1.99190509 5.61643028 1.07826555
H 0.84020883 6.94308662 1.31959927
C 1.12436259 5.60846519 3.05038142
H 0.31047922 6.11030722 3.58434772
H 2.07131171 5.91584015 3.49861312
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C 2.78967047 -5.68721104 -1.38149607
C 2.64238262 -4.91449738 -2.68339372
C 1.29231751 -4.19650078 -2.56170249
H 2.67798519 -5.54070139 -3.57775187
H 3.43481135 -4.16171837 -2.75923014
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O -1.77317417 -1.17221546 2.32134271
O -2.30380416 -2.00261021 4.24792671
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 H -3.60614443 -3.06070852 -2.94067430
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 H 1.84670281 -5.17277193 0.54702890
 H 1.05472052 3.90019870 -0.46154508
 H 0.37905076 5.45977497 -0.99724233
 H -0.66410887 4.04481697 -0.85162359
 H 1.86482835 3.55935693 2.89559507
 H 2.97651482 -3.95994616 -0.05761048
 H 0.29827785 -2.42733169 -3.38922715
 H 1.64039457 -3.06314993 -4.34108257
 H 1.95702171 -2.16168690 -2.83668756

Isomer II



PBE/L1 theoretical level

E= -10635.456307

G= 263.8496 kcal/mol, H= 340.8597 kcal/mol, U= 340.2672 kcal/mol, S= 258.2931 cal/mol at T= 298.150 K

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N 0.24370649 3.77230263 2.46521974
N -0.80805498 -1.52309060 -0.13760617
N 1.41516161 -4.23671532 -0.67281973
O 0.12814763 1.60229230 3.09068990
O 0.83987075 -3.14401793 1.22135508
C -1.31192017 2.19061804 1.32211983
C -2.42848706 2.99926877 1.02155817
H -2.52542853 3.99099398 1.46700001
C -3.40739727 2.50218916 0.18012422
C -3.26619029 1.21113038 -0.37496546
C -4.22332191 0.61320168 -1.25749648
H -5.11422634 1.18668199 -1.52814639
C -4.03769779 -0.64832687 -1.75166845
H -4.77852345 -1.09342933 -2.42167211
C -2.87960362 -1.41670275 -1.40410078
C -2.63699245 -2.72814655 -1.86916494
C -1.48653603 -3.39220667 -1.48338282
H -1.28657651 -4.40896082 -1.82620883
C -0.58456594 -2.74500394 -0.61229777
C -1.90920925 -0.85770273 -0.52742302
C -2.10509610 0.47771388 -0.00523797
C -0.24801534 2.52752399 2.34179187
C 0.62747389 -3.39295816 0.01670232
C 0.21797630 4.90050173 1.48258281
H -0.75318629 5.42459726 1.56495309
C 1.33157206 5.82615995 2.02034545
H 2.28651881 5.54257154 1.54542124
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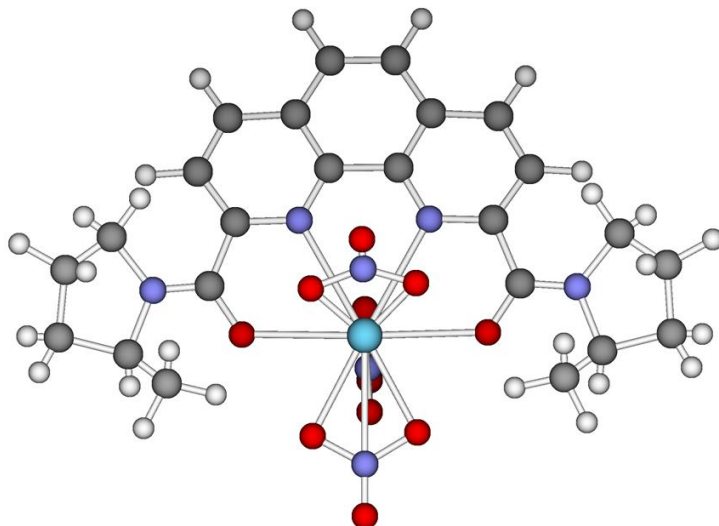
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C 1.57484221 -3.05143690 -2.91748595
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H -3.36505365 -3.21157670 -2.52648187
H 0.77744806 3.64219165 4.51477194
H 2.10229397 -5.37804413 0.97926021
H 1.34760404 3.80607057 -0.01772279
H 0.68115824 5.38141537 -0.56438327
H -0.37963432 3.96403742 -0.42139712
H 2.13548732 3.46958613 3.38253498
H 3.25076747 -4.15594864 0.39374107
H 0.57343763 -2.60616493 -2.99828243
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H 2.23330832 -2.32123017 -2.41993451
PBE0/L1 theoretical level
E= -10635.345939
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N -0.02002519 3.74397993 1.96948862
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N 1.13811362 -3.94141030 -1.03438938

O -0.38331860 1.64902425 2.68560886
O 0.32391596 -3.04366636 0.85393894
C -1.67762804 2.28700900 0.85069638
C -2.71956444 3.13643813 0.45922622
H -2.81301761 4.12423038 0.89086413
C -3.63685584 2.67963219 -0.45535111
C -3.50378871 1.39176595 -0.99345517
C -4.39577770 0.83613425 -1.96020830
H -5.23166037 1.43829787 -2.30148625
C -4.20850039 -0.41325933 -2.44692254
H -4.89259720 -0.82371122 -3.18266177
C -3.11249018 -1.21763766 -2.01018906
C -2.85790086 -2.51418018 -2.47919369
C -1.76742399 -3.20760918 -2.01385164
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C -2.22352624 -0.70706129 -1.04717636
C -2.42276263 0.62065089 -0.52961189
C -0.64508748 2.57191539 1.91110599
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N 2.90358567 -0.78010923 3.11625981
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H -4.46667719 3.30789900 -0.76308584
H -3.52641082 -2.96386456 -3.20645380
H 0.83540541 4.09505272 3.87827039
H 2.24482203 -5.23659801 0.22898404
H 1.63703883 2.86436033 2.89906335
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H 1.63971090 -6.05936670 -2.75364709
H 1.14366627 -5.19487381 -4.21771812
H -0.03657906 -5.55186319 -2.94649839

H	-0.64707118	6.74882603	0.45888644
H	-0.25551894	6.49600124	2.16793370
H	-1.75400901	5.84703779	1.50651395

Isomer III



PBE/L1 theoretical level

E= -10635.455985

G= 263.7182 kcal/mol, H= 340.8577 kcal/mol, U= 340.2652 kcal/mol, S= 258.7273 cal/mol at T= 298.150 K

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N	-0.26542661	4.05506277	1.80885231
N	-1.16483450	-1.28571105	-0.94009489
N	0.97218847	-4.10505056	-1.41020024
O	-0.25335339	1.84643412	2.31203604
O	0.50131565	-2.86733747	0.42462417
C	-1.70634890	2.45362401	0.54886776
C	-2.81886744	3.25369930	0.21365499
H	-2.96430492	4.22818279	0.67791969
C	-3.75048852	2.76972175	-0.68492573
C	-3.57646179	1.49319267	-1.25607371
C	-4.49958515	0.92372173	-2.19047880
H	-5.36677694	1.51627791	-2.49467516
C	-4.31026173	-0.33430812	-2.68532133

H -5.02320862 -0.76678813 -3.39270902
C -3.18342471 -1.12054002 -2.28342795
C -2.96615076 -2.43857408 -2.73224688
C -1.85541427 -3.13803625 -2.29995418
H -1.69941652 -4.16560602 -2.62502527
C -0.95775086 -2.51875710 -1.40464127
C -2.23347545 -0.58772475 -1.36552775
C -2.43396187 0.75094748 -0.84051734
C -0.67954683 2.78929710 1.61678660
C 0.23536849 -3.19269514 -0.74912375
C -0.60054797 5.25244093 1.00995338
H -1.61325514 5.61513615 1.26204860
C 0.43339497 6.29073906 1.46215880
H 1.35976493 6.19106007 0.87563354
H 0.05546110 7.31617880 1.33757687
C 0.67409670 5.90220547 2.92811871
H -0.17200972 6.23583746 3.55243874
H 1.59913230 6.32829332 3.34214878
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C 2.14298344 -4.75220537 -0.73343891
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C 2.14476466 -5.30481577 -3.08061218
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H 2.93428469 -4.60628653 -3.39808345
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O -0.36831233 -1.49891710 3.42454696
O -1.92138577 -1.05873311 1.93254876

O -2.47078085 -1.99639189 3.85006690
N 2.97513485 -0.62304306 2.81504297
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H 0.68738472 -3.68753171 -3.48561454
H -0.55764532 5.03259230 -0.06779330
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C 3.31392050 -3.78627062 -0.53392988
H -4.63065767 3.36309600 -0.94736385
H -3.68603754 -2.90315986 -3.41162133
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H 2.14360213 2.72940564 2.53378987
H 2.82077718 4.14912605 3.36068511
H 2.50230789 4.20975161 1.59988844
H 3.65044165 -3.35649824 -1.49036551
H 4.15196180 -4.33974648 -0.08044785
H 3.04896379 -2.96634340 0.14685173
H 1.80036569 -5.11521053 0.24923036
PBE0/L1 theoretical level
E= -10635.345749
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N -0.25153363 4.00571442 1.77695799
N -1.16983557 -1.28436470 -0.91777045
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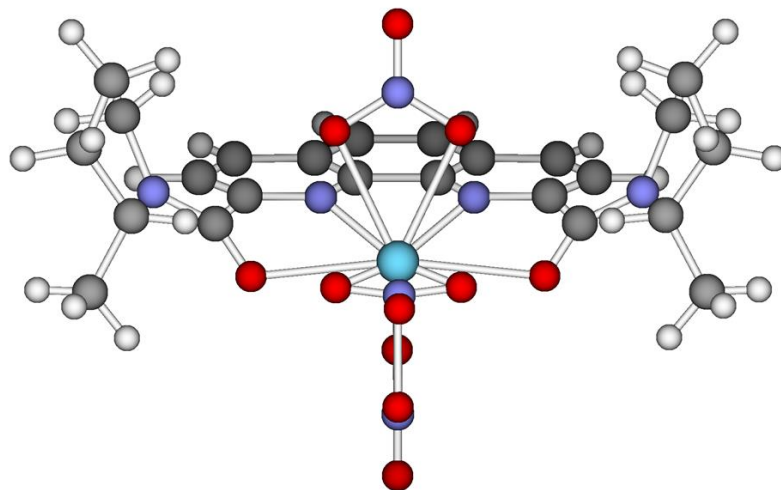
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C -3.74018836 2.73395252 -0.65021473
C -3.56789136 1.46613526 -1.21746504
C -4.49054718 0.89727920 -2.14492011
H -5.35387802 1.48332965 -2.44306421
C -4.30147886 -0.34773594 -2.63591671
H -5.01027203 -0.77913415 -3.33534861
C -3.17417383 -1.12715065 -2.24003696
C -2.95531631 -2.43478346 -2.68841267
C -1.84937263 -3.12496781 -2.26258898
H -1.68849516 -4.14423561 -2.58367753
C -0.96145278 -2.50253153 -1.37626946
C -2.23398447 -0.59657115 -1.33469534
C -2.43563366 0.73285323 -0.81070542
C -0.67202860 2.75509143 1.60892534
C 0.22752565 -3.17077708 -0.72723520
C -0.58343881 5.18107891 0.96717256
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C 0.87439221 -4.40668106 -2.81505680
H 2.10418630 -5.82036352 -3.92216969
H 2.96908855 -4.38515282 -3.34533572
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N -1.69364583 -1.48415780 3.11144114
O -0.47684544 -1.43549430 3.45436215
O -1.95463228 -1.05808222 1.93275809
O -2.55500984 -1.89980221 3.83383489
N 2.89972377 -0.69121778 2.87077761
O 2.17721939 0.35583732 2.89484739
O 2.47941971 -1.62290084 2.11296844
O 3.90538144 -0.79165775 3.51361465
N 1.90485346 0.70752978 -1.06337225
O 2.43310237 1.17182279 -2.03733373
O 1.75457323 -0.54458851 -0.90951598
O 1.45478559 1.43856609 -0.12677860
H 0.05001111 -5.11035442 -2.97872519
H 0.71780080 -3.52250767 -3.43743396
H -0.57043600 4.94208002 -0.09883195
C 2.13522339 3.76002955 2.48461032
C 3.27312255 -3.73365545 -0.46881467
H -4.61451006 3.32334661 -0.90726954
H -3.66952038 -2.89880013 -3.36109781
H 0.41444612 3.88745570 3.76134801
H 2.13207865 2.67030859 2.47033167
H 2.83892393 4.08107853 3.25859022
H 2.49040103 4.12197685 1.51589775
H 3.60966754 -3.24524879 -1.38737142
H 4.11048126 -4.29444122 -0.04259260

H 2.98757720 -2.96611381 0.25022846

H 1.78198385 -5.12106991 0.20875096

Isomer IV



PBE/L1 theoretical level

E= -10635.462096

G= 263.0940 kcal/mol, H= 340.8312 kcal/mol, U= 340.2387 kcal/mol, S= 260.7318 cal/mol at T= 298.150 K

N -1.62054837 1.18107092 0.09102554

N -0.16753648 3.96441054 1.68982363

N -1.24498236 -1.29039192 -0.89841092

N 1.02857292 -3.92182326 -1.47003460

O -0.33513951 1.80291641 2.36340666

O 0.39040676 -2.92324662 0.46612322

C -1.75181401 2.41318560 0.57538277

C -2.83636189 3.24699664 0.22998819

H -2.93016815 4.24006462 0.67336184

C -3.79126501 2.77108192 -0.65176922

C -3.65452981 1.47873592 -1.20483911

C -4.58048487 0.90402722 -2.13542390

H -5.44904327 1.49431086 -2.44033241

C -4.38993025 -0.35359275 -2.63803029

H -5.10478115 -0.77796936 -3.34843326

C -3.25717545 -1.14217365 -2.25253177
C -3.00080204 -2.44402838 -2.73644876
C -1.87008286 -3.12360668 -2.31776571
H -1.66025102 -4.13345909 -2.67508340
C -1.00526381 -2.50232792 -1.39204824
C -2.32359171 -0.60950768 -1.32146454
C -2.52545238 0.72072971 -0.78938383
C -0.69297713 2.72945905 1.60934210
C 0.20163496 -3.14728141 -0.74599302
C -0.18030541 4.97745800 0.61575550
H -0.84403181 5.81923866 0.88687092
C 1.28391409 5.42913389 0.56836092
H 1.87246382 4.67943859 0.01431258
H 1.40092230 6.40925407 0.08248914
C 1.67407656 5.43012810 2.05230403
H 1.29071581 6.33948898 2.54827404
H 2.76158953 5.38642645 2.21136308
C 0.97852230 4.18480492 2.63256860
C 0.51684541 4.33124733 4.07912493
C 2.28512430 -4.41730595 -0.81732035
C 2.02950811 -5.61228848 0.09587370
C 3.20844960 -4.71091509 -2.01431441
C 2.67717028 -3.81048799 -3.13739777
C 1.15975428 -3.90385723 -2.94055033
H 2.98632288 -4.13317251 -4.14275932
H 2.99575782 -2.76685834 -2.98000646
H 3.12222457 -5.77353144 -2.30289912
H 4.25991583 -4.50927496 -1.76208150
La 0.37771359 -0.45207366 1.27841938
N -1.62787914 -1.53690076 3.20778418
O -0.37170804 -1.46188366 3.49936438

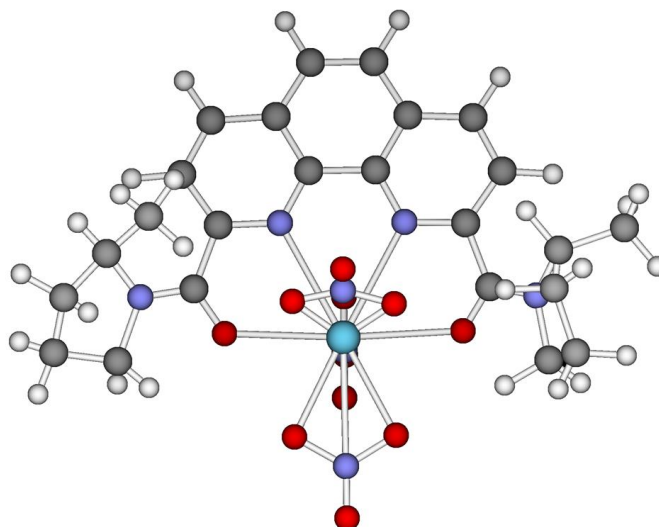
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O 2.22698402 0.42325351 2.78150630
O 2.54018879 -1.59047484 1.96558380
O 4.06220245 -0.69114733 3.28333855
N 1.85043931 0.73490673 -1.11100256
O 2.40651655 1.21283448 -2.08670449
O 1.68654346 -0.54313391 -0.96905929
O 1.38382161 1.47417080 -0.15363438
H 0.76279932 -4.83995962 -3.37504816
H 0.61711150 -3.04972053 -3.36862206
H -0.52535337 4.53679276 -0.32977891
H 2.98502445 -5.94908619 0.52880615
H 1.58500361 -6.45121765 -0.46417102
H 1.36404133 -5.33076763 0.92478460
H 0.02996120 3.40810513 4.42548656
H -0.17989007 5.17829323 4.18912172
H 1.39230180 4.51363277 4.72270823
H 1.62777102 3.29480815 2.54946017
H 2.67564774 -3.57884550 -0.21318129
H -4.65432978 3.38581228 -0.92181987
H -3.70091391 -2.90765953 -3.43686461
PBE0/L1 theoretical level
E= -10635.352441
N -1.61289525 1.17028272 0.09983227
N -0.15934543 3.92396307 1.67508602
N -1.23611057 -1.28111112 -0.88728690
N 1.03036380 -3.87698507 -1.45363569
O -0.32059598 1.78372526 2.33848643
O 0.39332154 -2.88800859 0.46009299

C -1.73981655 2.38793516 0.57990015
C -2.81206203 3.22138262 0.23736238
H -2.90220976 4.20662355 0.67856133
C -3.75759315 2.75154138 -0.64096093
C -3.62119460 1.46836686 -1.19077849
C -4.53993702 0.89998722 -2.12447453
H -5.40043736 1.48713684 -2.42878747
C -4.34803724 -0.34294543 -2.62631702
H -5.05315876 -0.76203334 -3.33693695
C -3.22050357 -1.12877941 -2.23895717
C -2.96022964 -2.41774750 -2.72696996
C -1.83933222 -3.09212852 -2.30857301
H -1.62419736 -4.09128189 -2.66755724
C -0.99165159 -2.47582150 -1.37938929
C -2.30417800 -0.60546780 -1.30870485
C -2.50770855 0.71537095 -0.77610296
C -0.67945242 2.70327568 1.60082555
C 0.21102382 -3.11421609 -0.73741579
C -0.18534441 4.92906666 0.61045182
H -0.86103326 5.75209522 0.87499851
C 1.25991440 5.40765858 0.57280171
H 1.86231756 4.67961884 0.02053692
H 1.35819817 6.38645029 0.09811467
C 1.64059639 5.40515709 2.04827595
H 1.23343897 6.29339218 2.54594970
H 2.71999121 5.38728952 2.21285200
C 0.97573507 4.14687490 2.60724735
C 0.52104598 4.26722527 4.04795456
C 2.26561999 -4.38456345 -0.80289620
C 1.98898125 -5.55746794 0.11678141
C 3.17209387 -4.71254683 -1.98975587

C 2.66996908 -3.80690885 -3.10776496
C 1.16047776 -3.85668015 -2.91192317
H 2.96780372 -4.13814116 -4.10505772
H 3.01598310 -2.78006411 -2.95352936
H 3.05037522 -5.76523113 -2.27167606
H 4.22251987 -4.54572964 -1.74212217
La 0.38035148 -0.45137867 1.27900124
N -1.61863565 -1.52710283 3.18708372
O -0.38694885 -1.45532358 3.47706103
O -1.93809462 -1.10566401 2.02265072
O -2.43740797 -1.95979559 3.94715238
N 3.00347233 -0.60307813 2.65235400
O 2.24915528 0.41909939 2.73719716
O 2.55179262 -1.55742288 1.94087780
O 4.06731462 -0.66097808 3.20038772
N 1.79082477 0.73159063 -1.12185335
O 2.29892731 1.20469332 -2.10321140
O 1.65402031 -0.52220535 -0.97241449
O 1.35202456 1.45595324 -0.17526565
H 0.74181378 -4.77209330 -3.34861732
H 0.64984369 -2.99118590 -3.33624291
H -0.50989133 4.48844194 -0.33312902
H 2.93173170 -5.91414452 0.54174381
H 1.52135479 -6.38110685 -0.43212759
H 1.34009588 -5.25580692 0.94133008
H 0.05806440 3.33787370 4.38546181
H -0.18898781 5.09209013 4.16564369
H 1.38826966 4.46298409 4.68536520
H 1.63969147 3.28000951 2.50994349
H 2.67783952 -3.55542803 -0.21597587
H -4.61120749 3.36459613 -0.91207206

H -3.64816093 -2.87517738 -3.43088198

Isomer V



PBE/L1 theoretical level

E= -10635.455224

G= 263.7891 kcal/mol, H= 340.7851 kcal/mol, U= 340.1926 kcal/mol, S= 258.2460 cal/mol at T= 298.150 K

H -4.50013685 3.34682775 -0.55275947

H -3.73768735 -3.01425028 -2.95088458

N -1.45774174 1.12382317 0.39231753

N 0.04129174 3.93025589 1.96447229

N -1.17408419 -1.38943899 -0.52872932

N 1.07611978 -4.03109932 -1.02100897

O -0.10449083 1.76957357 2.61465621

O 0.35455397 -3.06977034 0.90383488

C -1.55508900 2.36687660 0.85448140

C -2.64456344 3.20536065 0.53626990

H -2.71238518 4.20655060 0.96539718

C -3.63460755 2.72690701 -0.30310234

C -3.53150797 1.42423570 -0.83916706

C -4.49656010 0.84717125 -1.72722554

H -5.36434269 1.44616580 -2.01686311

C -4.34448624 -0.42467701 -2.20607018

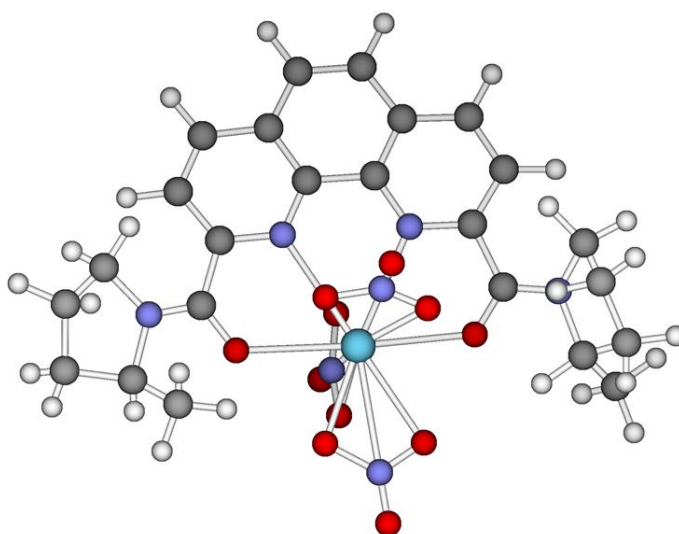
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C -3.21717000 -1.22677946 -1.83342397
C -3.00761509 -2.54861689 -2.28309727
C -1.88796508 -3.24837041 -1.86808586
H -1.71891952 -4.27496719 -2.19531560
C -0.98310530 -2.62633419 -0.98273015
C -2.24360847 -0.69092739 -0.94624156
C -2.40019751 0.65776521 -0.44550401
C -0.47332266 2.69238281 1.85894644
C 0.20711420 -3.28488803 -0.31596106
C 0.03945754 5.04153728 0.96168733
H -0.92080408 5.58648348 1.03272235
C 0.29115897 4.58831930 -0.47761443
C 1.17100585 5.95467472 1.48364294
H 2.11963844 5.64793396 1.01057732
H 0.98256373 7.00747395 1.22549379
C 1.22953224 5.68511772 2.98979187
H 0.41831574 6.21696711 3.51471853
H 2.18673325 5.98110962 3.44319153
C 1.00715816 4.17552519 3.06111550
H 1.93406057 3.60428786 2.87355304
H 0.58655274 3.81646872 4.01159334
C 2.34521031 -4.42203808 -0.34703815
H 2.20313787 -5.35349226 0.22322141
H 2.60820389 -3.62924600 0.37219504
C 3.36396098 -4.55113649 -1.49250054
C 2.74034834 -3.73111606 -2.63536358
C 1.23476279 -4.02551937 -2.49792290
H 3.12709188 -4.00293636 -3.62904000
H 2.90529704 -2.65518928 -2.46252656
H 3.49616051 -5.60370064 -1.78937602

