

Sterically crowded phenanthrolinediamides: conformational behavior and photophysics of their complexes with Eu-Gd-Tb triad

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Supplementary Materials

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1. NMR and IR spectra of synthesized compounds

N^2,N^9 -bis(2,5-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide (**L2**)

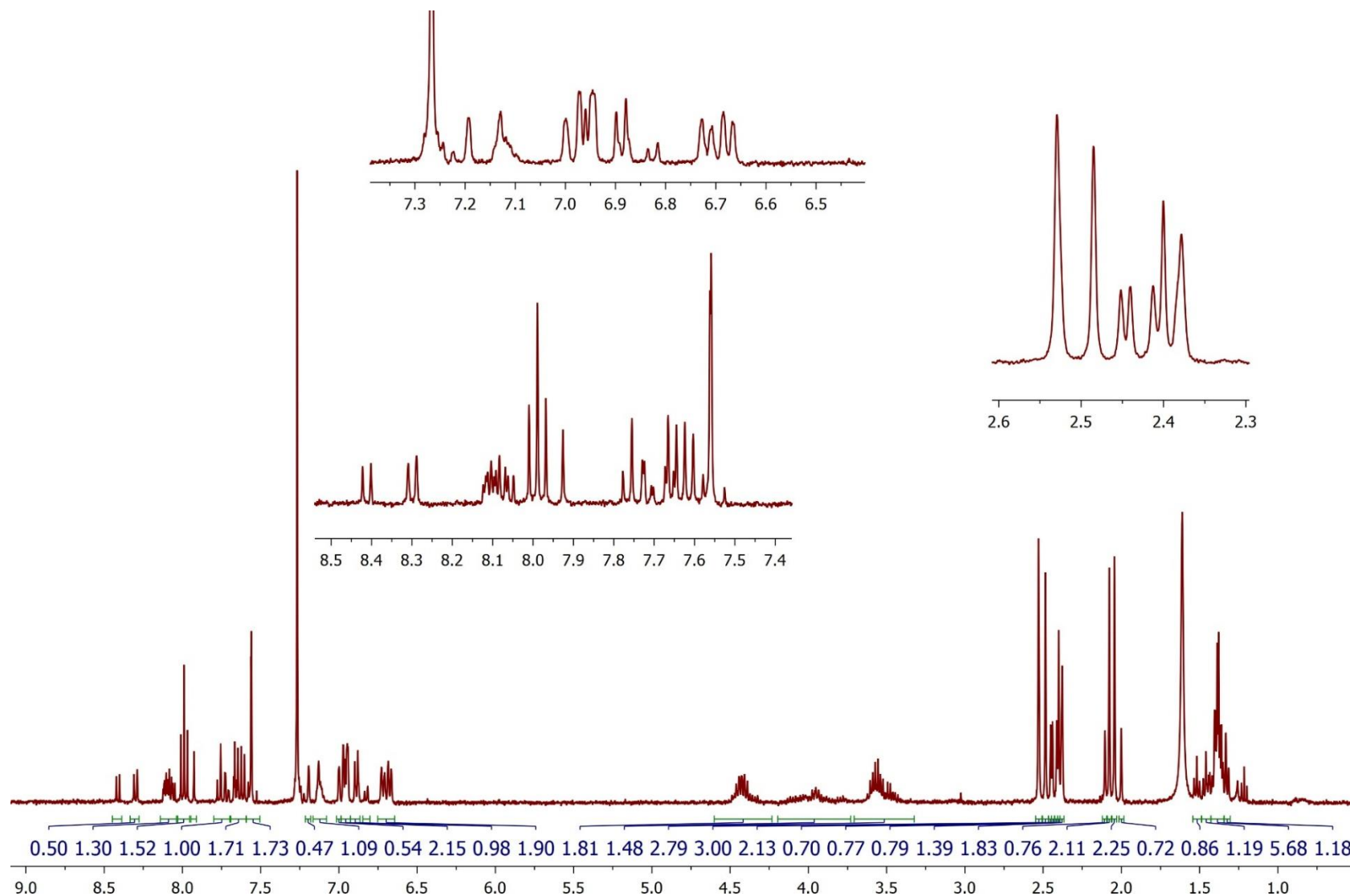


Figure S1. ^1H NMR spectrum in CDCl_3 at 25°C .