H 4.34841681 -4.16427660 -1.19021332
H 0.63167524 -3.20378184 -2.91434288
C 0.82545120 -5.36024380 -3.13003564
La 0.48491719 -0.55835307 1.61711633
N -1.56828308 -1.45312846 3.59198928
O -0.30904379 -1.42968094 3.87826490
O -1.87871182 -1.05701923 2.38529015
O -2.41768742 -1.81662655 4.38276482
N 3.10104895 -0.84228086 3.02199960
O 2.40749359 0.25574464 3.05942917
O 2.56538868 -1.81238496 2.34131122
O 4.17590094 -0.95442200 3.57970071
N 1.99464095 0.42751253 -0.84555244
O 2.54333472 0.82561713 -1.86116254
O 1.81083405 -0.83492333 -0.61359686
O 1.55598867 1.23764873 0.06405666
H 0.94646335 -5.30477428 -4.22352600
H 1.44824338 -6.18741751 -2.75654840
H -0.22439988 -5.61187506 -2.91493821
H 0.51048666 5.47450542 -1.09444034
H 1.15115523 3.90044641 -0.51735783
H -0.57318211 4.07685566 -0.92350250
PBE0/L1 theoretical level
E=-10635.345108
H -4.45968390 3.33162498 -0.56051290
H -3.68658519 -2.97851467 -2.95460582
N -1.45670366 1.11826146 0.39630508
N 0.04223683 3.88584352 1.95744860
N -1.17315555 -1.37800622 -0.51807320
N 1.07469344 -3.98184657 -1.00904310
O -0.12310933 1.74955928 2.60148311

O 0.36927888 -3.01513958 0.88915563
C -1.55347002 2.34604836 0.85619754
C -2.62940359 3.18412209 0.53723562
H -2.69695139 4.17609596 0.96648914
C -3.60475683 2.71325755 -0.30593050
C -3.49929023 1.42022872 -0.83947152
C -4.45357370 0.85071963 -1.73568726
H -5.31028080 1.44839764 -2.02996826
C -4.30004740 -0.40702724 -2.21256542
H -5.03192854 -0.82861984 -2.89403892
C -3.18173480 -1.20826650 -1.83091295
C -2.96990633 -2.51890683 -2.28141856
C -1.86279082 -3.21492910 -1.86202955
H -1.69128191 -4.23178148 -2.18949866
C -0.97655934 -2.59803581 -0.97070122
C -2.22837687 -0.68259019 -0.94001442
C -2.38588238 0.65799612 -0.44125697
C -0.47765270 2.66667032 1.85686517
C 0.21599007 -3.24364400 -0.31257352
C 0.03916321 4.98693228 0.96541250
H -0.90923518 5.53468180 1.03919959
C 0.28527394 4.53920603 -0.46625572
C 1.17030573 5.88803482 1.47696698
H 2.10866857 5.57666302 1.00483072
H 0.98900044 6.93447018 1.22125125
C 1.23353612 5.61955023 2.97282505
H 0.43052009 6.14925337 3.49617934
H 2.18626213 5.91000891 3.42007804
C 1.00647116 4.12061071 3.04149270
H 1.92313528 3.55114174 2.84904647
H 0.59232539 3.76666903 3.98719645

C 2.34105563 -4.35351753 -0.34699833
H 2.21023870 -5.26648617 0.23944202
H 2.61346245 -3.55092192 0.34392852
C 3.34078741 -4.50448036 -1.49378800
C 2.70325804 -3.72129297 -2.64083290
C 1.21118128 -4.01120996 -2.47343993
H 3.07277989 -4.01696444 -3.62557364
H 2.87016177 -2.64919114 -2.50031805
H 3.47453070 -5.55546904 -1.76468837
H 4.31839371 -4.10635185 -1.21455145
H 0.60646713 -3.20939064 -2.90425920
C 0.80420357 -5.35616684 -3.05960155
La 0.47626337 -0.55125773 1.62303185
N -1.57192898 -1.46850932 3.56003547
O -0.33809239 -1.44872761 3.84836793
O -1.87157178 -1.06429803 2.38406038
O -2.41030478 -1.83893561 4.33140659
N 3.09903312 -0.78225470 2.98476982
O 2.38254905 0.26616374 3.06232381
O 2.60714579 -1.72938621 2.28880644
O 4.16494703 -0.87233996 3.52417183
N 1.94499350 0.44758439 -0.83128721
O 2.47014761 0.85246921 -1.83457887
O 1.75487506 -0.79068345 -0.62467337
O 1.54142022 1.23209488 0.08122860
H 0.91289634 -5.33299637 -4.14768934
H 1.43062556 -6.16259050 -2.67001486
H -0.23434776 -5.60470104 -2.82637668
H 0.50657701 5.42076492 -1.07514107
H 1.13790178 3.85482931 -0.50719827
H -0.57415044 4.03547668 -0.91166234

Isomer VI



PBE/L1 theoretical level

E= -10635.459626

G= 264.0618 kcal/mol, H= 340.8097 kcal/mol, U= 340.2172 kcal/mol, S= 257.4137 cal/mol at T= 298.150 K

H	-4.60975075	3.42492580	-0.87970799
H	-3.74720287	-2.83993769	-3.44441271
N	-1.55314028	1.22242796	0.06020555
N	-0.12734939	4.04511499	1.71326125
N	-1.25327611	-1.29113483	-0.90187186
N	0.90055633	-4.03788996	-1.36439800
O	-0.06364904	1.83495581	2.17856908
O	0.20414659	-3.02605605	0.54887253
C	-1.66844857	2.45665169	0.54961008
C	-2.77269244	3.27927589	0.23654655
H	-2.88616967	4.26094151	0.69405609
C	-3.73842740	2.81105137	-0.63562369
C	-3.60462594	1.53013062	-1.20919991
C	-4.54329634	0.97557110	-2.13817954
H	-5.40536022	1.58011627	-2.43331432
C	-4.37250757	-0.28093025	-2.64732122
H	-5.09528303	-0.69417775	-3.35626101

C -3.25399208 -1.08834147 -2.26146245
C -3.03645325 -2.39863181 -2.74023795
C -1.93684387 -3.11696267 -2.30571008
H -1.75936222 -4.13699484 -2.65163851
C -1.06303918 -2.52219844 -1.37280869
C -2.30513406 -0.57389295 -1.33376276
C -2.47478390 0.76506537 -0.80581385
C -0.56262118 2.78270555 1.53964365
C 0.07769487 -3.23038840 -0.67502838
C -0.55381733 5.26984978 1.00591719
H -1.53119171 5.61542606 1.38904798
C 0.52603281 6.29428530 1.37427878
H 1.38083529 6.21205378 0.68514496
H 0.14003327 7.32306576 1.32612181
C 0.92742914 5.85751009 2.79055738
H 0.15707707 6.17012167 3.51572251
H 1.89370608 6.27062988 3.11374855
C 0.97705656 4.32295799 2.68863535
C 2.33149981 3.79680037 2.20492768
H 0.71417695 3.82970190 3.63838077
C 2.10128427 -4.59236383 -0.65644091
C 1.75240779 -5.79405403 0.21580201
H 2.48875356 -3.78048968 -0.01503039
C 3.07754517 -4.89558220 -1.80826187
C 2.64073229 -3.95176196 -2.93660498
C 1.11239374 -3.99535155 -2.82515478
H 2.99358320 -4.26273584 -3.93114805
H 2.98108864 -2.92299557 -2.73451352
H 4.11956263 -4.73654604 -1.49368989
H 0.62538463 -3.11282468 -3.26282001
La 0.41533017 -0.50699419 1.21536040

N -1.61605883 -1.23770201 3.28515267
O -0.35309747 -1.19921398 3.55219269
O -1.94192529 -0.94038463 2.05469036
O -2.45657706 -1.52791953 4.11555195
N 3.06574512 -0.86606562 2.54737663
O 2.47128916 0.29005885 2.46064186
O 2.41550565 -1.86106932 2.03115129
O 4.15456390 -0.99633616 3.07343531
N 1.90059662 0.32292944 -1.30671906
O 2.44898558 0.65012240 -2.34669232
O 1.79654562 -0.92185664 -0.94843531
O 1.38156521 1.18675566 -0.49646649
H 0.70604682 -4.90748072 -3.30031061
H 2.97018814 -5.94839573 -2.12479973
H 2.66944957 -6.17382288 0.69415790
H 1.31011307 -6.60595942 -0.38457435
H 1.05213916 -5.50357914 1.01260829
H -0.63658226 5.09269810 -0.07719749
H 2.33129144 2.70219493 2.11505556
H 3.09969473 4.06979322 2.94622636
H 2.61062837 4.23313427 1.23296118

PBE0/L1 theoretical level

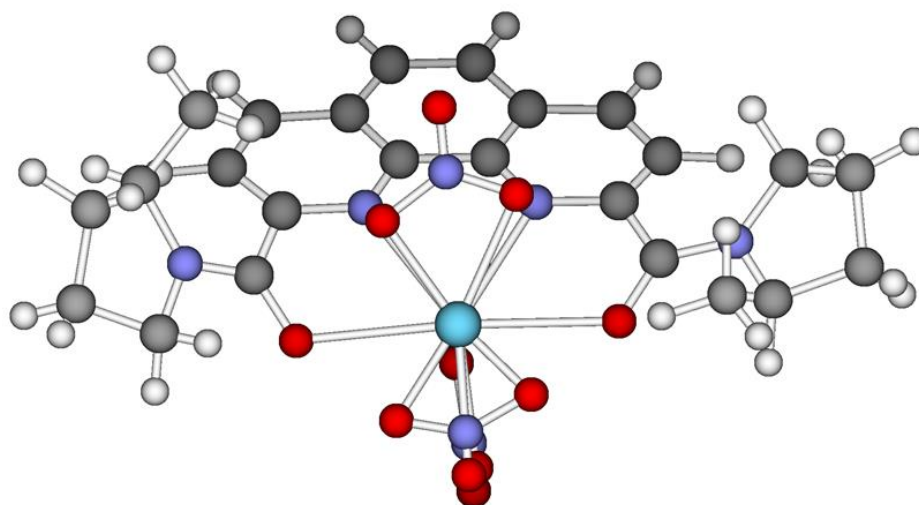
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N -0.13228488 4.00185490 1.70891786
N -1.24734497 -1.28145957 -0.88759202
N 0.90562904 -3.98581100 -1.35291135
O -0.07433111 1.81387532 2.17124677
O 0.21077564 -2.99027109 0.54125661

C -1.66925979 2.42880940 0.56413972
C -2.76354599 3.24864602 0.25519410
H -2.87643576 4.22082901 0.71267945
C -3.71753287 2.78615236 -0.61605930
C -3.57981181 1.51619840 -1.18916619
C -4.50918579 0.96795082 -2.12326550
H -5.36363602 1.56853855 -2.41800451
C -4.33380413 -0.27249011 -2.63388371
H -5.04485464 -0.68039310 -3.34506893
C -3.21973658 -1.07590640 -2.24574065
C -2.99811244 -2.37368226 -2.72801280
C -1.90837646 -3.08652139 -2.29342985
H -1.72544289 -4.09643078 -2.64018464
C -1.05187166 -2.49543858 -1.35791624
C -2.28901052 -0.56991976 -1.31827235
C -2.46334720 0.75853717 -0.78779382
C -0.56503880 2.75423002 1.54367328
C 0.08773321 -3.19563007 -0.66761875
C -0.54956043 5.21042156 0.99391824
H -1.51276159 5.56876707 1.37575400
C 0.53323448 6.22400904 1.34221387
H 1.37730777 6.12805748 0.65433145
H 0.15779528 7.24782944 1.28498006
C 0.93706566 5.80161524 2.75096250
H 0.17752661 6.12378788 3.47132730
H 1.90156782 6.20719767 3.06208444
C 0.97342581 4.27672815 2.66140699
C 2.31046081 3.74613166 2.16773367
H 0.72323596 3.79756379 3.61213541
C 2.09557104 -4.53551960 -0.65349030
C 1.74761569 -5.71851826 0.22727980

H 2.49641228 -3.72733116 -0.03075256
C 3.05222535 -4.86053514 -1.80099964
C 2.62762570 -3.91909909 -2.92158294
C 1.10954285 -3.93818235 -2.80249739
H 2.96804285 -4.23523664 -3.91010332
H 2.98396373 -2.90343833 -2.72453427
H 4.09213591 -4.72294426 -1.49710977
H 0.64182138 -3.05117130 -3.23211050
La 0.40285420 -0.51064080 1.23210454
N -1.63873243 -1.22957003 3.26481080
O -0.40204504 -1.20399296 3.53852820
O -1.94504881 -0.93759012 2.05795312
O -2.47506547 -1.50595212 4.07744598
N 3.04557586 -0.85989523 2.53540969
O 2.46615672 0.27326068 2.44773936
O 2.40622330 -1.83771360 2.03769135
O 4.12042141 -0.98750716 3.04893899
N 1.86216915 0.31895891 -1.28013003
O 2.39218974 0.64332628 -2.30906272
O 1.76631665 -0.90139234 -0.93097210
O 1.35762656 1.16469419 -0.48288935
H 0.69052172 -4.83367729 -3.27852893
H 2.92153192 -5.90428448 -2.11120105
H 2.65999770 -6.10378170 0.69195265
H 1.29121554 -6.52235889 -0.35926673
H 1.06516457 -5.41774654 1.02487910
H -0.63701725 5.02507114 -0.07925421
H 2.30413365 2.65963674 2.07942295
H 3.08384275 4.01457500 2.89353871
H 2.57777786 4.17658329 1.19851041

Isomer VII



PBE/L1 theoretical level

E= -10635.455567

G= 264.1066 kcal/mol, H= 340.6949 kcal/mol, U= 340.1024 kcal/mol, S= 256.8782 cal/mol at T= 298.150 K

N	-1.52543831	1.14852083	0.22032121
N	-0.24159265	3.96432066	1.96291697
N	-1.11107743	-1.35040343	-0.74850994
N	1.12208879	-4.07947063	-1.27253056
O	-0.36893517	1.78504789	2.55832624
O	0.67370898	-2.83482766	0.56111115
C	-1.70158744	2.37319565	0.71214110
C	-2.81332445	3.17111850	0.37213725
H	-2.93802810	4.15946627	0.81787986
C	-3.75272202	2.66586018	-0.50731659
C	-3.57977915	1.37621295	-1.05475175
C	-4.50923538	0.77522713	-1.96356535
H	-5.39232540	1.34707952	-2.26174808
C	-4.30695438	-0.48740748	-2.44460487
H	-5.02617550	-0.94008005	-3.13275838
C	-3.15791917	-1.24929380	-2.05727506
C	-2.91337824	-2.56607151	-2.49758077

C -1.77219284 -3.22888446 -2.08500719
H -1.59285927 -4.25331879 -2.40827370
C -0.87313193 -2.57636499 -1.21361482
C -2.20537615 -0.68676549 -1.16175640
C -2.42383313 0.65138233 -0.64895743
C -0.70323771 2.71398687 1.79410088
C 0.37078637 -3.19128227 -0.59465235
C -0.21410929 5.10199451 0.98974806
H -1.18577242 5.63046265 1.03376436
C 0.87742192 6.01499701 1.58933377
H 1.85342455 5.72191381 1.16570461
H 0.69488907 7.07047796 1.33761621
C 0.85229248 5.72013092 3.09139299
H 0.00525498 6.23378849 3.57674551
H 1.77763021 6.01945353 3.60490656
C 0.64616370 4.20692587 3.12499380
C 2.35129428 -4.65550995 -0.63641649
C 2.69708991 -5.80167818 -1.60354066
C 2.28233051 -5.24590826 -2.97359133
C 0.94986689 -4.55476189 -2.66057134
H 2.16412354 -6.02161741 -3.74437547
H 3.01832318 -4.51001358 -3.33293056
H 2.10352540 -6.70000792 -1.36343157
H 3.76294160 -6.06567621 -1.54850948
La 0.48272747 -0.41458520 1.44188380
N -1.48557663 -1.75027430 3.25793982
O -0.23108444 -1.67094553 3.55216932
O -1.83484685 -1.20191908 2.12362671
O -2.29874015 -2.29762292 3.97891259
N 3.05698800 -0.44736558 2.95153475
O 2.14717364 0.44881970 3.16497731

O 2.75778103 -1.33731818 2.04691482
O 4.11752319 -0.46193704 3.54676032
N 1.88828373 0.98912764 -0.85792363
O 2.37402391 1.57580578 -1.81223190
O 1.66627359 -0.28420162 -0.86768657
O 1.55317318 1.61241400 0.23133363
H 0.13212891 -5.29608870 -2.71593761
C 0.11066614 4.69804621 -0.44932726
H -4.63714361 3.24854660 -0.77864408
H -3.63310313 -3.05818057 -3.15748239
H 0.16938637 3.82864428 4.04107523
H 2.06867242 -5.02077723 0.36430031
C 3.47711635 -3.62699890 -0.49817619
H 0.34876060 5.60672522 -1.02505445
H -0.72697943 4.19587040 -0.95363081
H 0.97871256 4.01929712 -0.46922415
H 1.58971620 3.64847255 2.98954606
H 3.19702053 -2.80922318 0.17937513
H 3.75634789 -3.19971085 -1.47413099
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PBE0/L1 theoretical level

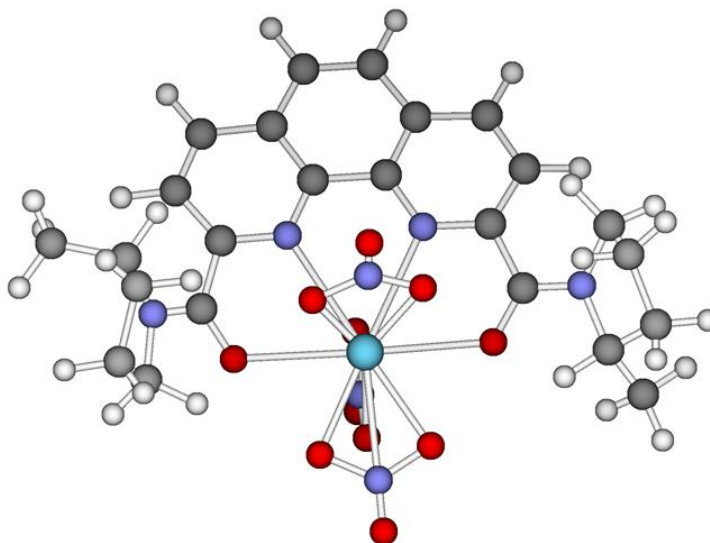
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N 1.10941792 -4.03881598 -1.25134015
O -0.36997882 1.76410758 2.53904843
O 0.65799689 -2.81127548 0.56506747
C -1.69178128 2.34696937 0.71306437
C -2.79148102 3.14476323 0.37711030

H -2.91300178 4.12415457 0.82310361
C -3.72123790 2.64684534 -0.50003010
C -3.54927468 1.36612463 -1.04412138
C -4.47451496 0.77078307 -1.95288503
H -5.34765053 1.34154665 -2.25222063
C -4.27682257 -0.48050436 -2.42699289
H -4.98903656 -0.92870468 -3.11222696
C -3.13559818 -1.24194551 -2.03497648
C -2.89572811 -2.55087161 -2.47010994
C -1.76664901 -3.21124411 -2.05593586
H -1.58869958 -4.22846985 -2.37385058
C -0.87821412 -2.56048203 -1.18891132
C -2.19524479 -0.68665594 -1.14617229
C -2.40949893 0.64531887 -0.63876826
C -0.69215631 2.68475270 1.78399456
C 0.36347657 -3.16703916 -0.57736379
C -0.20351930 5.03907681 0.96880370
H -1.16858530 5.56084156 1.01550186
C 0.88012367 5.95418549 1.55217481
H 1.84702837 5.67026711 1.12225103
H 0.68852377 7.00091982 1.30521083
C 0.87367660 5.65957975 3.04433846
H 0.03326019 6.16207790 3.53496337
H 1.79560745 5.96281385 3.54460597
C 0.67875141 4.15476894 3.07610297
C 2.33620214 -4.59695578 -0.62811130
C 2.69176006 -5.72551203 -1.59499574
C 2.27166057 -5.16785669 -2.95100331
C 0.94048375 -4.49922609 -2.63172984
H 2.16163039 -5.93335915 -3.72194862
H 2.99334145 -4.42615795 -3.30294132

H 2.11076951 -6.62455797 -1.36296141
H 3.75262499 -5.97737122 -1.54304135
La 0.46323460 -0.42529601 1.46014380
N -1.52338946 -1.76296651 3.22017574
O -0.29707047 -1.69319999 3.52825975
O -1.84964073 -1.20689857 2.11543417
O -2.33357072 -2.31390166 3.91069818
N 3.02694273 -0.43975404 2.94699192
O 2.11664343 0.41132414 3.18526793
O 2.75466228 -1.29083538 2.03517270
O 4.07299614 -0.44677562 3.53109169
N 1.86060524 0.97545010 -0.81789935
O 2.34339094 1.55864084 -1.75225782
O 1.62674582 -0.26882476 -0.84366745
O 1.54285443 1.57910013 0.25647777
H 0.14034371 -5.24625587 -2.69208527
C 0.11629130 4.63773680 -0.46189347
H -4.59610271 3.23047757 -0.76847988
H -3.60850739 -3.03857994 -3.12735605
H 0.22088869 3.77542925 3.99132538
H 2.06806111 -4.96842813 0.36500481
C 3.44316888 -3.56266379 -0.49588475
H 0.33330566 5.54242659 -1.03756940
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H 0.99110001 3.98136401 -0.48371875
H 1.61715782 3.60871577 2.92530298
H 3.15749764 -2.75103426 0.17332134
H 3.71239543 -3.13915110 -1.46758652
H 4.32664585 -4.04746389 -0.06989642
H 0.70416379 -3.66786671 -3.29997396

Isomer VIII



PBE/L1 theoretical level

E= -10635.459331

G= 263.5031 kcal/mol, H= 340.8417 kcal/mol, U= 340.2492 kcal/mol, S= 259.3948 cal/mol at T= 298.150 K

N	-1.61653864	1.09944475	0.18705942
N	-0.20395324	3.84218860	1.85224628
N	-1.14963889	-1.36029112	-0.79625589
N	1.18891776	-3.96145153	-1.26414514
O	-0.51574028	1.70876813	2.55768132
O	0.44943237	-2.96675730	0.63703656
7C	-1.79437196	2.32481003	0.67642695
C	-2.87608171	3.13938284	0.28156129
H	-3.01452613	4.12466574	0.72836852
C	-3.77391815	2.65489125	-0.65397793
C	-3.58537841	1.37112117	-1.21057677
C	-4.45023632	0.78951085	-2.19418359
H	-5.31165886	1.36776555	-2.53975224
C	-4.21075773	-0.45951566	-2.69699359
H	-4.87842083	-0.88929367	-3.44886875
C	-3.08675218	-1.23208916	-2.25732327
C	-2.78112268	-2.52423143	-2.73833370

C -1.66283989 -3.18855071 -2.26512551
H -1.41690230 -4.19088793 -2.62041259
C -0.86132944 -2.56275535 -1.28696871
C -2.21445608 -0.69307464 -1.27202570
C -2.46637559 0.62969720 -0.74203259
C -0.79219043 2.63538575 1.76949346
C 0.32067052 -3.19289160 -0.58259887
C -0.14478569 4.86538982 0.77734274
C -0.93830913 6.12689972 1.13470328
C 1.37244630 5.11352015 0.68675065
H 1.83177638 4.27962589 0.13115239
H 1.60933340 6.06091404 0.17959274
C 1.82344949 5.07763910 2.15759897
H 1.65258110 6.04986525 2.64637804
H 2.89156675 4.83529902 2.25803471
C 0.94803756 3.97892594 2.78571057
C 2.41233110 -4.45255470 -0.54841572
C 3.39242649 -4.75350380 -1.69738877
C 2.91885924 -3.85655260 -2.84858346
C 1.39319623 -3.94546175 -2.72628927
H 3.27535582 -4.18515015 -3.83621216
H 3.23362279 -2.81330466 -2.68145180
H 3.31730175 -5.81703186 -1.98567355
H 4.43092585 -4.55380535 -1.39486265
La 0.32638082 -0.51062894 1.47453094
N -1.75095987 -1.70298398 3.25583863
O -0.51251805 -1.61408973 3.61370349
O -2.02858520 -1.23481834 2.06727242
O -2.60919428 -2.18813705 3.96763921
N 2.87509823 -0.61727703 3.02686024
O 2.05081081 0.38425925 3.10992432

O 2.50336194 -1.57574749 2.23155975
O 3.92147708 -0.65291154 3.64553428
N 1.90386808 0.76553696 -0.80310780
O 2.49400783 1.28231645 -1.73851943
O 1.73244762 -0.51489919 -0.71823913
O 1.40515709 1.46841300 0.16667609
H 1.01716340 -4.88173294 -3.17897582
H -4.63199615 3.25764465 -0.96406013
H -3.43319726 -2.99243689 -3.48089242
H 0.59188038 4.22532654 3.79839826
C 2.11372662 -5.64274549 0.35794494
H 1.45939982 3.00412107 2.84127212
H 0.87440526 -3.09094214 -3.18223619
H -0.52953595 4.42185974 -0.15407695
H -0.53808373 6.60851860 2.03988266
H -2.00083733 5.90527582 1.31846488
H -0.87829548 6.84924126 0.30515000
H 1.40651572 -5.35864735 1.15059114
H 3.04710841 -5.97428989 0.84042633
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H 2.77398920 -3.61065149 0.06887393

PBE0/L1 theoretical level

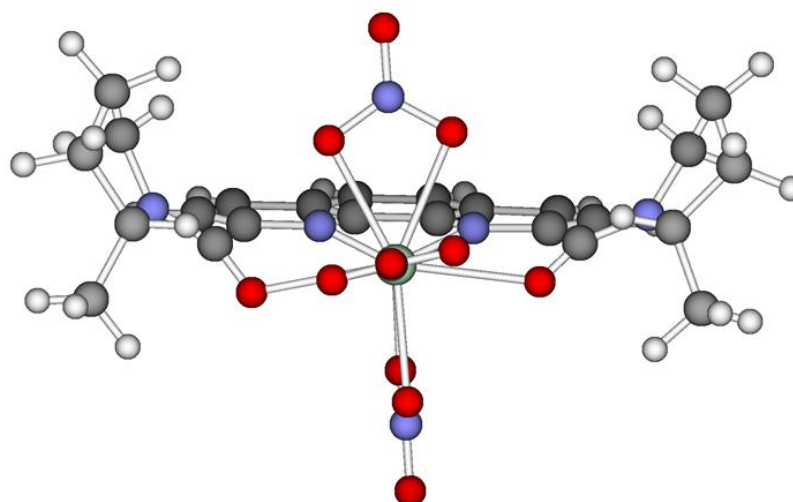
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N 1.18353891 -3.91335344 -1.24354410
O -0.49633521 1.68354368 2.52220082
O 0.42973459 -2.94818664 0.63918984
C -1.78242409 2.29724050 0.67344856
C -2.84732509 3.11507201 0.27630463

H -2.98015070 4.09426022 0.71715444
C -3.73552489 2.63794732 -0.65640688
C -3.55166769 1.36102128 -1.20558739
C -4.41027164 0.78610718 -2.19110799
H -5.26061678 1.36380267 -2.53892446
C -4.17446661 -0.45115092 -2.68789458
H -4.83363342 -0.87563533 -3.43829155
C -3.05956912 -1.22406304 -2.24238610
C -2.75611925 -2.50698566 -2.72124267
C -1.65081370 -3.16910648 -2.24570417
H -1.40306330 -4.16322184 -2.59761524
C -0.86376393 -2.54709458 -1.26834941
C -2.20286679 -0.69411314 -1.26035917
C -2.45217514 0.62154204 -0.73393244
C -0.77614725 2.60530448 1.75275028
C 0.31355056 -3.17023802 -0.56739223
C -0.15123530 4.81921959 0.77495408
C -0.93434620 6.06839514 1.15431690
C 1.35222948 5.07644701 0.66594374
H 1.80786896 4.25936747 0.09859999
H 1.57351983 6.02513218 0.17127675
C 1.81987512 5.02751112 2.12012196
H 1.65359724 5.98727131 2.61710238
H 2.88209534 4.78934145 2.20467520
C 0.96141225 3.92713237 2.74464202
C 2.39566731 -4.39569187 -0.53277624
C 3.36786914 -4.69888830 -1.67328405
C 2.90239263 -3.80112672 -2.81313872
C 1.38651586 -3.88519740 -2.69341779
H 3.25720406 -4.12239504 -3.79492807
H 3.21737337 -2.76736474 -2.63967204

H 3.28379703 -5.75304937 -1.96319818
H 4.40044403 -4.50981474 -1.37240815
La 0.31529498 -0.52466363 1.48092771
N -1.76989043 -1.68302202 3.23937321
O -0.55785209 -1.59965718 3.60125518
O -2.03022718 -1.23294461 2.07092166
O -2.62214327 -2.15166521 3.93852305
N 2.87118053 -0.62682974 2.98326230
O 2.07654428 0.36524355 3.05891991
O 2.48671985 -1.57752240 2.22899103
O 3.91111612 -0.66077566 3.57707977
N 1.85853779 0.72669929 -0.80638641
O 2.42299271 1.22866166 -1.74190068
O 1.70741069 -0.52906984 -0.70505553
O 1.37164927 1.42448354 0.13734557
H 1.01082373 -4.80828953 -3.15245795
H -4.58145475 3.24145722 -0.96978205
H -3.39856768 -2.96938229 -3.46382356
H 0.62142229 4.16205740 3.75648618
C 2.10149145 -5.57820320 0.36835754
H 1.47682476 2.96351647 2.78268003
H 0.87843013 -3.03010297 -3.14120102
H -0.54269636 4.39064837 -0.15086778
H -0.51836979 6.53796816 2.04933929
H -1.98509455 5.84776497 1.35885584
H -0.89117825 6.79339981 0.33650830
H 1.40570652 -5.29618645 1.16099691
H 3.03051925 -5.91368675 0.83853930
H 1.68266773 -6.41135311 -0.20507649
H 2.75874019 -3.55980492 0.07657798

L3*Nd(NO₃)₃ (Meso)



PBE/L1 theoretical level

E= -11766.855900

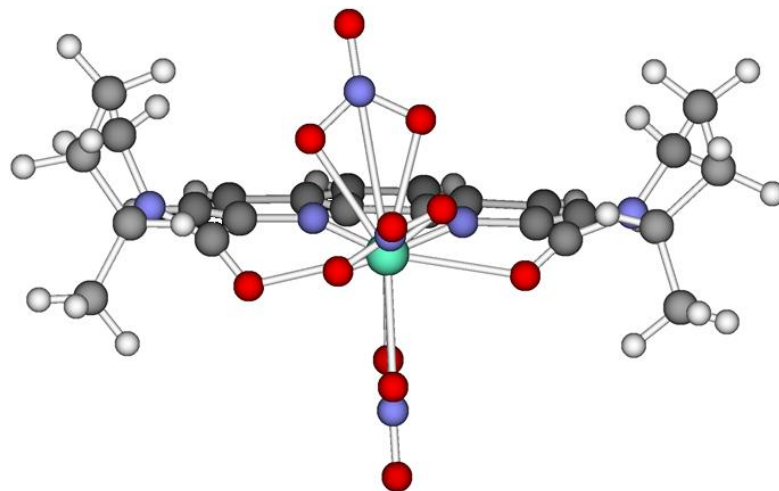
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N	-0.20141669	3.96346784	1.77016890
N	-1.18472338	-1.24086237	-0.93707585
N	1.04003239	-3.96734071	-1.45969784
O	-0.40968055	1.78396976	2.37951994
O	0.56689137	-2.73173261	0.38010094
C	-1.73910403	2.44219112	0.55134076
C	-2.82036495	3.27305818	0.19235241
H	-2.92710590	4.26080894	0.64453882
C	-3.75712085	2.80002809	-0.71101052
C	-3.60691166	1.51077414	-1.26676917
C	-4.52153540	0.93128198	-2.20565605
H	-5.38863611	1.51856315	-2.52038670
C	-4.32390451	-0.32819960	-2.70124483
H	-5.03176498	-0.75748801	-3.41571832
C	-3.19339085	-1.11297345	-2.30203128
C	-2.93416309	-2.42073369	-2.76681733

C -1.80149055 -3.09053850 -2.33714271
H -1.59623563 -4.10641098 -2.67789626
C -0.93369687 -2.45439243 -1.42340553
C -2.26589775 -0.57106048 -1.37067664
C -2.47735929 0.75737715 -0.84437370
C -0.72590482 2.73308015 1.63527977
C 0.28903139 -3.07280374 -0.78579026
C -0.16490267 5.00028276 0.72024781
H -0.83443063 5.84030628 0.98291475
C 1.30306149 5.44198608 0.74167728
H 1.90714443 4.69946146 0.19489077
H 1.44602871 6.43208218 0.28376287
C 1.63365436 5.40617132 2.23982739
H 1.23772907 6.30720377 2.74115872
H 2.71367502 5.34955263 2.44045234
C 0.90673560 4.15336323 2.76299763
C 0.38745376 4.27011299 4.19267941
C 2.28521585 -4.48140955 -0.80187166
C 1.98572648 -5.52012920 0.27521539
C 3.11149573 -5.01452017 -1.98626721
C 2.60828972 -4.21377182 -3.19374704
C 1.10095096 -4.12645197 -2.92598295
H 2.83004618 -4.69021034 -4.16037560
H 3.03772497 -3.19850111 -3.19062233
H 2.90705347 -6.09010220 -2.13075471
H 4.18957663 -4.89289856 -1.80604124
Nd 0.39027581 -0.31915566 1.13822198
N -1.43629241 -1.61334682 3.00256658
O -0.16762102 -1.49677622 3.22709870
O -1.84395790 -1.11117184 1.87219703
O -2.19668818 -2.15123343 3.78359056

N	2.98352122	-0.31665757	2.47167587
O	2.06005049	0.54574573	2.75531483
O	2.65549564	-1.18659866	1.56193304
O	4.07372761	-0.31478170	3.00957799
N	1.77323413	1.01120877	-1.12515223
O	2.33042288	1.57779443	-2.05015182
O	1.47747636	-0.24458034	-1.15410352
O	1.42989028	1.63868284	-0.03899303
H	0.59500653	-5.05898476	-3.23828888
H	0.62525910	-3.27375960	-3.42996264
H	-0.47375655	4.58289289	-0.24823157
H	2.93384957	-5.88405704	0.70236993
H	1.44042015	-6.37984180	-0.14719982
H	1.39522290	-5.07590914	1.08919847
H	-0.11776112	3.34176993	4.49652576
H	-0.30904216	5.11848259	4.29418135
H	1.23674309	4.43264008	4.87548876
H	1.55174637	3.25971627	2.68561530
H	2.77781105	-3.60935807	-0.33516786
H	-4.61748743	3.41289520	-0.99358672
H	-3.63193989	-2.89683485	-3.46103048

L3*Eu(NO₃)₃(Meso)



PBE/L1 theoretical level

E= -12987.853791

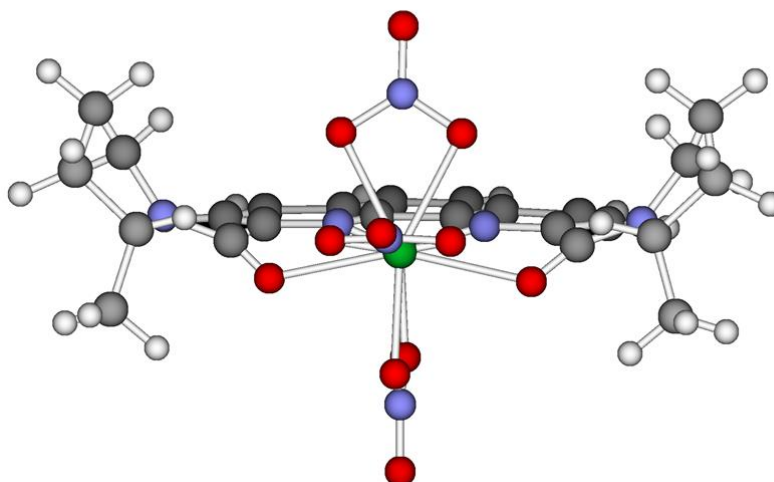
G= 264.8589 kcal/mol, H= 340.6332 kcal/mol, U= 340.0407 kcal/mol, S= 254.1483 cal/mol at T= 298.150 K

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N	-0.22671875	3.95122385	1.82265162
N	-1.16499746	-1.25603747	-0.95030785
N	1.03220212	-4.01877737	-1.41410971
O	-0.39743641	1.74781418	2.36789346
O	0.57837981	-2.72153473	0.38940278
C	-1.71544063	2.43342495	0.54027927
C	-2.80397034	3.25876427	0.18768373
H	-2.92580271	4.23644829	0.65771848
C	-3.72589874	2.79491568	-0.73496765
C	-3.56494451	1.51316929	-1.30613863
C	-4.47250795	0.93797266	-2.25459957
H	-5.33712578	1.52678585	-2.57341790
C	-4.27405500	-0.32082412	-2.75155234
H	-4.97784376	-0.74722832	-3.47170472
C	-3.15201449	-1.11119044	-2.33962202
C	-2.90306973	-2.42604280	-2.79009652
C	-1.78530514	-3.10807109	-2.34172583
H	-1.59219277	-4.12985802	-2.67126656
C	-0.92049456	-2.47554302	-1.42216563
C	-2.22862840	-0.57169765	-1.40276730
C	-2.43500447	0.76145107	-0.88361341
C	-0.71825612	2.71008039	1.64624405
C	0.29420757	-3.09433961	-0.76554638
C	-0.17127328	4.99759722	0.78197938
H	-0.84729415	5.83426666	1.03880799
C	1.29541981	5.44099283	0.83221179
H	1.90804887	4.70268774	0.28957385

H 1.44433498 6.43562508 0.38600680
C 1.59915972 5.39223289 2.33553028
H 1.19024432 6.28618813 2.83939528
H 2.67564583 5.33734941 2.55491972
C 0.86829859 4.13054800 2.83055472
C 0.33027360 4.22230864 4.25512981
C 2.26743722 -4.53768063 -0.74071503
C 1.94697523 -5.53088522 0.37276044
C 3.07718945 -5.13315678 -1.90637004
C 2.59325051 -4.36196899 -3.14032817
C 1.08900726 -4.22634649 -2.87497711
H 2.80045414 -4.87775373 -4.08983517
H 3.05069399 -3.35955453 -3.17427397
H 2.84366655 -6.20710850 -2.01278400
H 4.15851831 -5.03542233 -1.73155189
Eu 0.39535463 -0.29785982 1.03077829
N -1.39629388 -1.52928364 2.96400118
O -0.12845263 -1.37986791 3.16220784
O -1.84092677 -1.05907393 1.84269404
O -2.12408686 -2.07448959 3.77517438
N 3.12358046 -0.27755356 2.04343414
O 2.16456866 0.33317879 2.64729023
O 2.78151417 -0.91287446 0.96512973
O 4.27303314 -0.26296905 2.44891119
N 1.64197505 1.34701741 -1.09244287
O 2.16019249 2.00845361 -1.97973263
O 1.20670068 0.14658076 -1.29634237
O 1.47948682 1.80317605 0.10483665
H 0.55980611 -5.15560102 -3.15689468
H 0.63460964 -3.37898397 -3.40683007
H -0.46065593 4.58846855 -0.19602460

H 2.88772511 -5.90228891 0.80978352
 H 1.38095593 -6.39189196 -0.01846838
 H 1.36883223 -5.04586792 1.17215943
 H -0.17805423 3.28832221 4.53602076
 H -0.36975524 5.06731415 4.36055708
 H 1.16897750 4.37521362 4.95315313
 H 1.51784170 3.24107718 2.74511361
 H 2.78268623 -3.66100144 -0.30842978
 H -4.58763599 3.40677214 -1.01569963
 H -3.59980798 -2.89968133 -3.48704386

L3*Lu(NO₃)₃(Meso)



PBE/L1 theoretical level

E= -16710.257714

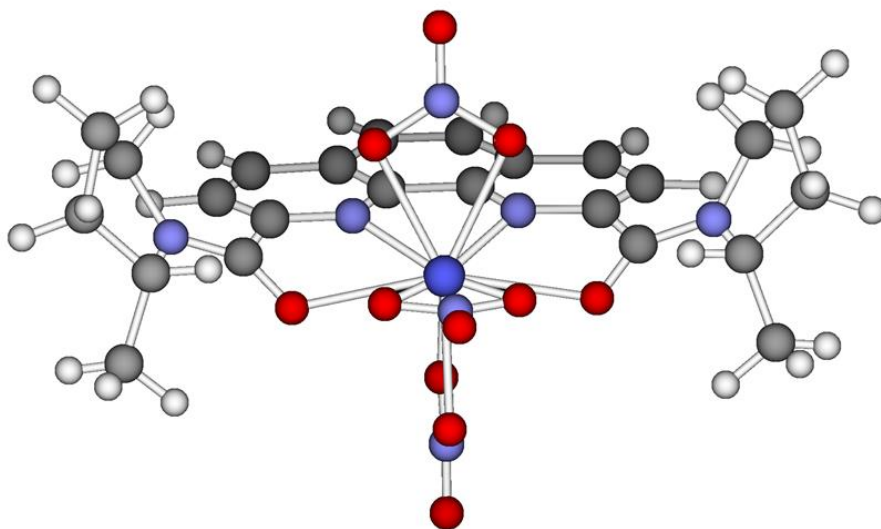
G= 267.7178 kcal/mol, H= 340.7519 kcal/mol, U= 340.1595 kcal/mol, S= 244.9576 cal/mol at T= 298.150 K

N -1.52900803 1.23280442 -0.06202852
 N -0.20515759 3.94277668 1.81466091
 N -1.16152298 -1.20228744 -1.03566515
 N 0.99819416 -4.00261450 -1.36763263
 O -0.17026410 1.69748259 2.11715984
 O 0.49261481 -2.64562798 0.37488514
 C -1.67259789 2.44327378 0.46987668

C -2.77012420 3.27361488 0.15476784
H -2.88347054 4.24742222 0.63400376
C -3.72087097 2.82036471 -0.74513108
C -3.57590985 1.54615319 -1.33599257
C -4.50005102 0.97121084 -2.26940656
H -5.37199736 1.55847442 -2.57060242
C -4.31062460 -0.28798237 -2.77191496
H -5.03045750 -0.71292061 -3.47700667
C -3.18062234 -1.08095586 -2.38450956
C -2.93603539 -2.39927959 -2.82722473
C -1.81463695 -3.07831955 -2.37935781
H -1.62818897 -4.10607195 -2.69467044
C -0.93667060 -2.43546844 -1.47993696
C -2.23864818 -0.53528631 -1.47213387
C -2.43862629 0.79204464 -0.94192952
C -0.62033677 2.69668579 1.52371001
C 0.25087696 -3.05181599 -0.77825749
C -0.31964454 5.12247801 0.93582922
H -1.08048081 5.82466030 1.32465780
C 1.08143020 5.74064541 1.01839948
H 1.76134014 5.18766022 0.34993717
H 1.08317935 6.80227327 0.72946024
C 1.46102035 5.50429678 2.48586416
H 0.97026581 6.25333405 3.13221812
H 2.54494715 5.55651188 2.66397476
C 0.91266179 4.10117483 2.80279231
C 0.44249636 3.91840100 4.24282598
C 2.21921158 -4.48945045 -0.64435327
C 1.87612462 -5.45565987 0.48559606
C 3.06919098 -5.10448408 -1.77096641
C 2.60607505 -4.37720442 -3.03980279

C 1.09333181 -4.25635672 -2.81799197
H 2.84652948 -4.91664314 -3.96810126
H 3.04680562 -3.36812115 -3.08905864
H 2.85809135 -6.18543959 -1.85237122
H 4.14338589 -4.97994328 -1.57108951
Lu 0.48461962 -0.28044760 0.88542473
N -1.05808425 -1.34096527 2.93731570
O 0.22144499 -1.18224084 3.02583790
O -1.56913984 -0.95964777 1.79867995
O -1.73550892 -1.80454826 3.83207536
N 3.08592796 -0.31610638 1.96479499
O 2.28230381 0.69326627 2.09227920
O 2.59005594 -1.30018198 1.28106022
O 4.20395756 -0.33809385 2.44259739
N 1.68020463 0.83582175 -1.43820274
O 2.16759920 1.31581819 -2.44571209
O 1.54619908 -0.44110733 -1.26389337
O 1.24947572 1.56061232 -0.45398054
H 0.58283204 -5.20122004 -3.08203769
H 0.64263785 -3.43145728 -3.38702965
H -0.59466821 4.82132578 -0.08451932
H 2.80785894 -5.80818462 0.95603806
H 1.32450938 -6.33062029 0.10449168
H 1.27740204 -4.95066690 1.25709534
H 0.07239864 2.89536071 4.40132523
H -0.35086283 4.64092970 4.49502039
H 1.29237580 4.08102560 4.92472124
H 1.65558624 3.31864405 2.56417346
H 2.70841122 -3.59505057 -0.21781346
H -4.58934689 3.43715882 -0.99209863
H -3.64001536 -2.88123441 -3.51112700

L3*Am(NO₃)₃(Meso)



PBE/L1 theoretical level

E= -32560.361975

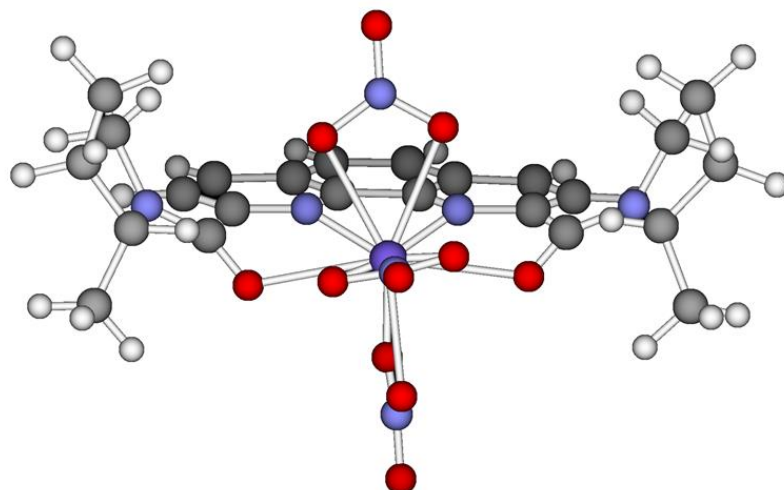
G= 265.2212 kcal/mol, H= 339.8748 kcal/mol, U= 339.2823 kcal/mol, S= 250.3893 cal/mol at T= 298.150 K

N	-1.50517559	1.23180234	-0.01343706
N	-0.21432635	4.01528168	1.79458916
N	-1.13221514	-1.22579300	-0.99850303
N	1.00664461	-4.04042864	-1.43326199
O	-0.16198023	1.77996254	2.18456388
O	0.52673113	-2.74678850	0.36872768
C	-1.65786946	2.45666456	0.50315952
C	-2.75598812	3.27716589	0.17419483
H	-2.87010932	4.25460005	0.64521313
C	-3.70367169	2.81234217	-0.72106493
C	-3.55327201	1.53136384	-1.29721463
C	-4.47662449	0.95928711	-2.22819042
H	-5.34805918	1.54791129	-2.52783298
C	-4.28586960	-0.29985526	-2.73241162
H	-5.00355434	-0.72645986	-3.43852878
C	-3.15631819	-1.08833683	-2.34642577
C	-2.91393661	-2.40094805	-2.80877209