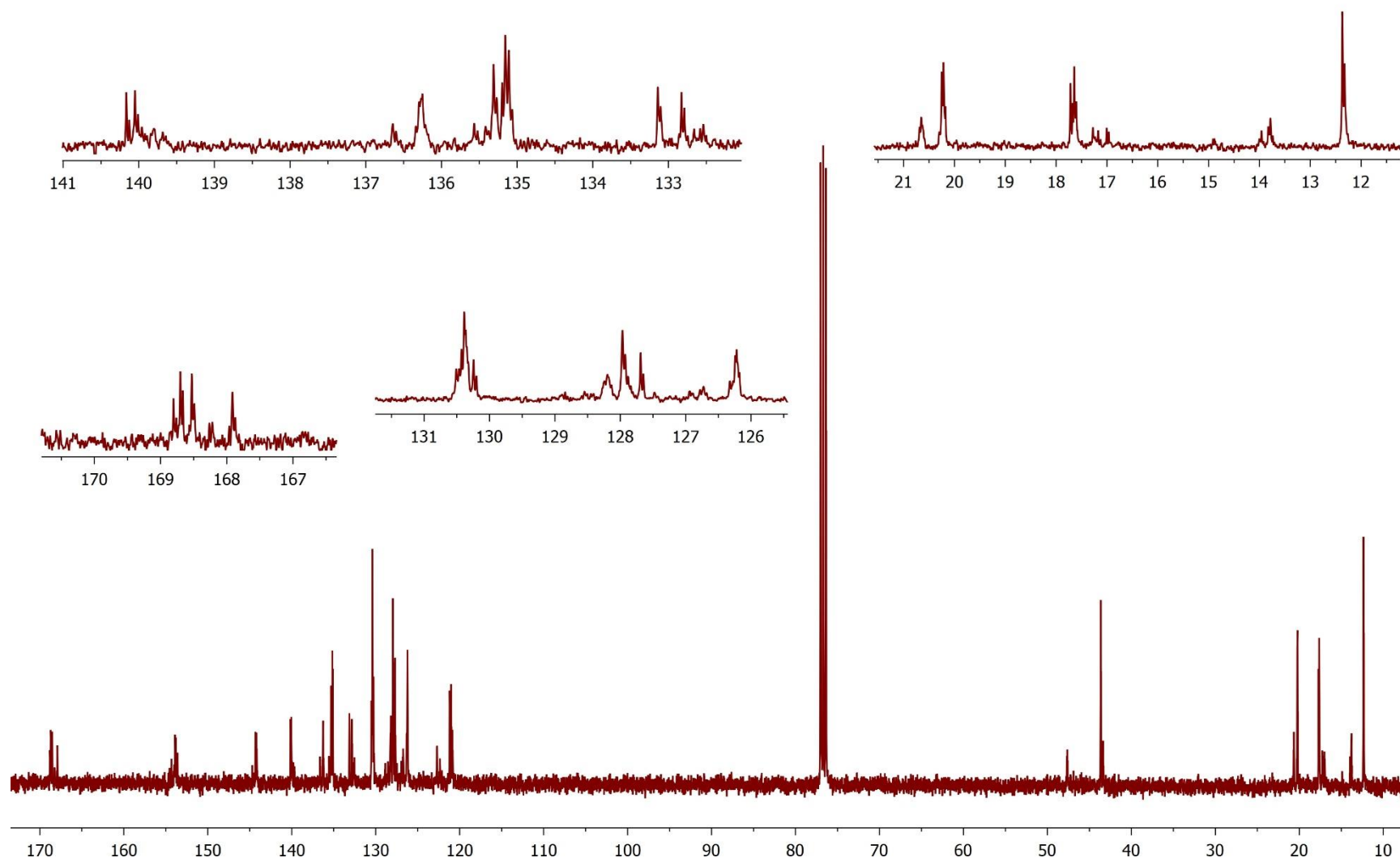


Figure S2. ^{13}C NMR spectrum in CDCl_3 at 25°C .