C -1.79196262 -3.08486509 -2.37396646
H -1.60334039 -4.10763884 -2.70348763
C -0.91225886 -2.45980406 -1.46691978
C -2.21524405 -0.54808378 -1.42619169
C -2.41612792 0.77649891 -0.89547420
C -0.62003750 2.75338912 1.54853106
C 0.26921448 -3.10601902 -0.80026847
C -0.31503901 5.15418291 0.86156106
H -1.09113812 5.86679697 1.19791901
C 1.07790875 5.78899431 0.95207244
H 1.78000104 5.21495819 0.32544798
H 1.07838440 6.83728743 0.61794251
C 1.42092669 5.61934280 2.43752551
H 0.90343434 6.38792419 3.03846598
H 2.49879384 5.69313955 2.64304924
C 0.87954628 4.22397995 2.79767418
C 0.38184384 4.09207010 4.23414087
C 2.21528482 -4.58231211 -0.73186117
C 1.85191131 -5.58928680 0.35557276
C 3.05446172 -5.16465855 -1.88359201
C 2.61452484 -4.36585999 -3.11700749
C 1.10407710 -4.22278309 -2.89449477
H 2.84789109 -4.86442709 -4.06965971
H 3.07839227 -3.36588979 -3.11525869
H 2.81510162 -6.23449230 -2.01702476
H 4.13074923 -5.07858133 -1.67460907
Am 0.44856462 -0.30668056 0.93636358
N -1.21221805 -1.41175592 3.06263375
O 0.06633497 -1.26747751 3.18728065
O -1.70321798 -1.02643728 1.91593301
O -1.91447997 -1.87128699 3.94220352

N	3.08378959	-0.40358686	2.17799711
O	2.30042315	0.62494683	2.26786184
O	2.60407257	-1.37541389	1.46739066
O	4.17353249	-0.45208767	2.71260858
N	1.85561514	0.83815408	-1.38521492
O	2.40147161	1.31389952	-2.36476254
O	1.69416976	-0.43887201	-1.22866261
O	1.38782239	1.57108414	-0.42323652
H	0.57492143	-5.14180326	-3.20863700
H	0.67224479	-3.36102915	-3.42239237
H	-0.56244522	4.80515623	-0.15075457
H	2.77520919	-5.97951746	0.81273609
H	1.28539550	-6.43626070	-0.06470953
H	1.25880086	-5.10809088	1.14639604
H	0.01538830	3.07322788	4.42497969
H	-0.42259264	4.81666994	4.44095039
H	1.21539712	4.28891373	4.92711878
H	1.63796711	3.44369960	2.60574245
H	2.72550011	-3.71900892	-0.26788452
H	-4.57322407	3.42280936	-0.97850710
H	-3.62014818	-2.87088609	-3.49832582

L3*Cm(NO₃)₃(Meso)



PBE/L1 theoretical level

E= -33396.683543

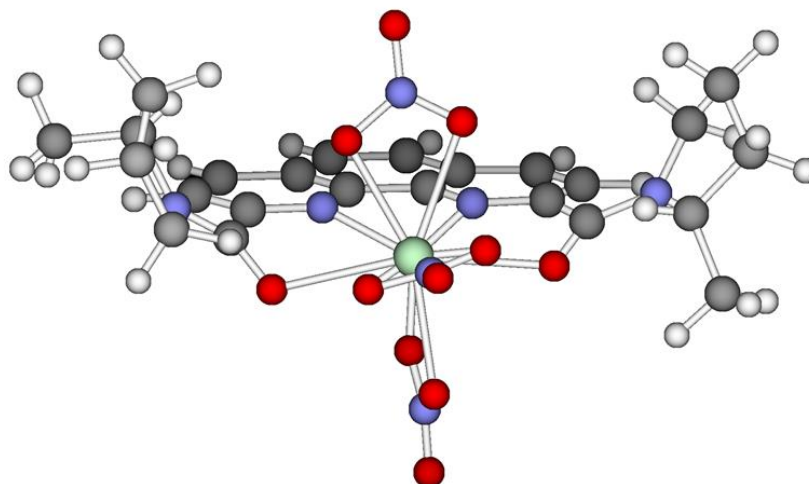
G= 263.9354 kcal/mol, H= 340.8541 kcal/mol, U= 340.2616 kcal/mol, S= 257.9866 cal/mol at T= 298.150 K

N	-1.58312285	1.22081554	0.01465227
N	-0.20209092	3.95349169	1.76634324
N	-1.20225906	-1.23916781	-0.96173429
N	1.02319050	-3.96209240	-1.43747020
O	-0.37699977	1.75802755	2.32258344
O	0.50683773	-2.73348522	0.39555559
C	-1.73470569	2.44094396	0.52613705
C	-2.81822228	3.27349162	0.17607743
H	-2.92609429	4.25757647	0.63607883
C	-3.75570297	2.80827212	-0.73057926
C	-3.60895205	1.52162302	-1.29441833
C	-4.52502823	0.94507587	-2.23406053
H	-5.39157629	1.53405440	-2.54724503
C	-4.33217669	-0.31522658	-2.73079658
H	-5.04342794	-0.74128789	-3.44385958
C	-3.20571661	-1.10560203	-2.33059645
C	-2.95212674	-2.41760564	-2.78776932
C	-1.82718861	-3.09456396	-2.34799790
H	-1.62825096	-4.11435652	-2.68155313
C	-0.95926744	-2.45883727	-1.43390763
C	-2.27659774	-0.56544244	-1.40052676
C	-2.48084188	0.76532710	-0.87525970
C	-0.71329987	2.72144318	1.60395372
C	0.25413412	-3.07578754	-0.77718318
C	-0.18251981	5.01470566	0.74026483
H	-0.85975617	5.84089518	1.02575994
C	1.28049660	5.47237682	0.76393467
H	1.88998735	4.75107002	0.19535242

H 1.40892994 6.47509575 0.32968804
C 1.62133884 5.40374756 2.25850606
H 1.21784568 6.28711081 2.78462267
H 2.70323467 5.35523033 2.45040154
C 0.91343707 4.12934685 2.75444841
C 0.40566841 4.20225716 4.19108200
C 2.26716614 -4.45972013 -0.76291382
C 1.96722829 -5.50450373 0.30794287
C 3.11722016 -4.97804260 -1.93716359
C 2.61656547 -4.18481636 -3.15090942
C 1.10467613 -4.12219763 -2.90268564
H 2.85834956 -4.65756750 -4.11454725
H 3.02900743 -3.16263175 -3.14186907
H 2.93328619 -6.05693531 -2.08456707
H 4.19052267 -4.83754730 -1.74305427
Cm 0.39113945 -0.32683438 1.11255634
N -1.36240220 -1.60392368 3.04369044
O -0.08868438 -1.48588479 3.23289204
O -1.80379927 -1.09531951 1.92503071
O -2.10146570 -2.14666080 3.84133577
N 3.00550795 -0.35362127 2.40551353
O 2.11350799 0.54762381 2.67094064
O 2.64001083 -1.23706257 1.52218938
O 4.09995317 -0.37469324 2.93511152
N 1.77116287 0.99210757 -1.15495706
O 2.31064916 1.54757202 -2.09706426
O 1.51057494 -0.27462515 -1.15043998
O 1.41170204 1.63651967 -0.08566717
H 0.61796188 -5.06382608 -3.21794748
H 0.62054259 -3.27823734 -3.41323209
H -0.49141777 4.61562300 -0.23584858

H 2.91480827 -5.85823727 0.74462712
H 1.43687093 -6.36971283 -0.12229043
H 1.36339068 -5.06855965 1.11663902
H -0.08132909 3.25867677 4.47696924
H -0.30346754 5.03640604 4.31942081
H 1.25880635 4.36205339 4.86961269
H 1.56804001 3.24561620 2.64697433
H 2.74030948 -3.58138180 -0.28786606
H -4.61561680 3.42478228 -1.00646818
H -3.64996815 -2.89296055 -3.48244214

L3*Nd(NO₃)₃(Rac)



PBE/L1 theoretical level

E= -11766.853441

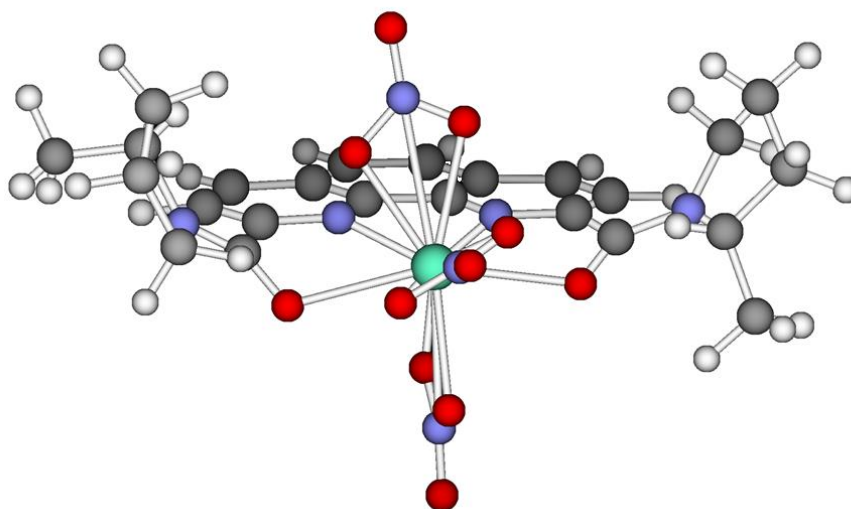
G = 264.5005kcal/mol, H= 340.7808 kcal/mol, U= 340.1883 kcal/mol, S= 255.8453 cal/mol at T= 298.150 K

N -1.57285821 1.12428236 0.14687414
N -0.25127152 3.84852672 1.93044662
N -1.09249854 -1.32844484 -0.82657534
N 1.19480944 -4.02085781 -1.25593543
O -0.54741788 1.68270445 2.54501104
O 0.62383294 -2.79375601 0.56154239
C -1.77402675 2.34155250 0.65181094

C -2.85675931 3.15012431 0.25017565
H -3.00887680 4.12943554 0.70547885
C -3.74055123 2.66697454 -0.69996309
C -3.54040432 1.38593888 -1.25749040
C -4.40120125 0.79650247 -2.23994827
H -5.26384783 1.37029743 -2.58987665
C -4.15884638 -0.45592749 -2.73315406
H -4.82586288 -0.89326262 -3.48127007
C -3.03447747 -1.22318053 -2.28574562
C -2.73360467 -2.52442265 -2.74331069
C -1.61237025 -3.17935085 -2.26362109
H -1.37624943 -4.19038630 -2.59878159
C -0.79924130 -2.53512502 -1.30662978
C -2.16040444 -0.67125654 -1.30931056
C -2.41706944 0.65151602 -0.78823245
C -0.81074607 2.63360333 1.78232777
C 0.40226981 -3.13722825 -0.61593074
C -0.16872983 4.90462685 0.88984525
C -0.99188322 6.14436197 1.25633585
C 1.34703934 5.17570972 0.85802794
H 1.83676445 4.36800671 0.29023412
H 1.58575273 6.14354467 0.39191452
C 1.75042188 5.09657288 2.34101748
H 1.55448115 6.05110788 2.85469937
H 2.81717467 4.86096287 2.46835232
C 0.86719376 3.97006869 2.90607524
C 2.41523099 -4.52070999 -0.54267144
C 3.30146527 -5.04142523 -1.68867040
C 2.84398746 -4.24466276 -2.91669202
C 1.32509756 -4.17706585 -2.71805072
H 3.11504889 -4.71612358 -3.87302637

H 3.26027465 -3.22416854 -2.89299631
H 3.11717987 -6.11926937 -1.84338737
H 4.36861372 -4.90672970 -1.45922315
Nd 0.35462490 -0.39634359 1.32699835
N -1.54173315 -1.75252450 3.07310653
O -0.28706732 -1.62242460 3.36108255
O -1.90198588 -1.23251820 1.93473542
O -2.33022261 -2.31788659 3.80502439
N 2.89482331 -0.34360284 2.76012993
O 1.92220855 0.46208459 3.04719496
O 2.63807964 -1.18924809 1.80583251
O 3.96612859 -0.31271279 3.33373022
N 1.83671391 0.99610245 -0.83817095
O 2.43939734 1.58962739 -1.71699345
O 1.52948689 -0.25291216 -0.92401809
O 1.45210421 1.59005415 0.25368050
H 0.84638137 -5.11600447 -3.05345106
H -4.59974146 3.26558423 -1.01484096
H -3.39113355 -3.00782061 -3.47093773
H 0.47382963 4.18362904 3.91244388
C 2.07963967 -5.56525087 0.51797658
H 1.38591564 2.99848461 2.94983840
H 0.86125386 -3.33022523 -3.24257207
H -0.51497245 4.48475266 -0.06738418
H -0.62897581 6.60434008 2.18821692
H -2.05668306 5.90310860 1.39812899
H -0.91498858 6.89190006 0.45086354
H 1.44750917 -5.13003016 1.30515897
H 3.01176715 -5.91860533 0.98723477
H 1.56484210 -6.43076181 0.06987244
H 2.87535834 -3.64386368 -0.05255690

L3*Eu(NO₃)₃(Rac)



PBE/L1 theoretical level

E= -12987.850930

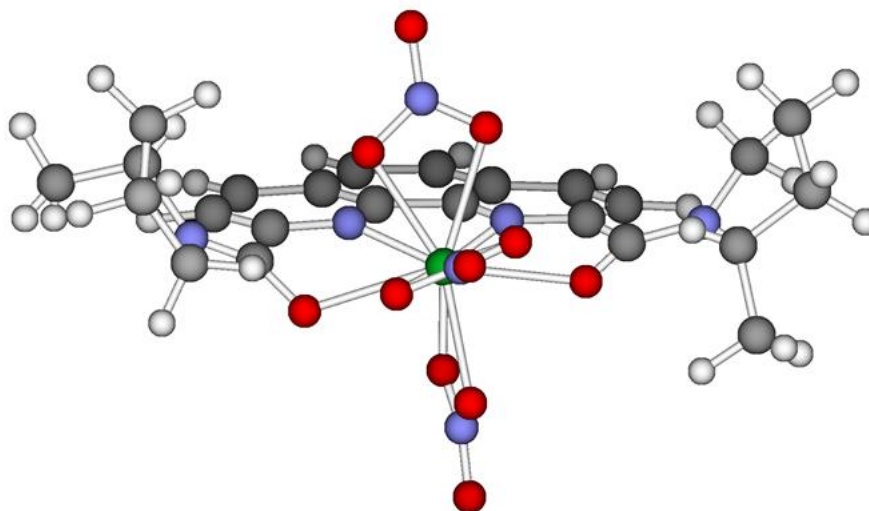
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N	-0.27230766	3.83455324	1.97394013
N	-1.07777357	-1.35203326	-0.84026361
N	1.18349433	-4.07384062	-1.21160281
O	-0.51781541	1.64168954	2.52051663
O	0.60642838	-2.81090474	0.58121562
C	-1.74540210	2.32758737	0.63617206
C	-2.83458877	3.13224816	0.24100050
H	-2.99977589	4.10189629	0.71215475
C	-3.70497084	2.65938830	-0.72587299
C	-3.49572015	1.38584280	-1.29819858
C	-4.34901094	0.80342627	-2.29145455
H	-5.20708942	1.38110137	-2.64627647
C	-4.10719156	-0.44810584	-2.78701901
H	-4.76888657	-0.88031495	-3.54272270
C	-2.99412036	-1.22397161	-2.32628584
C	-2.70447564	-2.53180504	-2.77277112

C -1.60064733 -3.20171189 -2.27439070
H -1.37598288 -4.21791935 -2.60136223
C -0.79317439 -2.56479120 -1.30730057
C -2.12523961 -0.67751127 -1.34224772
C -2.37385798 0.65070075 -0.82782948
C -0.79486573 2.60635662 1.78393149
C 0.39370182 -3.17263722 -0.59263504
C -0.19070198 4.90989876 0.95279086
C -1.03354836 6.13255835 1.33191156
C 1.32156634 5.20135832 0.93969840
H 1.82670188 4.41159725 0.36073685
H 1.55075788 6.18194103 0.49588451
C 1.71268249 5.09797668 2.42433572
H 1.50048280 6.03944016 2.95552254
H 2.78088927 4.87191057 2.55645370
C 0.83767313 3.95021486 2.95878601
C 2.39205909 -4.57604885 -0.47954103
C 3.27825546 -5.13375616 -1.60790610
C 2.84110379 -4.35727167 -2.85615396
C 1.32213366 -4.26082706 -2.66967773
H 3.11108565 -4.85458469 -3.79972911
H 3.27480078 -3.34379005 -2.85281873
H 3.07941532 -6.21182203 -1.74088120
H 4.34565592 -5.00930882 -1.37421954
Eu 0.36301607 -0.39408752 1.22265577
N -1.52215910 -1.63932598 3.05373883
O -0.26468509 -1.49906445 3.31338239
O -1.90929687 -1.16133428 1.91431153
O -2.29158330 -2.18413639 3.82555223
N 3.03404307 -0.34818009 2.37862253
O 2.03726864 0.24895726 2.93352938

O 2.75567746 -0.98598826 1.28383672
O 4.16098642 -0.31887245 2.84212279
N 1.71729195 1.26252913 -0.82662618
O 2.27689934 1.93364739 -1.68148947
O 1.29703856 0.06307696 -1.06077838
O 1.49417341 1.70927835 0.36451265
H 0.83068484 -5.19826937 -2.99011040
H -4.56427574 3.25825405 -1.04004407
H -3.35927320 -3.00968814 -3.50651717
H 0.43642724 4.13784695 3.96728325
C 2.03425622 -5.59425783 0.59940833
H 1.36698818 2.98394918 2.98339510
H 0.87604082 -3.41738939 -3.21457815
H -0.52099818 4.50350714 -0.01584273
H -0.68630701 6.57983398 2.27592373
H -2.09676433 5.87582302 1.45829523
H -0.95752198 6.89573956 0.54110926
H 1.39990342 -5.13595295 1.37152445
H 2.95778871 -5.94955635 1.08392620
H 1.51296270 -6.46249962 0.16449706
H 2.86190557 -3.69510579 -0.00612915

L3*Lu(NO₃)₃(Rac)



PBE/L1 theoretical level

E= -16710.256112

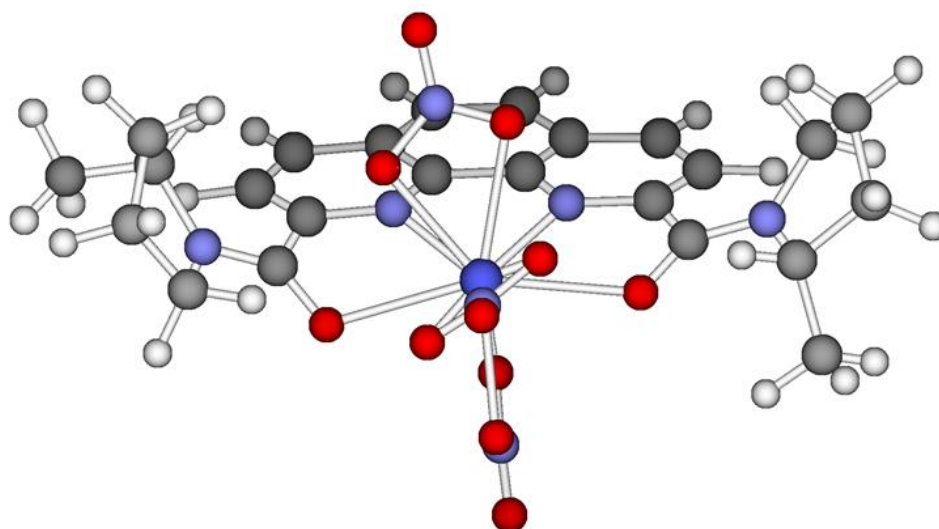
G= 267.4511 kcal/mol, H= 341.4316 kcal/mol, U= 340.8391 kcal/mol, S= 248.1315 cal/mol at T= 298.150 K

N	-1.49200165	1.13996017	0.01671871
N	-0.27305549	3.80064201	2.00467181
N	-1.04434383	-1.29854906	-0.93858236
N	1.16522574	-4.09238195	-1.19414937
O	-0.43722361	1.56839883	2.37008452
O	0.72716248	-2.59367275	0.44104120
C	-1.70062804	2.34087968	0.55671990
C	-2.78688002	3.15326667	0.17075728
H	-2.94906878	4.11880159	0.65054446
C	-3.66579223	2.69251466	-0.79540235
C	-3.46769881	1.42077851	-1.37374079
C	-4.33257771	0.83433604	-2.35558343
H	-5.19292212	1.41222548	-2.70448947
C	-4.10338020	-0.42321739	-2.84426594
H	-4.77898216	-0.85743147	-3.58647537
C	-2.98777246	-1.20127821	-2.39214993
C	-2.70618010	-2.51907420	-2.81439710
C	-1.59586287	-3.17983508	-2.31525612
H	-1.38517952	-4.20569038	-2.61925220
C	-0.76548278	-2.51974463	-1.38221860
C	-2.10305095	-0.64380980	-1.43094647
C	-2.34330416	0.68289733	-0.91591185
C	-0.75323224	2.57925272	1.71163547
C	0.44012681	-3.08524656	-0.66733718
C	-0.24880520	4.97247458	1.09383178
C	-1.15759861	6.10515022	1.58490193
C	1.24576986	5.34352684	1.12200451
H	1.79474139	4.64220095	0.47291508

H 1.42451358 6.37231398 0.77446896
C 1.63812876 5.11782598 2.59255672
H 1.36961210 5.98979807 3.20973897
H 2.71717882 4.94228983 2.71160626
C 0.83095086 3.87410975 3.00312567
C 2.37448192 -4.56046963 -0.44002819
C 3.17952251 -5.32008314 -1.50938225
C 2.73961449 -4.69162607 -2.83707070
C 1.23741317 -4.47203875 -2.61837053
H 2.94009757 -5.32782412 -3.71207929
H 3.23386383 -3.71784520 -2.98677206
H 2.91093898 -6.39083672 -1.48739612
H 4.26091242 -5.23527479 -1.32875705
Lu 0.44666222 -0.28712597 1.06040633
N -1.10866022 -1.67550039 2.90677691
O 0.15801086 -1.47611427 3.06135058
O -1.60463715 -1.16381514 1.81315720
O -1.78948903 -2.28802061 3.70474362
N 3.00374413 -0.12584303 2.22756457
O 2.02193379 0.59801841 2.64743137
O 2.69270205 -0.92436057 1.24516177
O 4.12401915 -0.07339477 2.69778538
N 1.68838692 1.17190707 -1.04253244
O 2.22176981 1.81162262 -1.93113732
O 1.36099958 -0.06991974 -1.16723931
O 1.39401639 1.69470203 0.11171533
H 0.67765355 -5.40824652 -2.80146289
H -4.52380800 3.29864311 -1.09887409
H -3.37177920 -3.01384521 -3.52686095
H 0.41875377 3.93568587 4.02252245
C 2.00847292 -5.39870596 0.78163862

H	1.41407430	2.94075990	2.93258381
H	0.82617319	-3.67656279	-3.25510097
H	-0.55288875	4.64458084	0.08765560
H	-0.84119976	6.47165585	2.57330847
H	-2.20546818	5.77823782	1.67206228
H	-1.11878085	6.94724703	0.87581444
H	1.44729733	-4.79804802	1.51157939
H	2.93194485	-5.75015593	1.26898742
H	1.41087186	-6.27816629	0.49118504
H	2.90999269	-3.65294909	-0.10753231

L3*Am(NO₃)₃(Rac)



PBE/L1 theoretical level

E= -32560.362122

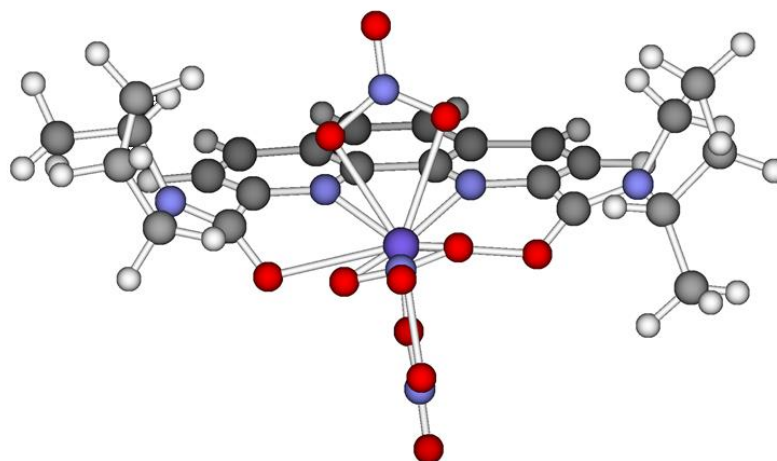
G= 265.3455 kcal/mol, H= 340.4623 kcal/mol, U= 339.8698 kcal/mol, S= 251.9427 cal/mol at T= 298.150 K