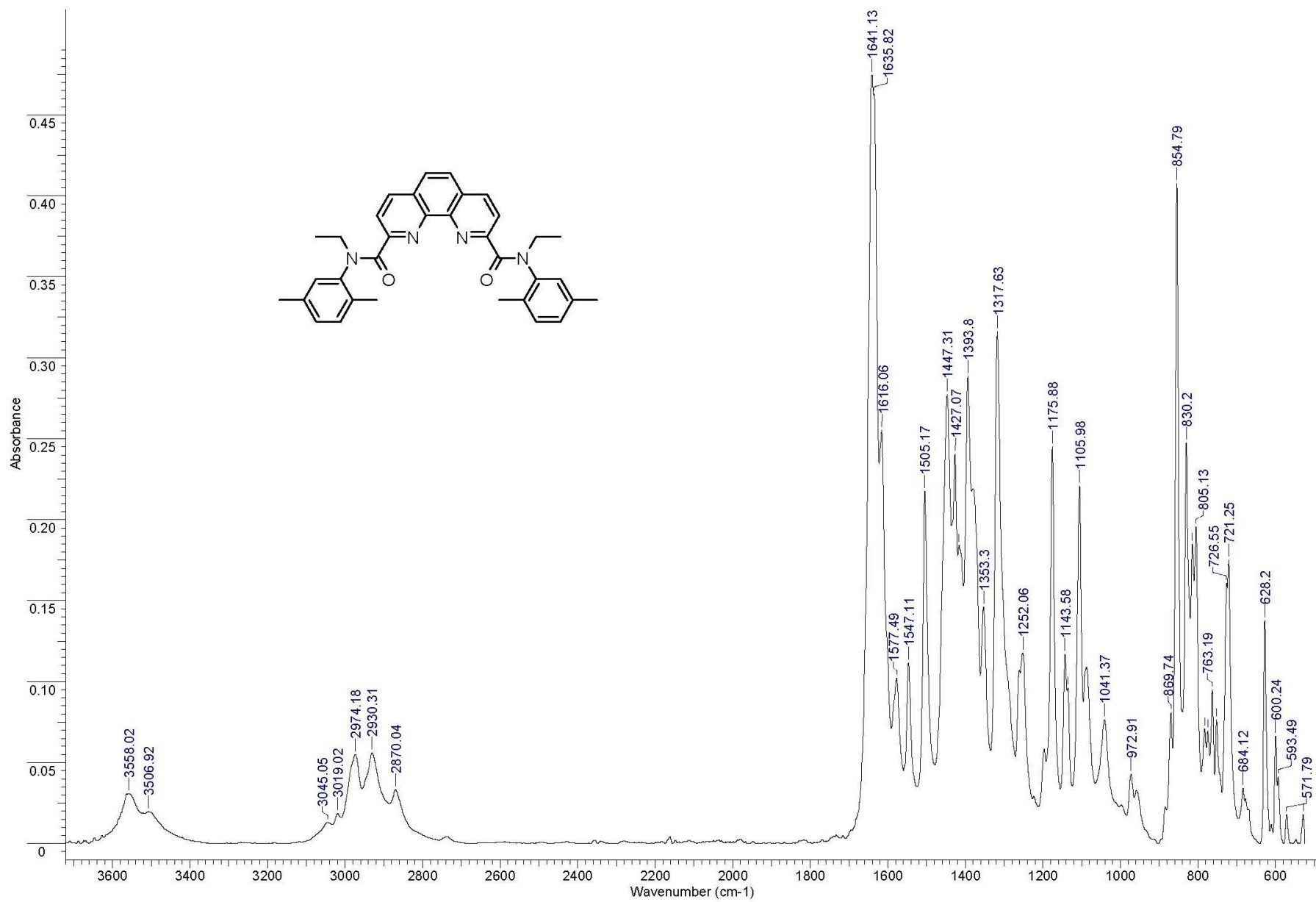


Figure S3. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,4-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide (**L3**)