N	-1.48201978	1.14206326	0.06658279
N	-0.29000026	3.85108972	2.01131654
N	-1.01460683	-1.32805300	-0.88907653
N	1.17371678	-4.14431715	-1.21489358
O	-0.43055981	1.62611222	2.43724680
O	0.74575651	-2.70329499	0.48158064
C	-1.70643985	2.34820843	0.60414547

C -2.79486156 3.14815569 0.20240709
H -2.97150636 4.11287069 0.67897373
C -3.65511036 2.67955828 -0.77529299
C -3.44035053 1.40634716 -1.35137856
C -4.28897095 0.82422668 -2.34381437
H -5.14706373 1.40033305 -2.70083213
C -4.04827785 -0.43336824 -2.83339310
H -4.71160316 -0.86903703 -3.58559060
C -2.94131827 -1.20768201 -2.36789346
C -2.66117668 -2.52485919 -2.79907227
C -1.56273007 -3.19597292 -2.29546475
H -1.35466051 -4.22049475 -2.60533428
C -0.73765379 -2.55435133 -1.34547257
C -2.06735444 -0.65675914 -1.38826203
C -2.31893706 0.67075223 -0.87642151
C -0.76541173 2.61678100 1.75045323
C 0.45084095 -3.15215445 -0.65056390
C -0.26053187 4.99192142 1.06120801
C -1.16940522 6.14277172 1.50743496
C 1.23348701 5.36573124 1.08276403
H 1.78731847 4.64440203 0.46032816
H 1.41229248 6.38325691 0.70360577
C 1.61790967 5.18883657 2.56179380
H 1.33877289 6.07706547 3.15048313
H 2.69719458 5.02455902 2.69453406
C 0.81449062 3.95400453 3.00429153
C 2.36689234 -4.66327906 -0.47104847
C 3.17918968 -5.37646627 -1.56653118
C 2.76915574 -4.67026186 -2.86418509
C 1.26630259 -4.44627523 -2.65712810
H 2.97782016 -5.25943279 -3.76965904

H 3.27694798 -3.69576144 -2.95169163
H 2.89498687 -6.44274521 -1.60726297
H 4.25856304 -5.31792164 -1.36435270
Am 0.42316610 -0.33880350 1.11028814
N -1.36702609 -1.63823116 3.00719738
O -0.11103614 -1.41055691 3.23793983
O -1.78873241 -1.22738242 1.85017014
O -2.09163117 -2.19233513 3.80951071
N 3.12555885 -0.22935781 2.18434000
O 2.10681057 0.30614981 2.77888870
O 2.83880544 -0.85079974 1.08033121
O 4.25703764 -0.15519339 2.62065005
N 1.73038173 1.37079418 -0.92748755
O 2.27581716 2.04492831 -1.78365338
O 1.27823400 0.17877544 -1.16858506
O 1.54496741 1.79186821 0.28054726
H 0.70070344 -5.36487818 -2.90107536
H -4.51363039 3.27756310 -1.09238100
H -3.32329941 -3.00818896 -3.52234244
H 0.40669560 4.03655243 4.02413988
C 1.97515368 -5.55896711 0.70104128
H 1.40215886 3.02299786 2.95398378
H 0.87089521 -3.61303115 -3.25461674
H -0.56137097 4.62863445 0.06619097
H -0.84698933 6.55323362 2.47660112
H -2.21676350 5.82166290 1.61702418
H -1.13562393 6.95315647 0.76197147
H 1.40160346 -4.99411440 1.44976604
H 2.88705325 -5.94075823 1.18742502
H 1.37827587 -6.41875505 0.35581270
H 2.91169739 -3.78152347 -0.08821142

L3*Cm(NO₃)₃(Rac)



PBE/L1 theoretical level

E= -33396.680655

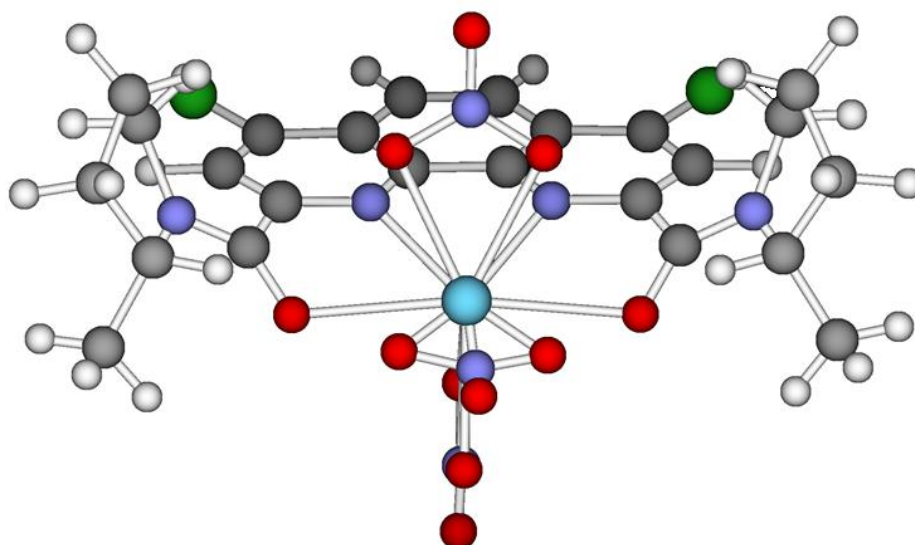
G= 264.5588 kcal/mol, H= 340.8870 kcal/mol, U= 340.2945 kcal/mol, S= 256.0059 cal/mol at T= 298.150 K

N	-1.56563902	1.13039362	0.11047891
N	-0.25685772	3.83911896	1.93473995
N	-1.09185684	-1.31893134	-0.86447597
N	1.18202853	-4.02675867	-1.24558449
O	-0.52418363	1.65639901	2.49694848
O	0.60245454	-2.77223659	0.54904389
C	-1.76855958	2.34221387	0.62737221
C	-2.85417128	3.15109992	0.23278280
H	-3.00979543	4.12593985	0.69651628
C	-3.73569608	2.67488599	-0.72273618
C	-3.53417373	1.39798617	-1.29021084
C	-4.39417410	0.81167537	-2.27552366
H	-5.25685310	1.38642061	-2.62384772
C	-4.15389776	-0.44054106	-2.77117538
H	-4.82271719	-0.87553900	-3.51901865
C	-3.03229046	-1.21154606	-2.32302713
C	-2.73625898	-2.51676679	-2.77336383

C -1.62164712 -3.17731833 -2.28563380
H -1.39307106 -4.19268894 -2.61302400
C -0.80595487 -2.53150058 -1.33136880
C -2.15641046 -0.66054702 -1.34821439
C -2.41046047 0.66266108 -0.82439363
C -0.80316073 2.62298512 1.75783360
C 0.38874778 -3.13131928 -0.62637752
C -0.18926717 4.92070246 0.91940624
C -1.02702296 6.14105225 1.31645250
C 1.32304096 5.21081400 0.89176512
H 1.82121217 4.42253447 0.30447996
H 1.54899037 6.19218636 0.44808152
C 1.72997463 5.10155058 2.37176061
H 1.51952505 6.03979921 2.90908241
H 2.80025029 4.87924814 2.49222994
C 0.86559343 3.94715309 2.90826535
C 2.39581919 -4.52094221 -0.51603371
C 3.28139067 -5.07397270 -1.64722073
C 2.83577967 -4.30035686 -2.89446783
C 1.31666470 -4.21404600 -2.70363379
H 3.10614157 -4.79644442 -3.83858919
H 3.26196218 -3.28379345 -2.89229584
H 3.08805227 -6.15326738 -1.77882349
H 4.34871960 -4.94340467 -1.41681671
Cm 0.37254778 -0.38671842 1.29007995
N -1.42949677 -1.76354802 3.10343885
O -0.16938362 -1.61615205 3.35374331
O -1.83476889 -1.23487687 1.98034739
O -2.18739033 -2.35008359 3.85067749
N 2.93112874 -0.34076628 2.69143438
O 1.98255563 0.49983957 2.96028709

O 2.64465451 -1.20440805 1.76080132
O 4.00643921 -0.32554388 3.25890732
N 1.83454621 1.02155352 -0.87414134
O 2.41243434 1.61434615 -1.76996863
O 1.56957424 -0.24151386 -0.93210077
O 1.43537152 1.62406003 0.20630457
H 0.83051962 -5.15527630 -3.02108598
H -4.59523916 3.27528024 -1.03316820
H -3.39430141 -3.00046134 -3.50034237
H 0.47436729 4.12551546 3.92218518
C 2.04795241 -5.53934622 0.56580573
H 1.39935505 2.98253131 2.92037463
H 0.86297166 -3.37379122 -3.24721336
H -0.53123093 4.51871252 -0.04694314
H -0.66846031 6.58279228 2.25873160
H -2.08866143 5.88367033 1.45384097
H -0.96030647 6.90860701 0.52912253
H 1.42191696 -5.08060074 1.34433353
H 2.97632480 -5.89382267 1.04141831
H 1.52293885 -6.40773916 0.13547508
H 2.86141205 -3.63715816 -0.04372763

L4*La(NO₃)₃ (Meso)



PBE/L1 theoretical level

E= -11557.266649

G= 248.7822 kcal/mol, H= 330.5046 kcal/mol, U= 329.9121 kcal/mol, S= 274.0981 cal/mol at T= 298.150 K

Cl -5.10346889 3.80653381 -1.07529879
Cl -4.05745983 -3.21315384 -3.88121367
N -1.61836505 1.16165257 0.09100277
N -0.13559902 3.94099236 1.67342746
N -1.25614023 -1.29521763 -0.88543433
N 1.03877211 -3.90124321 -1.44168806
O -0.32706460 1.78614986 2.36461353
O 0.33143547 -2.96634531 0.50536668
C -1.73376584 2.39658189 0.57011616
C -2.80093479 3.24726200 0.22558121
H -2.89156103 4.24313736 0.66029590
C -3.75871825 2.77917743 -0.65823573
C -3.65006471 1.48106861 -1.21956944
C -4.56895638 0.91228676 -2.15429401
H -5.42895222 1.50747514 -2.46561694
C -4.38178778 -0.34617731 -2.65650034
H -5.09096193 -0.76472396 -3.37250638
C -3.26056409 -1.14086187 -2.26531029
C -2.98204350 -2.44700885 -2.74366689
C -1.85573995 -3.12936664 -2.31517935
H -1.64718544 -4.13585424 -2.67945433
C -1.01099253 -2.50574517 -1.37811589
C -2.33058834 -0.61821127 -1.32266760
C -2.52821875 0.71657258 -0.79094189
C -0.67256516 2.71153092 1.60385084
C 0.18445268 -3.16030049 -0.71755821
C -0.13845389 4.94828272 0.59315526
H -0.80320710 5.79228306 0.85431254

C 1.32663441 5.39795685 0.55530190
H 1.91886353 4.64640045 0.00775934
H 1.44741344 6.37617254 0.06665414
C 1.70620430 5.40465164 2.04186797
H 1.32053506 6.31652927 2.53121400
H 2.79248977 5.36026287 2.20872903
C 1.00507557 4.16299057 2.62299800
C 0.53426093 4.31656504 4.06581259
C 2.28521252 -4.39881086 -0.77106428
C 2.02728796 -5.64236879 0.07402193
C 3.25554848 -4.61124372 -1.94818771
C 2.73111820 -3.68256211 -3.05155754
C 1.21203887 -3.82808352 -2.90660620
H 3.08011675 -3.95648408 -4.05823994
H 3.01049805 -2.63668108 -2.84322429
H 3.21637607 -5.66323948 -2.28204870
H 4.29029179 -4.38475227 -1.65192890
La 0.35907096 -0.48599595 1.30598402
N -1.67945862 -1.50758958 3.23172855
O -0.42494798 -1.44185281 3.53458714
O -1.98961377 -1.09833658 2.02887344
O -2.52334571 -1.91959476 4.00347996
N 2.97096872 -0.68830770 2.73160791
O 2.23200083 0.38052675 2.77903771
O 2.48446107 -1.66650581 2.02700520
O 4.04197216 -0.76551545 3.30158091
N 1.84627330 0.65224862 -1.09844863
O 2.39686346 1.10938537 -2.08672905
O 1.69689322 -0.62413657 -0.92233759
O 1.37023115 1.41048908 -0.16162519
H 0.85575283 -4.75995064 -3.38305378

H 0.65707856 -2.97546697 -3.32165408
H -0.47568288 4.50301456 -0.35303900
H 2.97531366 -5.97807550 0.52403229
H 1.62283528 -6.46304226 -0.54072565
H 1.32699656 -5.41750097 0.89179075
H 0.04326862 3.39632607 4.41407537
H -0.16128293 5.16560602 4.16732788
H 1.40624273 4.50050020 4.71362543
H 1.65318942 3.27144146 2.54713511
H 2.63365269 -3.58174801 -0.11423010

PBE0/L1 theoretical level

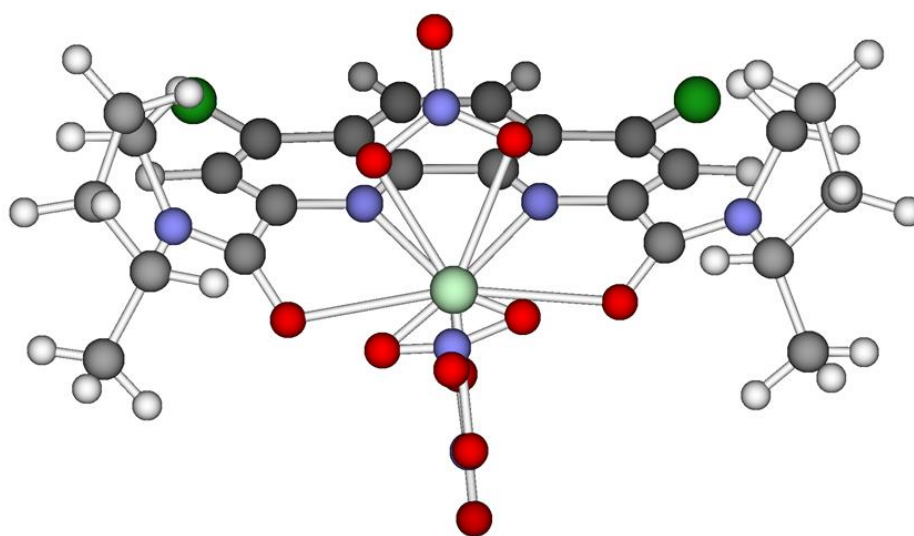
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O -0.32767507 1.77234685 2.35670996
O 0.38347220 -2.89955854 0.48319829
C -1.72869718 2.37349176 0.58582586
C -2.78933954 3.21796966 0.24792759
H -2.87905502 4.20599985 0.68043089
C -3.73909688 2.75141072 -0.62759829
C -3.62708640 1.46287227 -1.18417156
C -4.54396296 0.89458477 -2.11400461
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C -4.35505486 -0.35019490 -2.61272216
H -5.05966520 -0.76737374 -3.32147455
C -3.23256373 -1.13658345 -2.22566986
C -2.95252466 -2.43096638 -2.70398498
C -1.83006120 -3.10193253 -2.28430581
H -1.61850691 -4.09933853 -2.64723825

C -0.99246633 -2.47609878 -1.35745084
C -2.31324458 -0.61599463 -1.29476535
C -2.51441097 0.70924890 -0.76376480
C -0.66769636 2.68936849 1.60757554
C 0.21350965 -3.11348629 -0.71808624
C -0.14329205 4.89513493 0.58898264
H -0.81110919 5.72834444 0.84085780
C 1.30755210 5.35658979 0.55193621
H 1.90358627 4.61479712 0.01127202
H 1.41848600 6.32804251 0.06531326
C 1.68205988 5.36866570 2.02891636
H 1.28339922 6.26775074 2.51366663
H 2.76051474 5.34035540 2.19797611
C 1.00093389 4.12538385 2.60159254
C 0.54071116 4.26960039 4.03823709
C 2.28630662 -4.35126066 -0.79424298
C 2.02748370 -5.54015779 0.10915178
C 3.19999671 -4.64893675 -1.98347700
C 2.68519402 -3.73808789 -3.09129190
C 1.17635870 -3.81522202 -2.89971662
H 2.98998570 -4.05225134 -4.09190702
H 3.01337361 -2.70751357 -2.92385221
H 3.09634137 -5.69995832 -2.27820277
H 4.24687767 -4.46760845 -1.73127818
La 0.37541854 -0.46717015 1.31092751
N -1.64237666 -1.53370857 3.20108032
O -0.41250327 -1.46721351 3.50070906
O -1.94980860 -1.11082208 2.03316259
O -2.46916986 -1.96209860 3.95379639
N 2.99225926 -0.62168872 2.68965340
O 2.23767996 0.40085551 2.77351594

O 2.54056168 -1.57578039 1.97711456
O 4.05494928 -0.68003815 3.23860931
N 1.78827178 0.71183288 -1.09074354
O 2.29566526 1.18335140 -2.07274747
O 1.65049565 -0.54185832 -0.93966466
O 1.35090530 1.43741977 -0.14418611
H 0.77295280 -4.73223066 -3.34695220
H 0.65304017 -2.95309663 -3.31534600
H -0.46813133 4.44648838 -0.35072756
H 2.97547841 -5.88452053 0.53259641
H 1.57798612 -6.36604404 -0.45129222
H 1.37111664 -5.26205587 0.93608063
H 0.06571475 3.35035014 4.38653040
H -0.16006927 5.10411119 4.14200258
H 1.40738130 4.46385193 4.67677593
H 1.65526271 3.24978161 2.51805186
H 2.68318796 -3.52270746 -0.19610749
Cl -5.07467365 3.76615286 -1.04010439
Cl -4.01824808 -3.19424391 -3.82882071

L4*Nd(NO₃)₃(Meso)



PBE/L1 theoretical level

E= -12688.660431

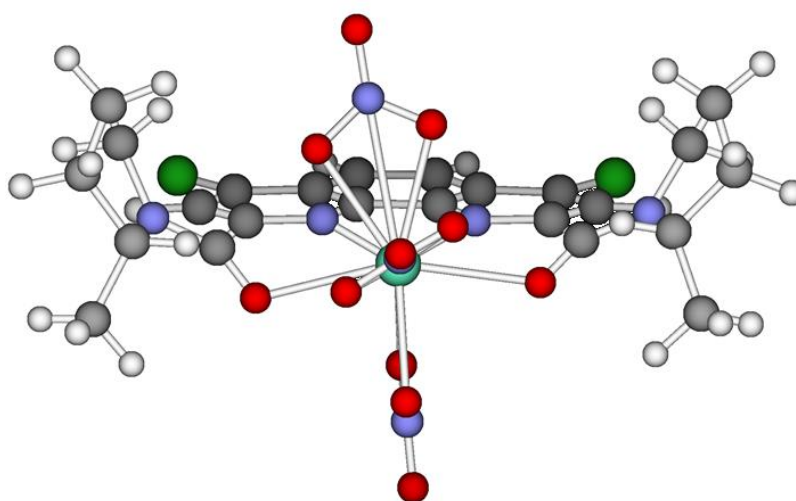
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Cl -3.99753070 -3.22403049 -3.85993290
N -1.57514548 1.20833290 0.05594091
N -0.18168329 3.95502234 1.76847088
N -1.17826247 -1.23493147 -0.92459422
N 1.05587018 -3.95576692 -1.45413613
O -0.40024456 1.77884889 2.39057326
O 0.57647502 -2.72956467 0.39152747
C -1.72448623 2.43185401 0.55947840
C -2.79803133 3.27077651 0.21050546
H -2.90884876 4.25879669 0.65828466
C -3.73822570 2.79966831 -0.69120145
C -3.60947132 1.50636053 -1.25776255
C -4.52162886 0.92628324 -2.19198370
H -5.38716841 1.51228726 -2.50531101
C -4.32403421 -0.33336863 -2.68747354
H -5.03067732 -0.76270473 -3.39959598
C -3.19600463 -1.11575615 -2.29236650
C -2.91385937 -2.42742634 -2.74999523
C -1.77753365 -3.09305310 -2.32192278
H -1.57569253 -4.10669422 -2.66758609
C -0.92060572 -2.44677067 -1.41072702
C -2.26436615 -0.57614112 -1.36059332
C -2.47654748 0.75548124 -0.83280414
C -0.70965743 2.72667122 1.64231932
C 0.30402330 -3.06657362 -0.77657479
C -0.14083590 4.98619604 0.71230644
H -0.81161737 5.82725000 0.96788156
C 1.32700121 5.42795658 0.73815739
H 1.93342400 4.68270016 0.19784805

H 1.47121739 6.41548967 0.27531931
C 1.65089190 5.40093374 2.23786163
H 1.25254059 6.30459213 2.73235798
H 2.73006368 5.34589911 2.44327426
C 0.92256492 4.15087652 2.76538038
C 0.39619353 4.27589607 4.19163847
C 2.29905009 -4.47617245 -0.79572469
C 1.99440026 -5.52031088 0.27448723
C 3.12728834 -5.00386286 -1.98104405
C 2.62899137 -4.19517088 -3.18517756
C 1.12098312 -4.10668039 -2.92166138
H 2.85208011 -4.66674280 -4.15380001
H 3.06031919 -3.18076682 -3.17558527
H 2.92142820 -6.07822037 -2.13189244
H 4.20505333 -4.88494253 -1.79735577
Nd 0.40091956 -0.32448241 1.15550983
N -1.43127477 -1.61593103 3.01388502
O -0.16291191 -1.50084436 3.24158168
O -1.83414888 -1.11307681 1.88111329
O -2.19486427 -2.15189838 3.79193234
N 2.98918390 -0.33061707 2.49381185
O 2.06786585 0.53729659 2.77081704
O 2.65926647 -1.20290089 1.58701682
O 4.07715750 -0.33076578 3.03483224
N 1.78284824 1.00528002 -1.10712516
O 2.34162021 1.57085097 -2.03096223
O 1.49173689 -0.25202182 -1.13284290
O 1.43231714 1.63448536 -0.02379660
H 0.61476648 -5.03692675 -3.23992801
H 0.64807338 -3.25054407 -3.42241096
H -0.44467950 4.56335115 -0.25536856

H 2.94106245 -5.88921356 0.70051908
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H -0.10945935 3.34928179 4.49993086
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H 1.24230039 4.44379473 4.87702560
H 1.56791770 3.25688267 2.69504166
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L4*Eu(NO₃)₃(Meso)



PBE/L1 theoretical level

E= -13909.657847

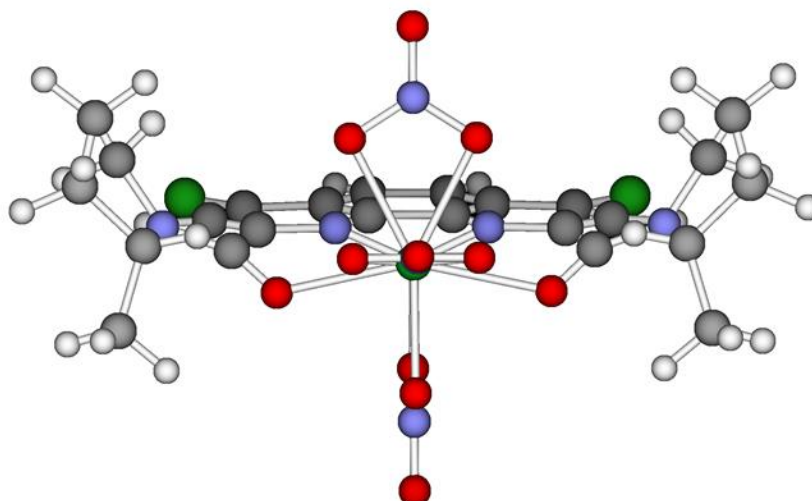
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N -0.19978689 3.93920660 1.81132805
N -1.17381179 -1.25938284 -0.92737991
N 1.04469287 -4.00064993 -1.40484512
O -0.39483953 1.74246144 2.37836528
O 0.56643730 -2.73370337 0.41504940
C -1.69984186 2.42147422 0.54212940

C -2.77612185 3.25913525 0.19513287
H -2.89529490 4.24061918 0.65503573
C -3.70375061 2.79739714 -0.72350198
C -3.57041144 1.50792027 -1.29929316
C -4.47682905 0.93291473 -2.24252534
H -5.33660460 1.52359056 -2.56298327
C -4.28283167 -0.32821217 -2.73552823
H -4.98572397 -0.75368077 -3.45357132
C -3.16700745 -1.11983514 -2.32388282
C -2.89732885 -2.44006562 -2.76526403
C -1.77697349 -3.11902237 -2.31704760
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C -2.23987460 -0.58427352 -1.38576794
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C -0.70154566 2.70191216 1.64764726
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C -0.13396733 4.97687531 0.76208925
H -0.81044632 5.81670046 1.00654018
C 1.33316720 5.41778183 0.82111597
H 1.94911444 4.67492294 0.28872183
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H 1.21370995 6.27791977 2.82105064
H 2.69968557 5.32509136 2.55520988
C 0.88861465 4.12313604 2.82624364
C 0.34075373 4.22640944 4.24623489
C 2.28595853 -4.51244020 -0.73558301
C 1.97681868 -5.52420998 0.36419076
C 3.10587192 -5.08138180 -1.90760064
C 2.60976100 -4.30567265 -3.13405585

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H 2.82383919 -4.80937958 -4.08839893
H 3.05214548 -3.29630971 -3.15873265
H 2.89225912 -6.15830612 -2.02534366
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Eu 0.39495873 -0.31353065 1.05940425
N -1.40605712 -1.53046584 2.99008107
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O 1.22781110 0.09284188 -1.26640832
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H 0.58717799 -5.12806892 -3.15718365
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H -0.35805827 5.07360792 4.34059668
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H 1.53674984 3.23165607 2.75128937
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L4*Lu(NO₃)₃(RS)



PBE/L1 theoretical level

E= -17632.062357

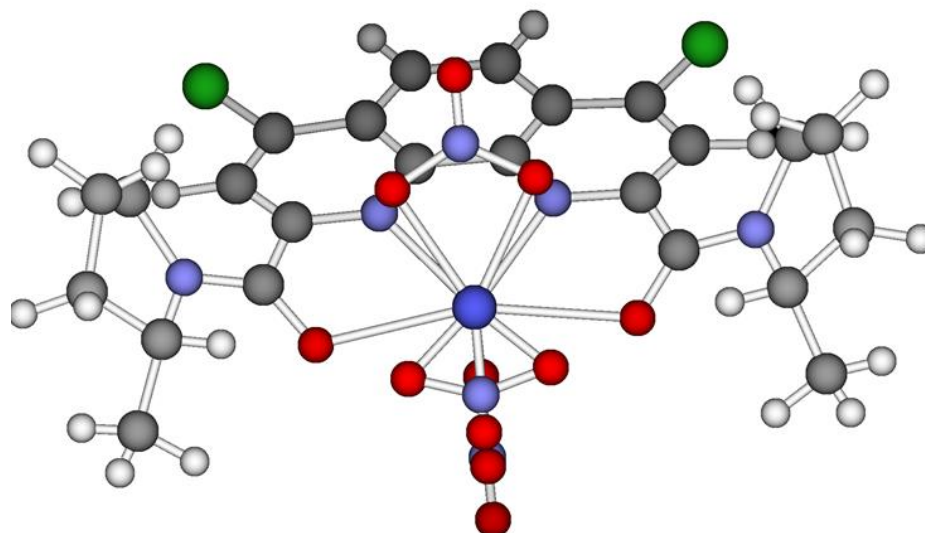
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Cl	-4.00664043	-3.20299125	-3.91261053
N	-1.52108610	1.22319877	-0.05450095
N	-0.18761857	3.93530798	1.81443262
N	-1.15484285	-1.19716454	-1.02394283
N	1.01424003	-3.99153996	-1.36156964
O	-0.16214570	1.69031894	2.12947369
O	0.49726591	-2.64766645	0.38933086
C	-1.66086674	2.43235135	0.48020110
C	-2.75357795	3.26782298	0.17905433
H	-2.87420487	4.23859596	0.65976208
C	-3.70461655	2.81742954	-0.72277552
C	-3.57787108	1.54143405	-1.32722580
C	-4.49794817	0.96803445	-2.25908160
H	-5.36773443	1.55497944	-2.55901837
C	-4.30738449	-0.29031155	-2.76327348
H	-5.02398396	-0.71476561	-3.46848249

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C -2.91379118 -2.40346026 -2.81449819
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C -2.23548865 -0.53947800 -1.46401727
C -2.43682075 0.79063100 -0.93117774
C -0.60635900 2.68969631 1.53276277
C 0.26379681 -3.04839897 -0.76699120
C -0.29974186 5.11080313 0.92876863
H -1.05862403 5.81665993 1.31440544
C 1.10298681 5.72566605 1.00799298
H 1.78144062 5.16783667 0.34218314
H 1.10631776 6.78562784 0.71328717
C 1.48211253 5.49701357 2.47680354
H 0.99423647 6.25161648 3.11868382
H 2.56628132 5.54672575 2.65390968
C 0.92981368 4.09762049 2.80328441
C 0.45657253 3.92613149 4.24362135
C 2.23203039 -4.48558903 -0.63645226
C 1.88211536 -5.46124458 0.48318502
C 3.08643508 -5.09131765 -1.76475072
C 2.62812924 -4.35505819 -3.03018546
C 1.11455381 -4.23552799 -2.81377125
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H 3.06924701 -3.34585786 -3.07151556
H 2.87670827 -6.17175961 -1.85487568
H 4.15967798 -4.96716976 -1.55982983
Lu 0.49724078 -0.28637388 0.90445697
N -1.05259120 -1.34490764 2.95048571
O 0.22702582 -1.18798435 3.04257965

O -1.55935419 -0.96240151 1.80959511
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O 2.59735465 -1.30914617 1.30273950
O 4.20976210 -0.34937897 2.46834755
N 1.68931127 0.82953769 -1.41960418
O 2.17505717 1.30930221 -2.42740083
O 1.55695462 -0.44774044 -1.24395728
O 1.25896394 1.55418396 -0.43469989
H 0.60494924 -5.17865086 -3.08522296
H 0.66637528 -3.40677094 -3.37915039
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H 1.33169627 -6.33227968 0.09168208
H 1.28065836 -4.96318436 1.25707972
H 0.08409724 2.90518641 4.40997410
H -0.33525571 4.65246201 4.48935652
H 1.30586004 4.09214115 4.92535782
H 1.67061102 3.31128383 2.57069755
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L4*Am(NO₃)₃(RS)



PBE/L1 theoretical level

E= -33482.166813

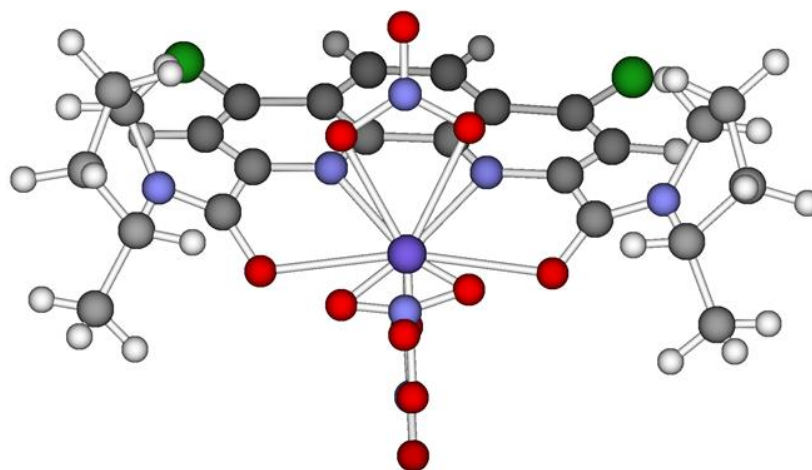
G= 250.7916 kcal/mol, H= 329.5601 kcal/mol, U= 328.9677 kcal/mol, S= 264.1912 cal/mol at T= 298.150 K

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Cl	-3.98552608	-3.19207525	-3.90334082
N	-1.49735618	1.22284365	-0.00845731
N	-0.19598915	4.00737667	1.79380572
N	-1.12516689	-1.21889091	-0.98893642
N	1.02372813	-4.02820730	-1.42694771
O	-0.15142263	1.77208114	2.19019890
O	0.53486586	-2.74178743	0.37905946
C	-1.64468515	2.44734454	0.50997072
C	-2.73636413	3.27461433	0.19242869
H	-2.85630178	4.25152540	0.66034037
C	-3.68613911	2.81148481	-0.70193309
C	-3.55641341	1.52718103	-1.29036367
C	-4.47653151	0.95527726	-2.21725821
H	-5.34706736	1.54213238	-2.51445675
C	-4.28453827	-0.30367661	-2.72297597
H	-5.00052261	-0.73017746	-3.42726541
C	-3.15748429	-1.08906150	-2.34124541
C	-2.89075089	-2.40561843	-2.79737592
C	-1.76689410	-3.08657169	-2.36191416
H	-1.58254671	-4.10745716	-2.69575667
C	-0.89831150	-2.45160747	-1.45681965
C	-2.21264863	-0.55183595	-1.41958702
C	-2.41506076	0.77560425	-0.88642848
C	-0.60483724	2.74701118	1.55291128
C	0.28407130	-3.09874392	-0.79222149
C	-0.29756126	5.14591980	0.85948038
H	-1.07513416	5.85696554	1.19537473

C 1.09425724 5.78290892 0.95097578
H 1.79758275 5.21059561 0.32424498
H 1.09198940 6.83110237 0.61683792
C 1.43669522 5.61430120 2.43654537
H 0.91773170 6.38214254 3.03699493
H 2.51432252 5.68995762 2.64245224
C 0.89777678 4.21832371 2.79766846
C 0.39974341 4.08678436 4.23398161
C 2.22870064 -4.57699442 -0.72326446
C 1.85796940 -5.58490562 0.36080059
C 3.06747556 -5.16077566 -1.87449789
C 2.63495755 -4.35710764 -3.10730219
C 1.12461185 -4.20674086 -2.88902998
H 2.86734891 -4.85532999 -4.06025934
H 3.10374808 -3.35951614 -3.10306811
H 2.82302570 -6.22905111 -2.01066875
H 4.14360762 -5.08056784 -1.66270924
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O 0.07578292 -1.27169168 3.19794416
O -1.69328046 -1.02910364 1.92622173
O -1.90548551 -1.87577021 3.95179486
N 3.09276724 -0.40838599 2.19322872
O 2.30789590 0.61915290 2.28507280
O 2.61170554 -1.38032770 1.48322189
O 4.18305588 -0.45611241 2.72533655
N 1.86791992 0.83330280 -1.36638331
O 2.41493201 1.30874574 -2.34452152
O 1.70528805 -0.44385070 -1.20964706
O 1.39843667 1.56577253 -0.40446755
H 0.59132850 -5.12180614 -3.20730138

H 0.69903833 -3.34108996 -3.41567326
 H -0.54345411 4.79609013 -0.15290301
 H 2.77880788 -5.98199129 0.81695664
 H 1.28705263 -6.42731905 -0.06259604
 H 1.26757717 -5.10334110 1.15340626
 H 0.03647325 3.06727386 4.42717695
 H -0.40665364 4.80951786 4.43938303
 H 1.23268223 4.28753805 4.92651796
 H 1.65713084 3.43900800 2.60541654
 H 2.74133968 -3.71638060 -0.25697190

L4*Cm(NO₃)₃(Meso)



PBE/L1 theoretical level

E= -34318.488033

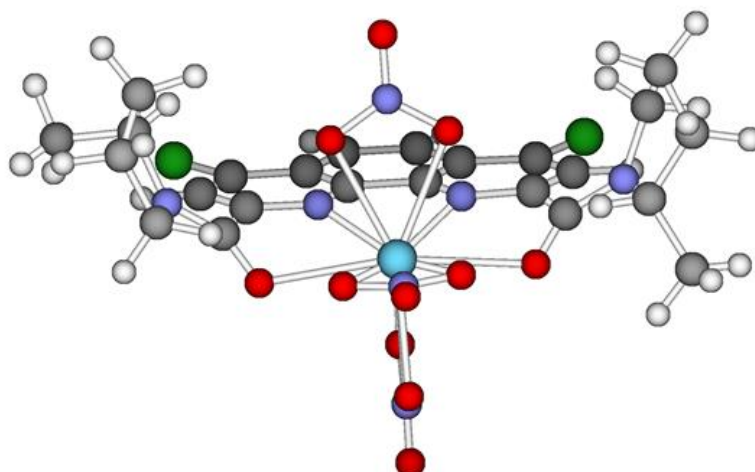
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 Cl -4.02333307 -3.21747112 -3.88362813
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 N -0.17505597 3.94388580 1.75452638
 N -1.20285332 -1.23867059 -0.94683504
 N 1.03675890 -3.94534636 -1.42592168
 O -0.35033149 1.75042868 2.32057214

O 0.48215342 -2.75842357 0.42560339
C -1.71750045 2.42736006 0.53122967
C -2.79310226 3.26928306 0.19321406
H -2.90166235 4.25483847 0.64703071
C -3.73698759 2.80627751 -0.70877224
C -3.61413503 1.51536298 -1.28342021
C -4.52897739 0.93979961 -2.21829987
H -5.39307976 1.52915537 -2.52952838
C -4.33782053 -0.32079601 -2.71517611
H -5.04809427 -0.74623191 -3.42609382
C -3.21495461 -1.11058140 -2.31900096
C -2.93993258 -2.42673802 -2.76992631
C -1.81316519 -3.10191917 -2.33039045
H -1.61714566 -4.11915588 -2.66993880
C -0.95658249 -2.45793700 -1.41713727
C -2.28125811 -0.57436973 -1.38845551
C -2.48399901 0.76005584 -0.86199242
C -0.68771738 2.71250606 1.60129547
C 0.25327542 -3.08095360 -0.75734442
C -0.16394745 5.00500107 0.72753501
H -0.84882003 5.82498407 1.01224029
C 1.29482782 5.47597599 0.75291407
H 1.91186357 4.76195049 0.18337826
H 1.41345227 6.48032522 0.31985605
C 1.63557625 5.40904188 2.24748731
H 1.22250843 6.28753185 2.77415705
H 2.71769524 5.37164211 2.44034362
C 0.94048750 4.12725735 2.74199176
C 0.43402106 4.19299793 4.17938900
C 2.27833200 -4.44617462 -0.74779171
C 1.97603524 -5.51545572 0.29772219

C 3.14522815 -4.93172312 -1.92369211
C 2.64972019 -4.11810017 -3.12604260
C 1.13471794 -4.07563543 -2.89361072
H 2.90633607 -4.56820345 -4.09656620
H 3.05097651 -3.09208179 -3.09088707
H 2.97369862 -6.00905371 -2.09517241
H 4.21493721 -4.78455782 -1.71531940
Cm 0.40004516 -0.34847957 1.13312352
N -1.37238169 -1.57344878 3.07691121
O -0.09882248 -1.45948136 3.27140450
O -1.80242729 -1.08699918 1.94332397
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N 3.00682759 -0.40189594 2.43513823
O 2.14148784 0.53843105 2.65435982
O 2.61725998 -1.31153262 1.59010208
O 4.09678841 -0.43279502 2.97215223
N 1.78793955 0.92042094 -1.15730095
O 2.32676506 1.45376801 -2.11187029
O 1.55358756 -0.35150579 -1.11176431
O 1.40302408 1.59268034 -0.11466331
H 0.66032630 -5.01552534 -3.23158073
H 0.64802653 -3.22625780 -3.39259982
H -0.46772715 4.60290289 -0.24893092
H 2.92229652 -5.86989594 0.73657066
H 1.45795584 -6.37612343 -0.15581930
H 1.36041594 -5.10203981 1.10937667
H -0.04480207 3.24517417 4.46486044
H -0.28141066 5.02126741 4.31023979
H 1.28696322 4.35858679 4.85665560
H 1.60273421 3.24958324 2.63125801
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L4*La(NO₃)₃(Rac)



PBE/L1 theoretical level

E= -11557.263659

G= 249.0797 kcal/mol, H= 330.5259 kcal/mol, U= 329.9334 kcal/mol, S= 273.1718 cal/mol at T= 298.150 K

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N	-1.14714360	-1.35650766	-0.77950454
N	1.20726764	-3.94107747	-1.25319290
O	-0.50789082	1.70352960	2.56770277
O	0.44961196	-2.97342753	0.65626329
C	-1.78306222	2.31272244	0.68500513
C	-2.85757732	3.13537836	0.30021790
H	-2.99751472	4.12200022	0.74071103
C	-3.76035929	2.65167880	-0.63174844
C	-3.59249735	1.36316204	-1.19921720
C	-4.45585060	0.77950251	-2.17665792
H	-5.31643581	1.35580719	-2.52020335
C	-4.21621656	-0.46990266	-2.67850542
H	-4.88343000	-0.90076441	-3.42676616
C	-3.09393406	-1.23959506	-2.24329209
C	-2.76673985	-2.53698087	-2.71384311

C -1.64456165 -3.19599843 -2.24092031
H -1.40124130 -4.19678688 -2.59880567
C -0.85285103 -2.55784917 -1.26788878
C -2.21693444 -0.70126504 -1.25914896
C -2.46980762 0.62509310 -0.72850871
C -0.77819258 2.62815762 1.77552485
C 0.33150926 -3.18884087 -0.56606400
C -0.12395992 4.84946966 0.76757485
C -0.91474420 6.11444569 1.11778700
C 1.39376318 5.09417439 0.67480874
H 1.85160899 4.25875330 0.12051120
H 1.63027132 6.04035950 0.16541614
C 1.84658480 5.06279802 2.14515281
H 1.67915249 6.03714228 2.63078165
H 2.91414452 4.81807852 2.24553537
C 0.96997684 3.96897864 2.77930999
C 2.43035936 -4.43605614 -0.53838247
C 3.41506791 -4.71972704 -1.68768299
C 2.94122767 -3.81234908 -2.83051562
C 1.41563463 -3.90933180 -2.71505618
H 3.30278945 -4.12757444 -3.82055545
H 3.24969459 -2.76941991 -2.65017200
H 3.34575534 -5.78038597 -1.98749948
H 4.45165825 -4.51840544 -1.37984669
La 0.33289981 -0.51956403 1.49781549
N -1.75579643 -1.69875634 3.27217007
O -0.51880020 -1.61197329 3.63574195
O -2.02527380 -1.23443198 2.07944965
O -2.61920357 -2.17776465 3.98088789
N 2.87748957 -0.62923187 3.05158448
O 2.05849195 0.37790513 3.12602472

O 2.49943352 -1.59249532 2.26472378
O 3.92349386 -0.66531616 3.66988158
N 1.90941834 0.74497366 -0.78643495
O 2.49916744 1.25643837 -1.72447169
O 1.74225998 -0.53570932 -0.69190240
O 1.40647829 1.45308948 0.17739320
H 1.04415882 -4.84202290 -3.17825699
Cl -5.11182070 3.64810443 -1.09920192
Cl -3.77672744 -3.32279658 -3.89717412
H 0.61572784 4.21921682 3.79162741
C 2.13228369 -5.63756514 0.35301033
H 1.47861195 2.99282503 2.83700728
H 0.89532942 -3.05181837 -3.16366696
H -0.50896776 4.40132380 -0.16155882
H -0.50935441 6.60313606 2.01687241
H -1.97710001 5.89771605 1.30864704
H -0.85761392 6.82940626 0.28187910
H 1.42437828 -5.36480379 1.14902902
H 3.06591082 -5.97402096 0.83150196
H 1.72030354 -6.47411394 -0.23469055
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PBE0/L1 theoretical level

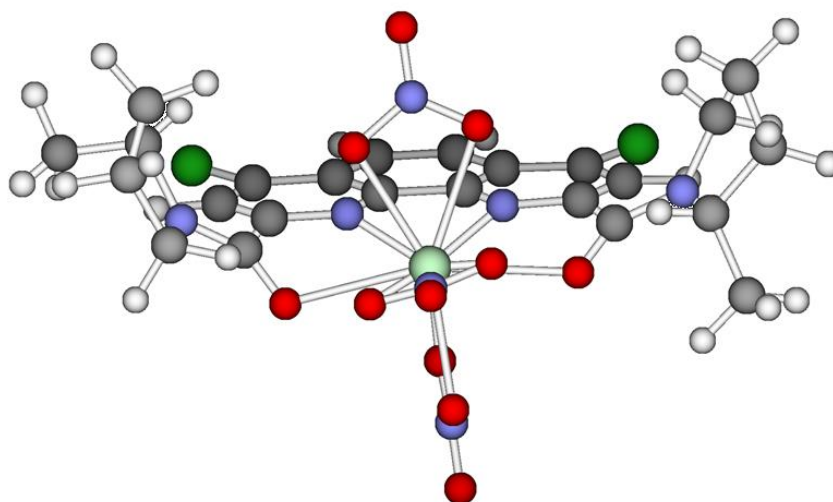
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N 1.20036495 -3.89384484 -1.23145866
O -0.48284695 1.67757416 2.53030443
O 0.42359215 -2.95996976 0.65961534
C -1.76963031 2.28393841 0.68226582
C -2.82894516 3.10862899 0.29660624

H -2.96351814 4.08917809 0.73130435
C -3.72333694 2.63252068 -0.63065535
C -3.55967832 1.35203600 -1.19118834
C -4.41740608 0.77595145 -2.17128634
H -5.26755571 1.35076594 -2.51722598
C -4.18122482 -0.46107411 -2.66866159
H -4.84057474 -0.88448012 -3.41618323
C -3.06733179 -1.23143923 -2.22835088
C -2.74200797 -2.51774979 -2.69954848
C -1.63326752 -3.17475843 -2.22498345
H -1.38739073 -4.16622019 -2.58249617
C -0.85658556 -2.54332972 -1.25030100
C -2.20673776 -0.70306778 -1.24681878
C -2.45655704 0.61551261 -0.71904707
C -0.75807291 2.59666777 1.75653124
C 0.32181183 -3.16824198 -0.55039102
C -0.13139287 4.80490351 0.76375788
C -0.91344976 6.05498695 1.14185572
C 1.37185884 5.06166887 0.65083486
H 1.82649362 4.24363422 0.08410463
H 1.59134066 6.00917578 0.15330628
C 1.84327245 5.01663160 2.10392022
H 1.67834258 5.97756863 2.59888315
H 2.90569878 4.77873325 2.18615079
C 0.98675483 3.91809344 2.73404932
C 2.41192603 -4.37895966 -0.52047628
C 3.39174199 -4.66006899 -1.66007006
C 2.92661095 -3.74986696 -2.79015017
C 1.41065300 -3.84520507 -2.68034101
H 3.28821301 -4.05594921 -3.77420616
H 3.23364615 -2.71642184 -2.60130310

H 3.31645155 -5.71074724 -1.96445823
H 4.42135143 -4.46802473 -1.35110533
La 0.32232383 -0.53764647 1.50517929
N -1.77819276 -1.67140722 3.25833988
O -0.56769013 -1.59174216 3.62660646
O -2.02815676 -1.22938097 2.08377099
O -2.63735104 -2.12871647 3.95544171
N 2.87557817 -0.64773548 3.00551748
O 2.09241843 0.35513341 3.06602407
O 2.47810364 -1.60565937 2.26688457
O 3.91548848 -0.68438792 3.59806800
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O 2.42885017 1.18721592 -1.73251319
O 1.71992481 -0.56163734 -0.67628837
O 1.36983979 1.40035486 0.14046723
H 1.04284728 -4.76453161 -3.15280557
Cl -5.05472469 3.62713647 -1.10170579
Cl -3.73439884 -3.28910065 -3.88437128
H 0.64834625 4.15571833 3.74571109
C 2.11949682 -5.57536077 0.36257166
H 1.50216901 2.95450377 2.77363777
H 0.90016782 -2.98716426 -3.11971688
H -0.52446824 4.37377834 -0.16024072
H -0.49546868 6.52644253 2.03488779
H -1.96439338 5.83737659 1.34860814
H -0.87128597 6.77755308 0.32202244
H 1.41778541 -5.30889034 1.15539193
H 3.04802632 -5.91156721 0.83310699
H 1.70910954 -6.40309763 -0.22454078
H 2.76613259 -3.54880500 0.10179243

L4*Nd(NO₃)₃(Rac)