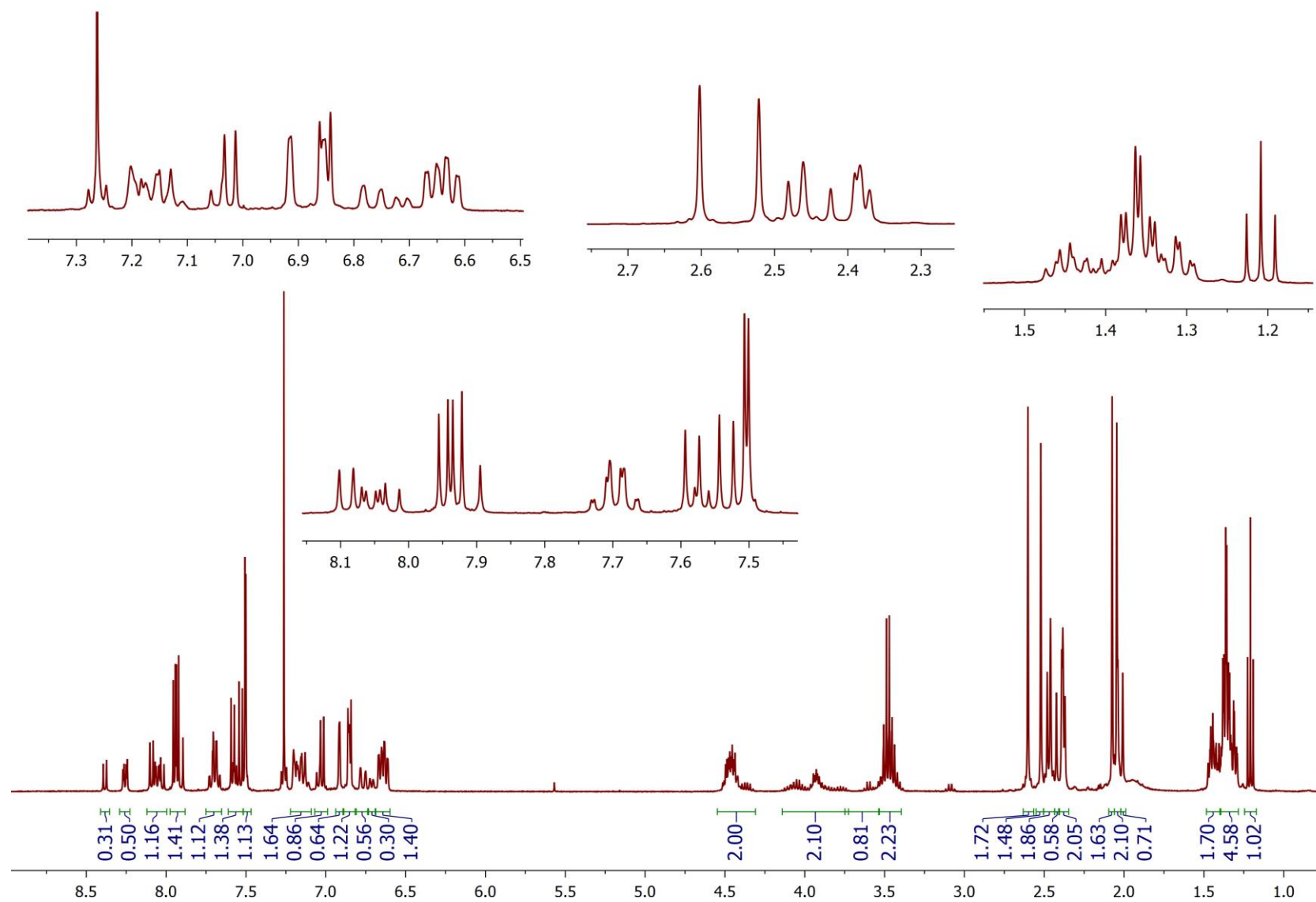


Figure S4. ^1H NMR spectrum in CDCl_3 at 25°C

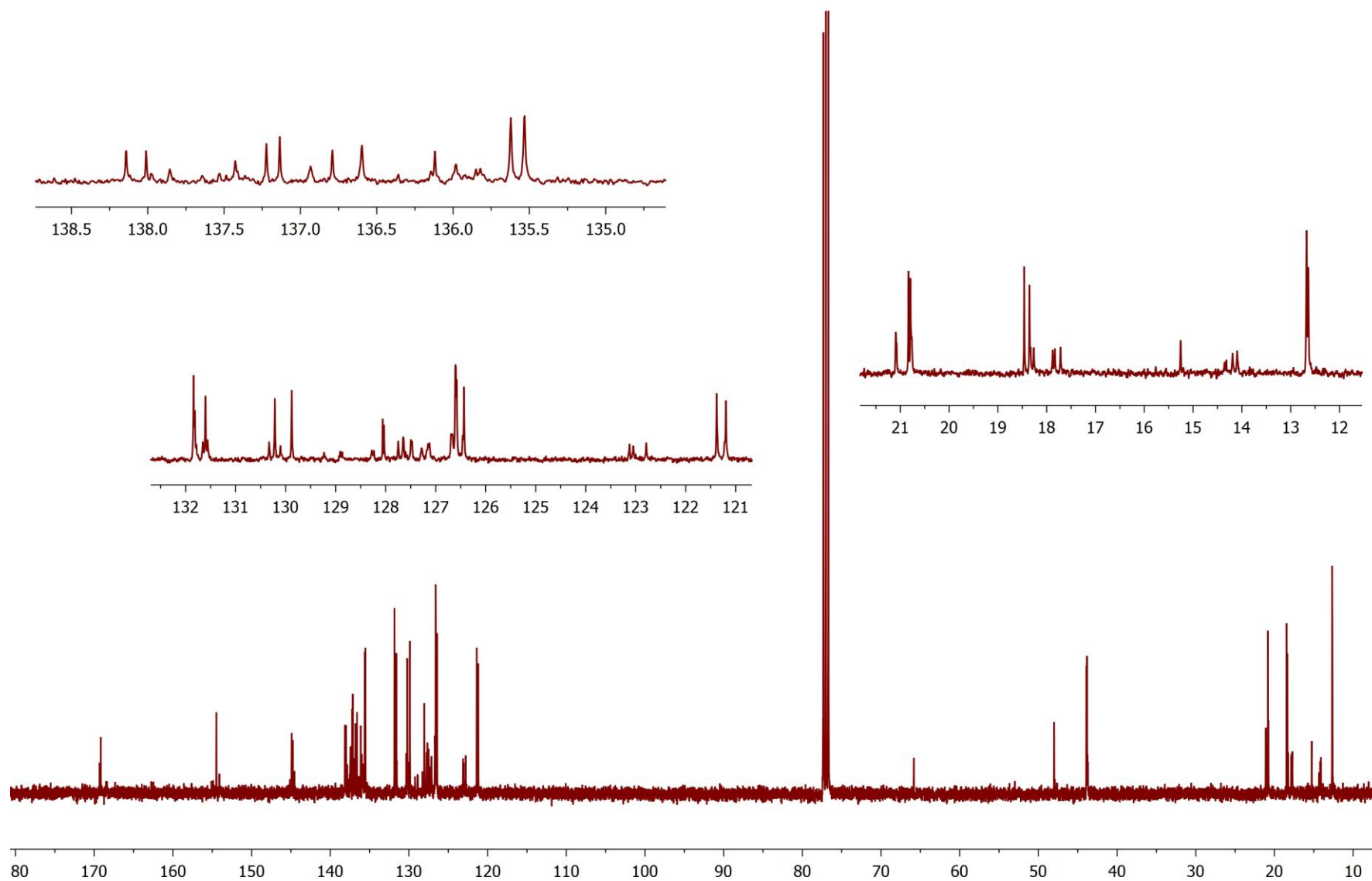