PBE\L1 theoretical level

E= -12688.657934

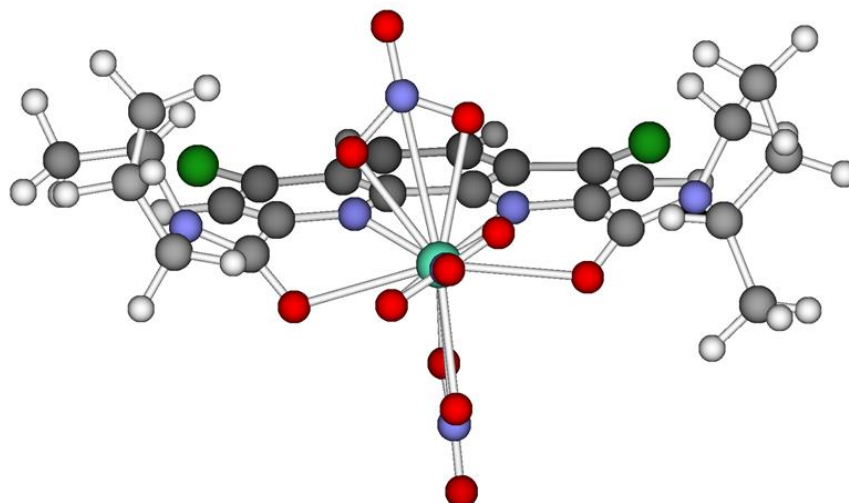
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N	-0.22738720	3.83964944	1.92294705
N	-1.09371388	-1.32525837	-0.80994129
N	1.20790923	-4.00298643	-1.24400926
O	-0.53662419	1.67893302	2.55176234
O	0.61171156	-2.80516720	0.58656716
C	-1.75976956	2.33161283	0.65716475
C	-2.83369708	3.14991832	0.26471177
H	-2.98527288	4.13155460	0.71228355
C	-3.72335958	2.66796374	-0.68134403
C	-3.54679418	1.38110101	-1.24818242
C	-4.40639448	0.79085666	-2.22490430
H	-5.26632929	1.36459100	-2.57433939
C	-4.16611242	-0.46288472	-2.71593070
H	-4.83242512	-0.90050602	-3.46111441
C	-3.04530430	-1.22906744	-2.27161503
C	-2.72339749	-2.53495407	-2.71936631

C -1.59911680 -3.18620706 -2.24035215
H -1.36596453 -4.19526911 -2.57981968
C -0.79632068 -2.53154612 -1.28713357
C -2.16601682 -0.67894876 -1.29603863
C -2.42134547 0.64805597 -0.77529514
C -0.79298973 2.62788129 1.78472614
C 0.40542537 -3.13613605 -0.59690207
C -0.14402035 4.89280939 0.87858617
C -0.96431559 6.13526201 1.24183834
C 1.37231159 5.16062689 0.84593838
H 1.86055815 4.35039616 0.28051975
H 1.61233020 6.12638283 0.37639278
C 1.77609861 5.08613014 2.32907343
H 1.58274102 6.04293966 2.83930945
H 2.84231758 4.84831524 2.45658255
C 0.89071190 3.96392107 2.89914274
C 2.42831564 -4.50427818 -0.53046805
C 3.32387352 -5.00323200 -1.67881167
C 2.86604881 -4.19537020 -2.89949799
C 1.34568703 -4.14107990 -2.70775676
H 3.14521265 -4.65403795 -3.85975170
H 3.27434301 -3.17207289 -2.86186361
H 3.14972305 -6.08058739 -1.84741449
H 4.38868570 -4.86209393 -1.44261515
Nd 0.35938379 -0.40678206 1.34809208
N -1.54629111 -1.74347973 3.09504962
O -0.29173103 -1.61615288 3.38568282
O -1.90006459 -1.22956312 1.95118904
O -2.33927441 -2.30001068 3.82773781
N 2.89051080 -0.36662820 2.79322171
O 1.92917764 0.46140084 3.05656433

O 2.62513876 -1.22674239 1.85429132
O 3.95761299 -0.34210974 3.37372303
N 1.85191810 0.95458794 -0.82839036
O 2.45861936 1.53564537 -1.71202242
O 1.55463958 -0.29844451 -0.89318067
O 1.45267212 1.56573975 0.24899100
H 0.87509602 -5.07932711 -3.05583572
Cl -5.07336426 3.66195321 -1.15940690
Cl -3.74255967 -3.34279370 -3.88104367
H 0.49607259 4.18291903 3.90377975
C 2.09410906 -5.56502676 0.51426619
H 1.40763187 2.99161935 2.94812202
H 0.87871104 -3.29124260 -3.22457623
H -0.49077171 4.47042036 -0.07736411
H -0.59983748 6.59687328 2.17223334
H -2.03017759 5.89930248 1.38453627
H -0.88541323 6.87982130 0.43400115
H 1.45570612 -5.14509773 1.30469596
H 3.02649689 -5.91840696 0.98287445
H 1.58737469 -6.42785549 0.05214185
H 2.87919641 -3.63030386 -0.02678502

L4*Eu(NO₃)₃(Rac)



PBE/L1 theoretical level

E= -13909.655372

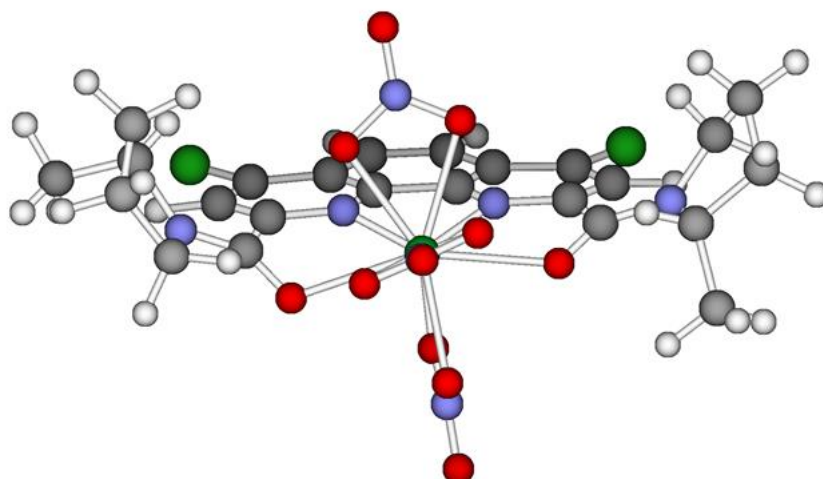
G= 250.4028 kcal/mol, H= 330.3367 kcal/mol, U= 329.7443 kcal/mol, S= 268.0998 cal/mol at T= 298.150 K

N	-1.52827489	1.11064613	0.11755731
N	-0.25017777	3.82453585	1.97074723
N	-1.08105659	-1.34973907	-0.82109892
N	1.19874108	-4.05410862	-1.20594966
O	-0.51322955	1.63665128	2.53193402
O	0.60289377	-2.81761169	0.60069531
C	-1.73326683	2.31725073	0.64409882
C	-2.81450486	3.13105559	0.25887901
H	-2.98016214	4.10301018	0.72252196
C	-3.68989086	2.65948987	-0.70469511
C	-3.50350785	1.38039958	-1.28705621
C	-4.35458040	0.79784733	-2.27598214
H	-5.20983076	1.37541783	-2.63052821
C	-4.11377382	-0.45411098	-2.77092910
H	-4.77375984	-0.88559371	-3.52517533
C	-3.00452018	-1.22906673	-2.31293106
C	-2.69247627	-2.54089618	-2.75118732
C	-1.58496118	-3.20641208	-2.25385022
H	-1.36182582	-4.21968699	-2.58704209
C	-0.78921950	-2.55987954	-1.28867567
C	-2.13235259	-0.68575484	-1.32736969
C	-2.37967849	0.64678949	-0.81305140
C	-0.78053522	2.59986711	1.79035366
C	0.40099409	-3.16844082	-0.57795697
C	-0.16537499	4.89639330	0.94535261
C	-1.00620651	6.12222528	1.31799912
C	1.34754503	5.18474388	0.93450868
H	1.85265434	4.39228439	0.35929206

H 1.57885182 6.16335392 0.48766249
C 1.73549414 5.08624268 2.42033553
H 1.52292860 6.02955818 2.94789886
H 2.80319834 4.85976362 2.55536151
C 0.85874891 3.94116426 2.95719433
C 2.40857458 -4.55908394 -0.47660145
C 3.29890823 -5.10064793 -1.60953283
C 2.86026192 -4.31357861 -2.85053802
C 1.34057999 -4.22573662 -2.66618204
H 3.13334322 -4.80050755 -3.79851508
H 3.28936815 -3.29827070 -2.83681130
H 3.10587335 -6.17826080 -1.75341821
H 4.36521244 -4.97304487 -1.37272537
Eu 0.36669698 -0.40405372 1.24817431
N -1.52734756 -1.63917816 3.07465219
O -0.27029091 -1.50103903 3.33828163
O -1.90882111 -1.16208339 1.93242157
O -2.30060840 -2.18044829 3.84422040
N 3.02917647 -0.35823214 2.42056394
O 2.03205800 0.25154316 2.96128488
O 2.75338674 -1.00819731 1.33195698
O 4.15301991 -0.32939985 2.89038444
N 1.73716021 1.22521865 -0.80987036
O 2.30744529 1.88395023 -1.66650844
O 1.31818771 0.02287780 -1.03244197
O 1.50052440 1.68793106 0.37307319
H 0.85383826 -5.16225910 -2.99600554
Cl -5.04002571 3.65345716 -1.18249345
Cl -3.70567203 -3.33981180 -3.92399883
H 0.45566919 4.13157988 3.96435165
C 2.05313897 -5.59031582 0.59058613

H	1.38687289	2.97429156	2.98488474
H	0.89221954	-3.37877369	-3.20371532
H	-0.49407148	4.48661852	-0.02243823
H	-0.65501249	6.57739687	2.25654364
H	-2.06967998	5.86983728	1.45037234
H	-0.93268967	6.87833929	0.52009267
H	1.41799116	-5.14317417	1.36855114
H	2.97792578	-5.94862461	1.07039583
H	1.53436971	-6.45495319	0.14570326
H	2.87353277	-3.68075562	0.00638773

L4*Lu(NO₃)₃(Rac)



PBE/L1 theoretical level

E= -17632.060677

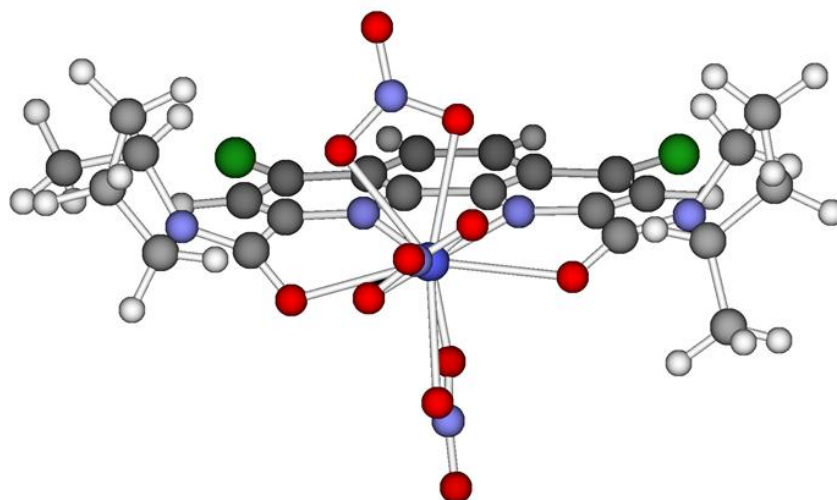
G= 252.7284 kcal/mol, H= 331.0392 kcal/mol, U= 330.4467 kcal/mol, S= 262.6558 cal/mol at T= 298.150 K

N	-1.49641395	1.12728274	0.03337539
N	-0.25430170	3.78705239	2.00620008
N	-1.05358243	-1.29574442	-0.91745168
N	1.17985570	-4.06736851	-1.19094229
O	-0.44817808	1.55912316	2.39401627
O	0.70486176	-2.60822082	0.47128952
C	-1.69702184	2.32909966	0.57306790

C -2.77306056 3.15240598 0.19510880
H -2.93565536 4.11972713 0.66892165
C -3.65433455 2.69488454 -0.77128112
C -3.47844243 1.41855097 -1.36103010
C -4.33835697 0.83551025 -2.34312248
H -5.19400215 1.41546226 -2.69310069
C -4.10925531 -0.42137852 -2.83367419
H -4.78025389 -0.85312015 -3.57817149
C -2.99921036 -1.19993412 -2.38219357
C -2.69383478 -2.51951170 -2.80022669
C -1.58200955 -3.17901349 -2.30119967
H -1.37348008 -4.20129299 -2.61485052
C -0.76666069 -2.51324153 -1.36451030
C -2.11421371 -0.64920080 -1.41474879
C -2.35453773 0.68041933 -0.89704710
C -0.74846768 2.56933045 1.72783649
C 0.43846387 -3.08230233 -0.64945233
C -0.21626873 4.94826698 1.08137619
C -1.10604584 6.10030174 1.56074488
C 1.28368556 5.29761600 1.10283852
H 1.82139456 4.58025694 0.46200034
H 1.47620022 6.31924772 0.74205011
C 1.67501247 5.08563471 2.57587743
H 1.42192841 5.96997356 3.18174148
H 2.75134277 4.89440203 2.69505143
C 0.84909314 3.86068010 3.00565314
C 2.39073467 -4.53481722 -0.43762147
C 3.21385193 -5.25978231 -1.51726663
C 2.77157831 -4.61293602 -2.83537745
C 1.26500499 -4.42031813 -2.62178588
H 2.98623037 -5.22958946 -3.72083306

H 3.25155234 -3.62911868 -2.96411347
H 2.96343422 -6.33513308 -1.51751995
H 4.29259634 -5.16018200 -1.32868791
Lu 0.43848929 -0.30485907 1.09804678
N -1.13665617 -1.68322146 2.93134665
O 0.13010874 -1.48969376 3.09505796
O -1.62132359 -1.16883206 1.83320796
O -1.82635140 -2.29175830 3.72367549
N 2.98390722 -0.15804932 2.28696609
O 2.00440073 0.58047366 2.68810368
O 2.67472172 -0.96329302 1.30936217
O 4.09876966 -0.11220355 2.76916885
N 1.70287323 1.13285780 -1.00521779
O 2.24705482 1.76388860 -1.89281285
O 1.37855864 -0.11071896 -1.12079477
O 1.39273047 1.66714776 0.14015001
H 0.72035939 -5.36140442 -2.82367301
Cl -4.99945068 3.70050812 -1.23713887
Cl -3.72261477 -3.33716822 -3.94645452
H 0.43489915 3.94530153 4.02250195
C 2.02753234 -5.40393782 0.76301223
H 1.41849208 2.91786122 2.95149016
H 0.84558088 -3.61976981 -3.24666500
H -0.52705985 4.61261368 0.07989556
H -0.77280378 6.48193073 2.53787041
H -2.15810585 5.79349756 1.66840553
H -1.06402230 6.92785931 0.83508301
H 1.45175648 -4.82790661 1.50138438
H 2.95263076 -5.75137711 1.25004733
H 1.44609702 -6.28620195 0.44939187
H 2.91019154 -3.62656713 -0.08235258

L4*Am(NO₃)₃(Rac)



PBE/L1 theoretical level

E= -33482.167024

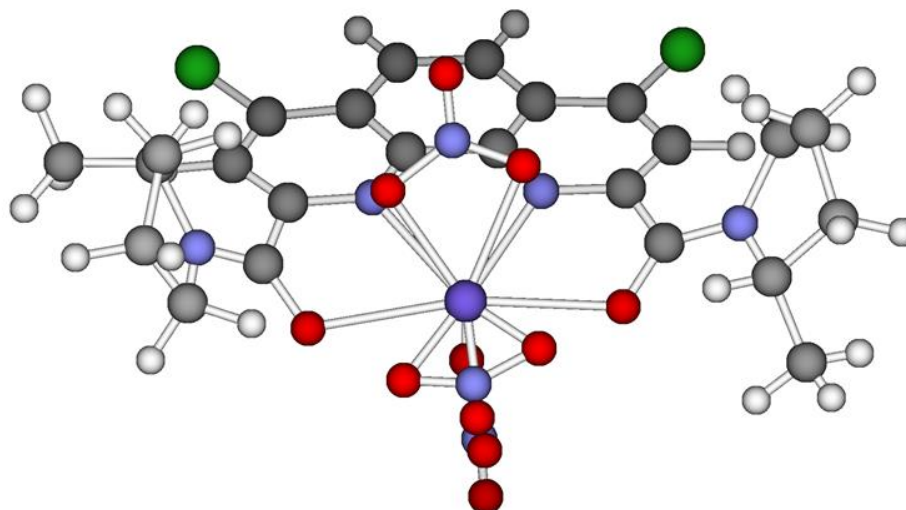
G= 250.8120 kcal/mol, H= 330.1333 kcal/mol, U= 329.5408 kcal/mol, S= 266.0449 cal/mol at T= 298.150 K

N	-1.47323287	1.13153386	0.07039306
N	-0.26949552	3.84230423	2.01204181
N	-1.01404274	-1.32636368	-0.87502611
N	1.18614173	-4.13445902	-1.20783365
O	-0.41465610	1.61768854	2.43837452
O	0.75001085	-2.70284534	0.49557874
C	-1.68944585	2.33949399	0.60772544
C	-2.76859498	3.14917707	0.21371645
H	-2.94728208	4.11533260	0.68387574
C	-3.63042402	2.68348694	-0.76429880
C	-3.43876290	1.40455782	-1.35117698
C	-4.28356409	0.82435381	-2.34091544
H	-5.13701868	1.40193748	-2.69937301
C	-4.04533863	-0.43529361	-2.82859135
H	-4.70662355	-0.86966228	-3.57988071
C	-2.94569707	-1.21029329	-2.36232471
C	-2.64547539	-2.53366423	-2.78177071

C -1.54658544 -3.20290279 -2.27654958
H -1.34362996 -4.22616053 -2.58983517
C -0.73158586 -2.55188179 -1.32942700
C -2.06866288 -0.66390955 -1.37961686
C -2.31788421 0.66877860 -0.86877114
C -0.74716443 2.61023760 1.75245523
C 0.45956957 -3.14950562 -0.63884968
C -0.24582940 4.98996592 1.06945419
C -1.15811861 6.13434553 1.52525830
C 1.24688089 5.36859751 1.09265649
H 1.80327034 4.65368366 0.46515483
H 1.42148721 6.38908052 0.71981132
C 1.63315380 5.18402147 2.57034063
H 1.35236490 6.06799078 3.16443706
H 2.71297836 5.02165794 2.70067596
C 0.83357990 3.94468451 3.00705671
C 2.38007665 -4.65541887 -0.46528965
C 3.19177842 -5.36543465 -1.56315994
C 2.78096199 -4.65655470 -2.85906506
C 1.27819169 -4.43306208 -2.65141940
H 2.98875999 -5.24401855 -3.76573920
H 3.28867435 -3.68193722 -2.94524145
H 2.90829921 -6.43174744 -1.60596406
H 4.27119970 -5.30654716 -1.36151814
Am 0.43340153 -0.34425598 1.12358117
N -1.35694206 -1.63065028 3.02445912
O -0.10138648 -1.39587700 3.25498486
O -1.77708781 -1.23096907 1.86306298
O -2.07992959 -2.18017960 3.83006430
N 3.13538837 -0.23764768 2.19560695
O 2.11812305 0.30215156 2.78888106

O 2.84538245 -0.86164463 1.09338343
O 4.26691246 -0.16541804 2.63038802
N 1.74802339 1.34876812 -0.91857928
O 2.30241704 2.01212883 -1.77614188
O 1.28703022 0.15815358 -1.15364325
O 1.56019008 1.77793252 0.28629631
H 0.71229243 -5.35094786 -2.89684176
Cl -4.97780657 3.67802596 -1.25135744
Cl -3.67254353 -3.34063435 -3.93781734
H 0.42335907 4.02155304 4.02629137
C 1.98881233 -5.55439663 0.70435518
H 1.42407501 3.01566529 2.95379639
H 0.88305402 -3.59830284 -3.24697423
H -0.54674280 4.63310242 0.07215568
H -0.83627564 6.53798008 2.49740362
H -2.20509887 5.81130028 1.63300467
H -1.12678719 6.95018005 0.78588706
H 1.41602635 -4.99236727 1.45576012
H 2.90132165 -5.93747282 1.18848717
H 1.39194179 -6.41325092 0.35700527
H 2.92458463 -3.77417421 -0.08086818

L4*Cm(NO₃)₃(Rac)



PBE/L1 theoretical level

E= -34318.485149

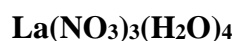
G= 249.8737 kcal/mol, H= 330.5476 kcal/mol, U= 329.9552 kcal/mol, S= 270.5818 cal/mol at T= 298.150 K

N	-1.56577730	1.11511827	0.12199934
N	-0.22679725	3.82629347	1.92214906
N	-1.10057771	-1.31913757	-0.84314448
N	1.19539523	-4.00147247	-1.23317742
O	-0.50913668	1.64995670	2.50331497
O	0.56986451	-2.79914141	0.58425474
C	-1.75707555	2.32932639	0.63621610
C	-2.83414745	3.14850211	0.25223821
H	-2.98857379	4.12622929	0.70762163
C	-3.72269011	2.67387128	-0.69840193
C	-3.54595923	1.39119709	-1.27590895
C	-4.40478373	0.80510205	-2.25622296
H	-5.26491928	1.37990665	-2.60341120
C	-4.16601610	-0.44758138	-2.75168967
H	-4.83370113	-0.88185620	-3.49762034
C	-3.04787850	-1.21792972	-2.30739450
C	-2.72900033	-2.52635479	-2.75136232
C	-1.61170661	-3.18388176	-2.26407123
H	-1.38361764	-4.19584656	-2.59881902
C	-0.80924857	-2.53000379	-1.30958903
C	-2.16855335	-0.67066312	-1.33104420
C	-2.42097712	0.65656453	-0.80673730
C	-0.78314841	2.61414957	1.75963008
C	0.38309154	-3.13429713	-0.60252458
C	-0.16161989	4.90435076	0.90205473
C	-0.99415702	6.12836075	1.29835463
C	1.35139585	5.19014692	0.86724246
H	1.84529972	4.39893436	0.28030583

H 1.57755125 6.16928244 0.41894224
C 1.76472998 5.08542728 2.34578991
H 1.55902576 6.02602053 2.88064218
H 2.83496070 4.86097670 2.46224070
C 0.90025908 3.93524122 2.89068532
C 2.40861464 -4.49643469 -0.50185436
C 3.31556392 -5.00508308 -1.63690376
C 2.87111616 -4.20692587 -2.86905861
C 1.34871709 -4.15020514 -2.69441724
H 3.15993643 -4.67417240 -3.82228446
H 3.27971482 -3.18373370 -2.83581686
H 3.14255857 -6.08374500 -1.79820812
H 4.37779522 -4.86216831 -1.39088678
Cm 0.37016290 -0.40917599 1.31989992
N -1.45459807 -1.74353468 3.13780546
O -0.19450574 -1.60399699 3.39412427
O -1.84657383 -1.22762001 2.00332308
O -2.22298193 -2.31082749 3.88798642
N 2.91975212 -0.39049619 2.73381376
O 1.99229109 0.48459274 2.96797991
O 2.61529994 -1.27463043 1.82870293
O 3.99025822 -0.38658881 3.30928636
N 1.85051358 0.95249373 -0.86112440
O 2.43430614 1.52540493 -1.76537311
O 1.59937286 -0.31508473 -0.88657165
O 1.43076193 1.58042717 0.19683161
H 0.88086760 -5.09072495 -3.03973651
Cl -5.07292557 3.67043543 -1.16890347
Cl -3.74619603 -3.33046627 -3.91679192
H 0.51312286 4.11798573 3.90532327
C 2.06356287 -5.54814434 0.54838187

H 1.43166101 2.96932673 2.90408444
H 0.88826245 -3.30335999 -3.22189951
H -0.50812030 4.49942923 -0.06149057
H -0.62907374 6.57326412 2.23655033
H -2.05615997 5.87652874 1.44287896
H -0.92954725 6.89174271 0.50695366
H 1.42130506 -5.12017441 1.33125079
H 2.99181366 -5.90032578 1.02581358
H 1.55778575 -6.41308165 0.08915222
H 2.85405493 -3.61772299 -0.00138486

Nitrates



PBE/L1 theoretical level

E= -9642.097318

G= 53.3819 kcal/mol, H= 105.8898 kcal/mol, U= 105.2973 kcal/mol, S= 176.1123 cal/mol at T= 298.150 K

La -0.01745072 0.03941465 -0.08009092
N -2.88875771 0.66897988 -0.56789005
O -1.92837203 1.52223504 -0.78965306
O -4.05084801 0.92287028 -0.77512562
O -2.48932242 -0.48393327 -0.10402510
N 0.24982727 -2.03345084 -2.26907063
O 0.46912551 -2.31057143 -1.00930166
O -0.07948777 -0.79881620 -2.50240612
O 0.34689739 -2.86435509 -3.14117336
N 0.09314170 2.14140987 2.08958840
O 0.72087282 2.24467993 0.95873511
O 0.02993391 3.04302406 2.89206719
O -0.47006425 0.97196674 2.30463123
O 0.69057828 1.79106164 -1.94979513
H -0.02730745 2.45715356 -1.97258639
H 0.55669630 1.24782395 -2.75659680