Figure S5. ^{13}C NMR spectrum in CDCl_3 at 25°C

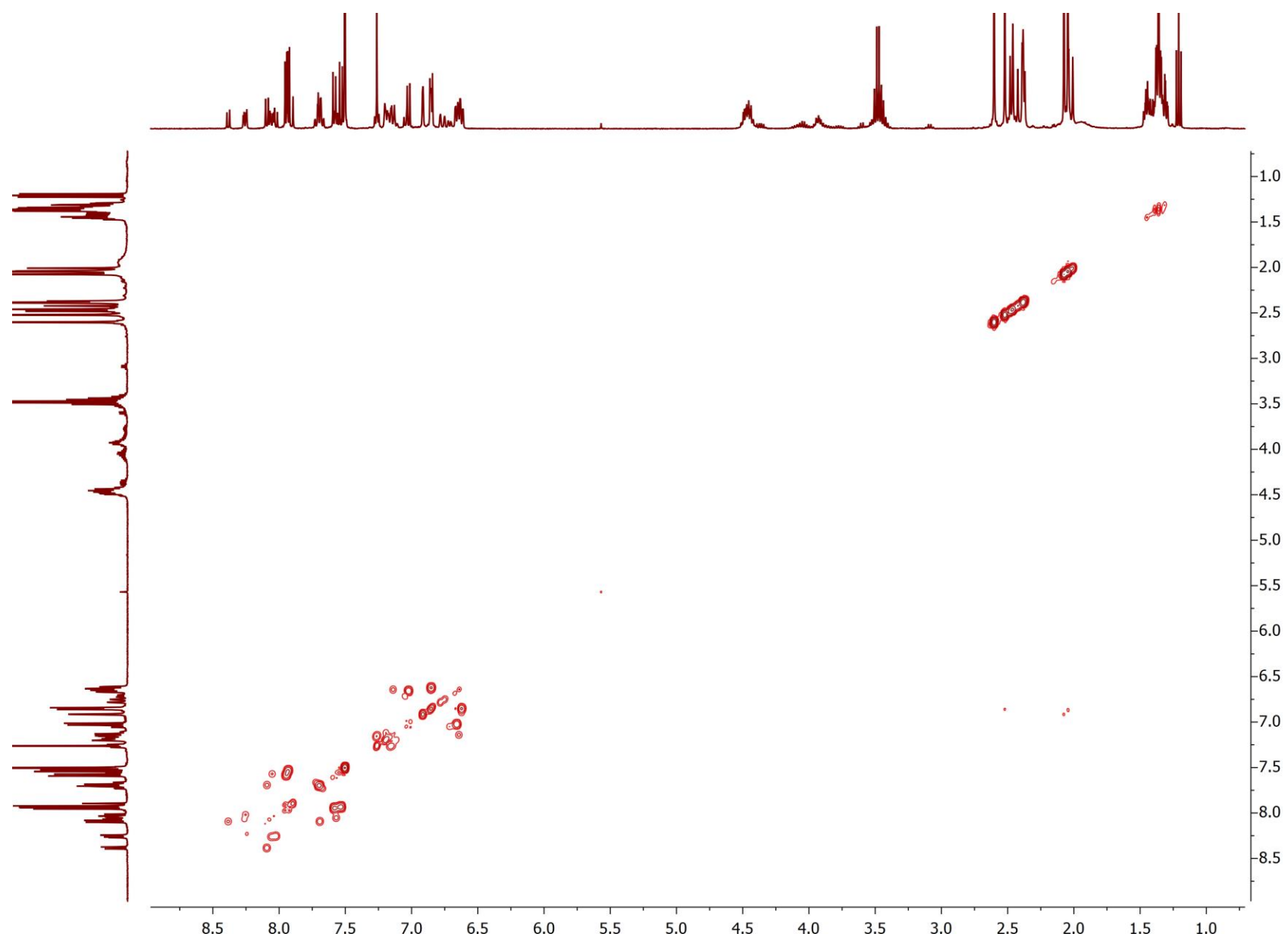


Figure S6. $^1\text{H}/^1\text{H}$ COSY NMR spectrum in CDCl_3 at 25°C.