O 1.56816590 -0.82050055 2.01577806
H 1.02049017 -0.21734004 2.58009863
H 1.15512693 -1.69574893 2.17421746
O 2.59965801 0.17230313 -0.40205047
H 2.86960483 1.10862684 -0.48422387
H 2.88411617 -0.11630398 0.49250901
O -0.82267028 -2.17092156 1.33470869
H -0.68676341 -2.76558900 0.56091714
H -1.79319084 -2.05401897 1.40073824
PBE0/L1 theoretical level
E= -9641.90411563
La -0.02973660 -0.01643320 -0.05039048
N -2.85563040 0.68312019 -0.61486340
O -1.89039898 1.49601591 -0.80304956
O -3.98921037 0.96606022 -0.84288192
O -2.50848508 -0.46106812 -0.16331235
N 0.30149275 -2.05739784 -2.21207833
O 0.38962287 -2.35492110 -0.97064960
O 0.05274607 -0.83215630 -2.45374012
O 0.44143066 -2.86829662 -3.07335567
N 0.03753816 2.06705070 2.10004807
O 0.66495377 2.17938662 0.99891722
O -0.03150741 2.95142961 2.89578414
O -0.51345420 0.92351210 2.29911208
O 0.72722709 1.77785838 -1.87621176
H 0.11463277 2.52475595 -1.81691980
H 0.52906656 1.33517170 -2.71527171
O 1.57842588 -0.80243385 1.98836398
H 1.00824416 -0.32604322 2.62054205
H 1.43289626 -1.73700559 2.18709517
O 2.54031301 0.18323997 -0.49348837

H 2.69439268 1.06862950 -0.85215640
H 3.00600362 0.12764271 0.35205156
O -0.94614947 -2.10533190 1.37118721
H -0.85619795 -2.77988744 0.67843556
H -1.89821577 -1.94289792 1.44683218

Nd(NO₃)₃(H₂O)₄

PBE/L1 theoretical level

E= -10773.492766

G= 54.2571kcal/mol, H= 105.8958 kcal/mol, U= 105.3034 kcal/mol, S= 173.1973 cal/mol at T= 298.150 K

Nd 0.02021915 0.01166109 -0.08434540
N -2.78535986 0.60743934 -0.54352832
O -1.83417118 1.47301483 -0.73809993
O -3.95070672 0.85009933 -0.74078512
O -2.36504269 -0.55249572 -0.11462208
N 0.16858573 -1.96648109 -2.26481867
O 0.39970762 -2.27045560 -1.01441967
O -0.09988253 -0.71291602 -2.46538568
O 0.20339151 -2.78575873 -3.15106010
N -0.01843936 2.11770582 1.97429729
O 0.67321289 2.20859909 0.88139814
O -0.15231565 3.03387260 2.75060225
O -0.56242400 0.93933868 2.17814398
O 0.79025263 1.77881324 -1.85691988
H 0.16008550 2.52367067 -1.77821743
H 0.54644805 1.31811285 -2.68792892
O 1.56711614 -0.78899258 2.01599741
H 1.03195083 -0.17503770 2.57482982
H 1.08447707 -1.63791442 2.13131595
O 2.55918097 0.07194296 -0.42564288
H 2.80818582 1.00372231 -0.58892435
H 2.84546351 -0.14286901 0.48918524

O -0.73587757 -2.16449833 1.38373792
H -0.65855688 -2.74720025 0.59370673
H -1.69550073 -1.99337339 1.48148346

Eu(NO₃)₃(H₂O)₄

PBE/L1 theoretical level

E= -11994.497997

G= 54.1542 kcal/mol, H= 105.7015 kcal/mol, U= 105.1090 kcal/mol, S= 172.8905 cal/mol at T= 298.150 K

N -2.74106860 0.22598195 0.01776200
O -2.17184520 1.22799683 -0.56652075
O -3.93982434 0.10236165 0.11109148
O -1.90453625 -0.65733540 0.50886905
N -0.01424715 -1.70417202 -2.21535850
O 0.42451546 -1.89757991 -1.00594270
O -0.35052702 -0.47876206 -2.47153473
O -0.10478565 -2.59533930 -3.02917290
N 0.14335951 2.76792932 1.53033042
O 0.28633529 2.85805821 0.24475501
O 0.13983190 3.73357582 2.25992537
O 0.01132500 1.55293941 1.96798527
O 1.01058364 1.84728324 -2.15551949
H 0.76053965 2.78958297 -2.08212161
H 0.62084270 1.50895333 -2.98714590
O 0.88793862 -1.04726923 1.71804178
H 0.60404843 -0.57602167 2.52639318
H 0.33954483 -1.91536725 1.67790461
O 2.59570003 0.20145746 0.12479670
H 3.29220533 0.84873402 0.33680367
H 2.48089361 -0.39127678 0.90928328
O -0.66292977 -3.10786319 1.28486013
H -0.34402812 -3.17482162 0.35548779
H -1.48381722 -2.57699943 1.17517054

Lu(NO₃)₃(H₂O)₄

PBE/L1 theoretical level

E= -15716.911897

G= 56.7595 kcal/mol, H= 106.3943 kcal/mol, U= 105.8018 kcal/mol, S= 166.4759 cal/mol at T= 298.150 K

Lu	0.12668742	0.35841832	-0.20042945
N	-2.62425399	0.35054472	-0.29543921
O	-1.90557230	1.30995774	-0.79433483
O	-3.82842660	0.34133789	-0.30528688
O	-1.90943384	-0.62477821	0.22348505
N	0.17094085	-1.78774416	-2.02344322
O	0.55622333	-1.91212308	-0.77958149
O	-0.18877026	-0.58001471	-2.33218980
O	0.14686915	-2.71088982	-2.79986167
N	0.24010830	2.45321631	1.70221746
O	1.03164172	2.33433628	0.65940946
O	0.32507646	3.37442040	2.47858071
O	-0.62326503	1.49553275	1.81062424
O	0.73080158	1.88078153	-1.97037554
H	0.44796687	2.80497503	-1.82483065
H	0.30917731	1.57729650	-2.80044103
O	0.77543509	-0.81970644	1.74968612
H	0.39504921	-0.27447397	2.47114968
H	0.24111941	-1.70166075	1.76875579
O	2.51866770	0.14566690	-0.34323007
H	2.88954473	1.01294971	-0.07739831
H	2.73322892	-0.46658224	0.39247599
O	-0.69520992	-2.96099830	1.46360791
H	-0.31985083	-3.09278703	0.56127381
H	-1.54375529	-2.50767541	1.26557612

Am(NO₃)₃(H₂O)₄

PBE/L1 theoretical level

E= -31261.185570

G= 54.1532 kcal/mol, H= 105.7675 kcal/mol, U= 105.1750 kcal/mol, S= 173.1151 cal/mol at T= 298.150 K

Am 0.06713514 0.46687964 -0.24284039
N -2.79886293 0.02605263 0.01149526
O -2.27314067 0.70795095 -0.95175278
O -3.98163986 -0.19636983 0.10788497
O -1.92476392 -0.42099205 0.89427108
N 0.13592091 -1.64116311 -2.27282357
O 0.07820817 -1.89856589 -0.99310911
O 0.16058552 -0.37241259 -2.55145907
O 0.16165528 -2.50507379 -3.11551929
N 0.11141367 2.81689000 1.48616779
O -0.42412046 2.81345582 0.29727316
O 0.12208175 3.79167414 2.19891024
O 0.63490289 1.67503357 1.83576417
O 1.11655056 2.11161590 -1.90257215
H 0.64308649 2.96747279 -1.86902094
H 1.01431656 1.76169217 -2.81134510
O 0.91491777 -1.07239008 1.68158519
H 0.77815431 -0.58801961 2.51986933
H 0.29322875 -1.89474750 1.70708072
O 2.57597685 -0.08615001 -0.14185189
H 3.25181055 0.58746982 0.06114447
H 2.44765568 -0.62261635 0.68156582
O -0.85840148 -2.96349478 1.46347153
H -0.65836138 -3.16133070 0.52195871
H -1.58831000 -2.30286121 1.38385177

Cm(NO₃)₃(H₂O)₄

PBE/L1 theoretical level

E= -32403.327034

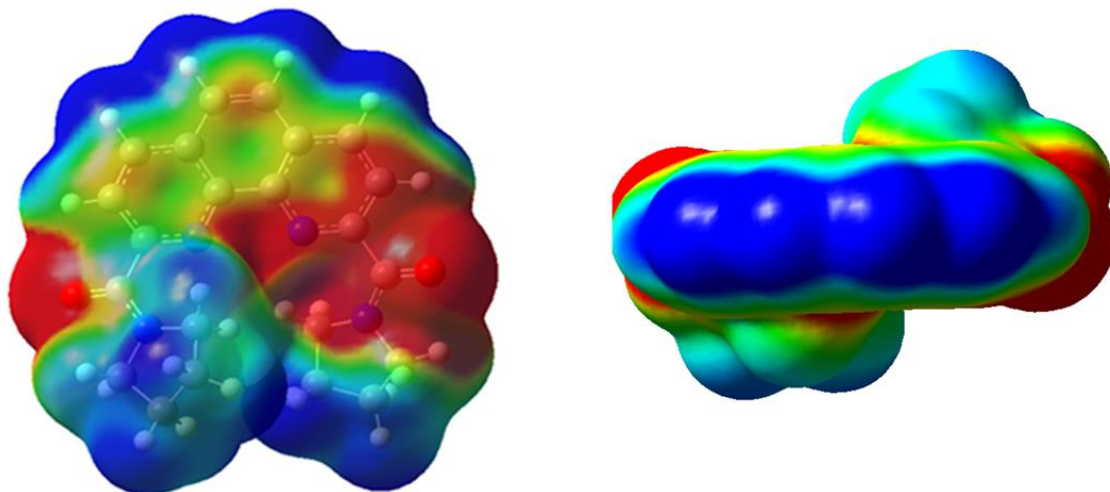
G= 54.7254 kcal/mol, H= 105.8937 kcal/mol, U= 105.3012 kcal/mol, S= 171.6193 cal/mol at T= 298.150 K

Cm 0.15520579 0.41810909 -0.19832096
N -2.72203827 0.06833909 -0.18989702
O -2.09969997 0.66250682 -1.15310752
O -3.91591835 -0.10410449 -0.16617562
O -1.93341780 -0.35140899 0.78443229
N 0.34402183 -1.66690385 -2.22729659
O 0.02165945 -1.92169440 -0.98386335
O 0.58591336 -0.41337365 -2.46276426
O 0.40835574 -2.52468777 -3.07399559
N 0.40501738 2.80899453 1.44601929
O -0.63250899 2.59557343 0.69520336
O 0.54196626 3.80205727 2.12078547
O 1.30245769 1.85184979 1.41445768
O 0.56330711 2.26871443 -1.87551916
H -0.10888156 2.97256207 -1.77229524
H 0.46319327 1.91228354 -2.78223228
O 0.81837857 -1.07368577 1.76596069
H 0.77476394 -0.65953147 2.64925265
H 0.16159032 -1.87639976 1.76945066
O 2.64212871 -0.24390469 -0.07299761
H 3.18172669 0.51307493 0.23118652
H 2.47065926 -0.77601337 0.74214077
O -0.98641187 -2.90197062 1.46679401
H -0.74668479 -3.13408732 0.54173040
H -1.69478405 -2.22629881 1.33105147

ESP maps of ligands

Gaussian 16¹¹ was used for optimization of ligands at B3LYP/6-31G(d,p) and to create ESP maps.

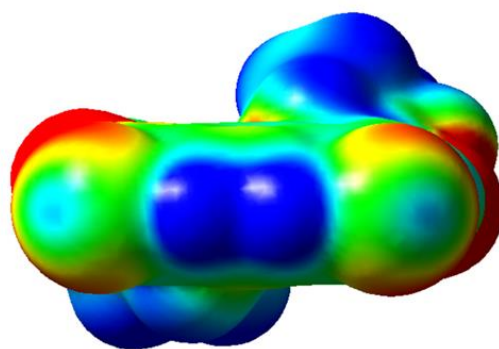
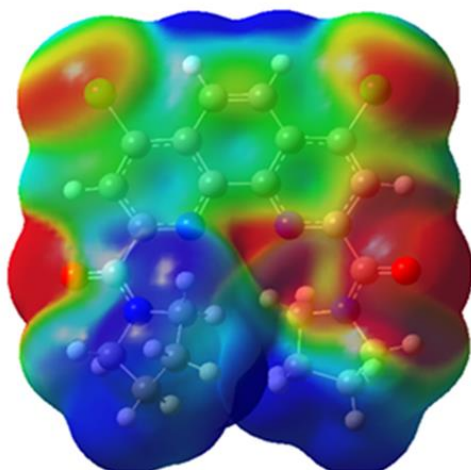
L1



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N	-2.90557718	-1.28621435	0.20480818
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O	-4.50823021	-0.26214826	-1.02372181
C	2.63914585	1.29034078	0.30650815
C	3.36834192	2.49392271	0.45793816
H	4.43502283	2.44001579	0.63657820
C	2.68768883	3.68666077	0.37683818
C	1.28767884	3.68378687	0.17900819
C	0.52360594	4.89185476	0.07602818
H	1.04469287	5.84254694	0.14957818
C	-0.82440406	4.85260201	-0.11465182
H	-1.39814615	5.77140999	-0.20014182
C	-1.51998115	3.60251975	-0.20211181
C	-2.91784000	3.52704573	-0.40001184
C	-3.53178716	2.29789376	-0.46556184
H	-4.59429693	2.18129086	-0.63940179
C	-2.73706412	1.13871574	-0.30182183
C	-0.80492705	2.37643170	-0.08904182
C	0.64163297	2.41904593	0.08188818

C 3.42388892 -0.00069723 0.42547816
C -3.44679022 -0.19430524 -0.39579183
C 1.90388286 -1.27139115 -1.20042181
H 2.17099094 -0.75537020 -2.13371181
H 0.97690195 -0.83546323 -0.83359182
C 1.84088695 -2.78825116 -1.41826189
H 1.20743787 -3.24833322 -0.65045178
H 1.42366791 -3.04807210 -2.39489198
C 3.29996800 -3.23547721 -1.23629189
H 3.87026691 -3.03382611 -2.15042186
H 3.40222096 -4.30004740 -1.00967181
C 3.80494595 -2.34510612 -0.09332182
H 3.64557695 -2.80832624 0.88892817
H 4.86623478 -2.09349322 -0.16052182
C -3.61751413 -2.56953621 0.07472818
H -3.76073313 -2.81887627 -0.98013180
H -4.61609411 -2.48724914 0.52255821
C -2.72444105 -3.56019306 0.83196819
C -2.06423306 -2.68423223 1.90819812
C -1.78921711 -1.36738133 1.16737819
H -1.15290213 -3.11957908 2.32712817
H -2.76425409 -2.51273417 2.73427820
H -1.96090007 -3.97039127 0.16065818
H -3.29190922 -4.39931536 1.24279809
H -1.77296913 -0.49838126 1.82679808
H -0.82770705 -1.39073825 0.64525819
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H 3.21108699 4.63498306 0.46712816

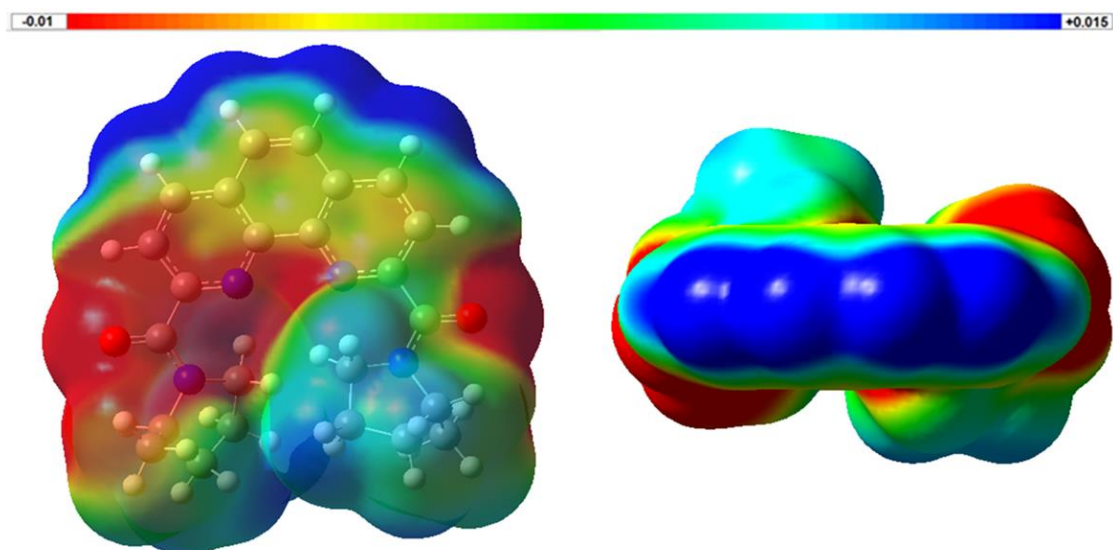
L2



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Cl	4.16207314	-3.59611607	-0.46989000
N	-1.33147800	-0.30457500	0.08970000
N	-3.13962603	1.95556903	-0.32675999
N	1.37852097	-0.02488500	-0.07314000
N	2.65915203	2.54526901	0.32799000
O	-4.57184219	0.73954397	0.94410998
O	4.35595512	1.66217506	-0.88600999
C	-2.64269805	-0.42088899	0.22141001
C	-3.30267406	-1.66274095	0.36214000
H	-4.37392378	-1.68159497	0.51191998
C	-2.54312992	-2.80640888	0.30726999
C	-1.13443995	-2.73516393	0.14843000
C	-0.27848601	-3.87794089	0.06567000
H	-0.72073299	-4.86526299	0.12396000
C	1.06769300	-3.73921704	-0.09109000
H	1.70054603	-4.61556387	-0.16265000
C	1.67550898	-2.44625401	-0.15871000
C	3.06936789	-2.23228002	-0.31983000
C	3.58314395	-0.95884800	-0.36324000
H	4.63592291	-0.75848401	-0.51234001
C	2.68695998	0.12272900	-0.21012001

C 0.86739498 -1.27520704 -0.06061000
C -0.57866502 -1.42458200 0.06632000
C -3.51950192 0.81399798 0.30256999
C 3.29349494 1.50889099 -0.27645999
C -2.03125691 2.16788292 -1.28398001
H -2.21061492 1.59422195 -2.20393991
H -1.08364606 1.83404601 -0.86587000
C -2.09464192 3.67594290 -1.55973995
H -1.52633405 4.21835518 -0.79479003
H -1.67206299 3.93411398 -2.53437996
C -3.59111309 4.00116777 -1.43431997
H -4.11579180 3.71244597 -2.35225010
H -3.79106688 5.06085682 -1.25569999
C -4.04794979 3.11661601 -0.26783001
H -3.93897200 3.62479591 0.69896001
H -5.08511877 2.78129292 -0.34053999
C 3.27476692 3.88116097 0.23083000
H 3.41082597 4.16048098 -0.81734002
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C 2.30171394 4.78695822 0.99492002
C 1.69666696 3.84335589 2.04632998
C 1.52832198 2.52441502 1.27789998
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L3

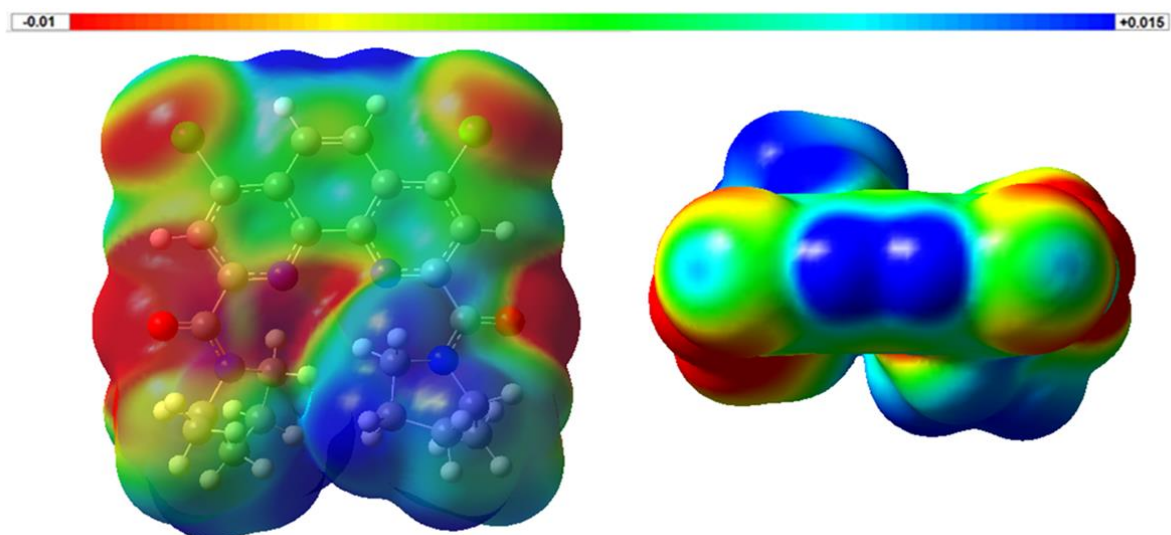


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H	-3.42201638	4.86860752	0.26880679
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N	2.87356782	-0.86179918	0.27552676
N	-1.40758514	1.55526280	0.05286678
N	-2.93791223	-0.89386326	-0.31729323
O	4.51097107	0.24230577	-0.85076320
O	-4.55917883	0.21075076	0.82765681
C	2.67109466	1.57139087	-0.17915322
C	3.43721771	2.75668883	-0.27900323
H	4.51132774	2.67636585	-0.39134324
C	2.78186059	3.96552086	-0.23678322
C	1.37304080	3.99539495	-0.12224322
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H	1.18025684	6.15920448	-0.11501322
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H	-1.28001320	6.14908171	0.08586678
C	-1.45386922	3.98341274	0.09417678
C	-2.86234927	3.93868685	0.21027677
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H	-4.57867193	2.63319087	0.37014678

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C 0.69234776 2.74630690 -0.06113322
C 3.42248058 0.25930876 -0.26633322
C -3.47216940 0.22687778 0.23885678
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H 0.83764678 -1.13194418 0.82978678
H 1.72163987 0.00009376 1.84205675
C 2.25803375 -2.11506820 2.17080665
H 3.00391459 -1.77579021 2.89896679
H 1.42713284 -2.56236506 2.72345662
C 2.89890170 -3.06939912 1.15532684
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H 3.58659959 -3.78937125 1.60729682
C 3.61708379 -2.14272118 0.15432678
H 4.65103483 -1.95603418 0.47176677
C 3.63820267 -2.67990112 -1.27707314
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H -2.00905132 -0.43340623 -2.17203331
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H 4.15594482 -1.98384309 -1.93868315
H -4.20932007 -3.72907996 1.15583682
H -2.54637837 -3.12593412 1.30833685
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L4



Cl 4.37977839 -4.90177155 -0.25780594
Cl 6.12345743 2.47765732 0.22914705
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N -1.52046049 -2.54835987 0.32970303
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C 3.56719160 -2.27216387 -0.09064296
C 4.92857170 -1.83492470 -0.04976895
H 5.71546030 -2.57886577 -0.08313996
C 5.24206066 -0.51143271 0.03125605

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H -3.02008247 -4.00314045 0.51076609
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C -1.25460041 4.08661556 -0.34817696
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C -2.21395922 3.66326833 -1.47627497
C -2.08198738 2.13357711 -1.51914597
C -0.59037244 1.89522326 -1.25840294
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H -2.67978144 1.67706633 -0.72213292
H -1.88478529 4.09323025 -2.42913985

H -3.23697948 4.00357723 -1.29398203
H -0.37097442 0.94049037 -0.78470194
H -0.01874340 1.93832624 -2.19566584
H -4.52837944 -3.09510779 -1.26480901
H -3.35836363 -1.80162871 -1.59332097
H -2.92001057 -3.50005078 -1.89625895
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H -2.43479538 3.25021529 1.28989804
H -1.16489136 4.38714933 1.79378295

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