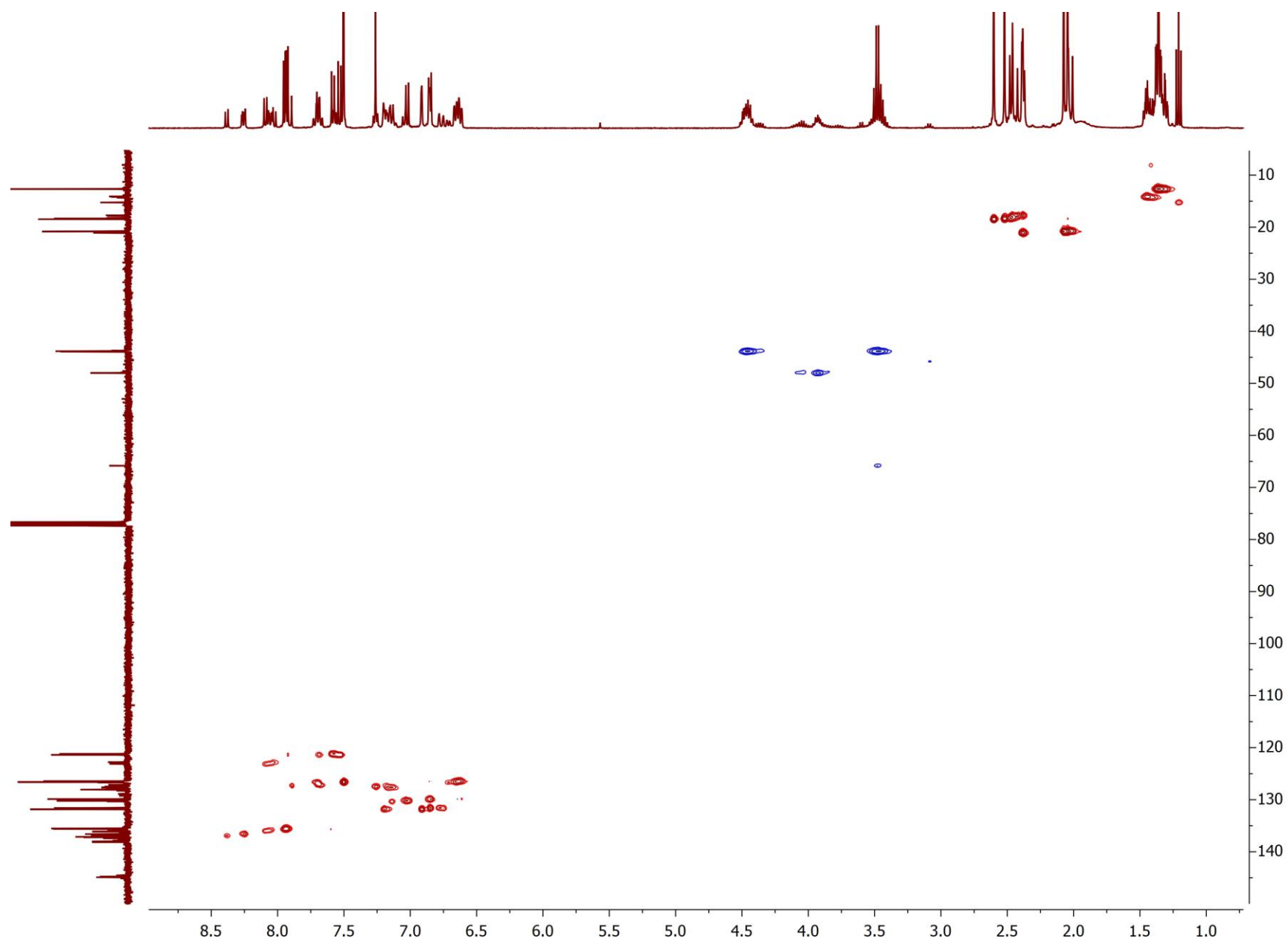


Figure S7. $^1\text{H}/^{13}\text{C}$ HSQC NMR spectrum in CDCl_3 at 25°C .

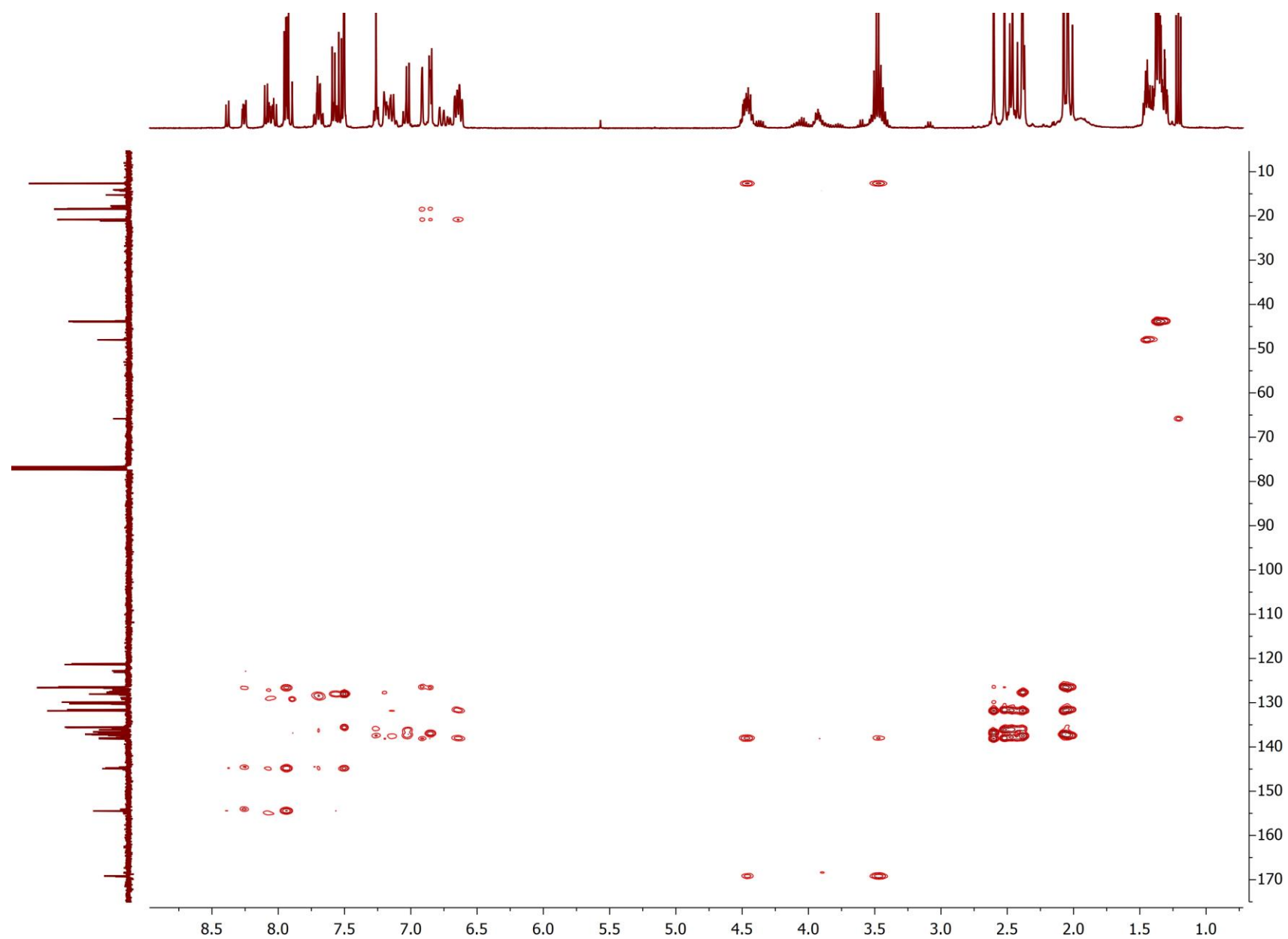


Figure S8. $^1\text{H}/^{13}\text{C}$ HMBC NMR spectrum in CDCl_3 at 25°C.

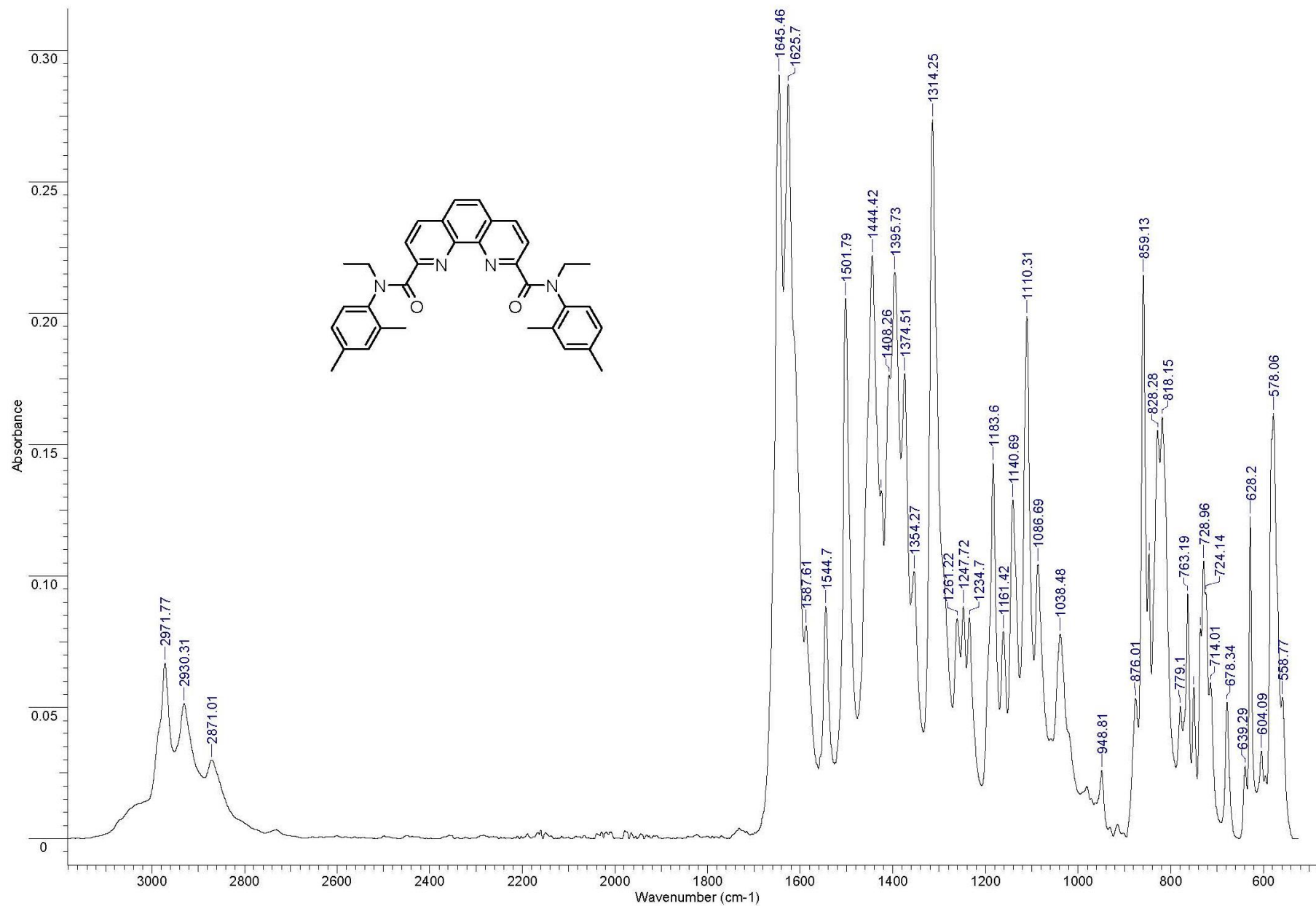


Figure S9. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,6-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide europium trinitrate **L1**•Eu(NO₃)₃

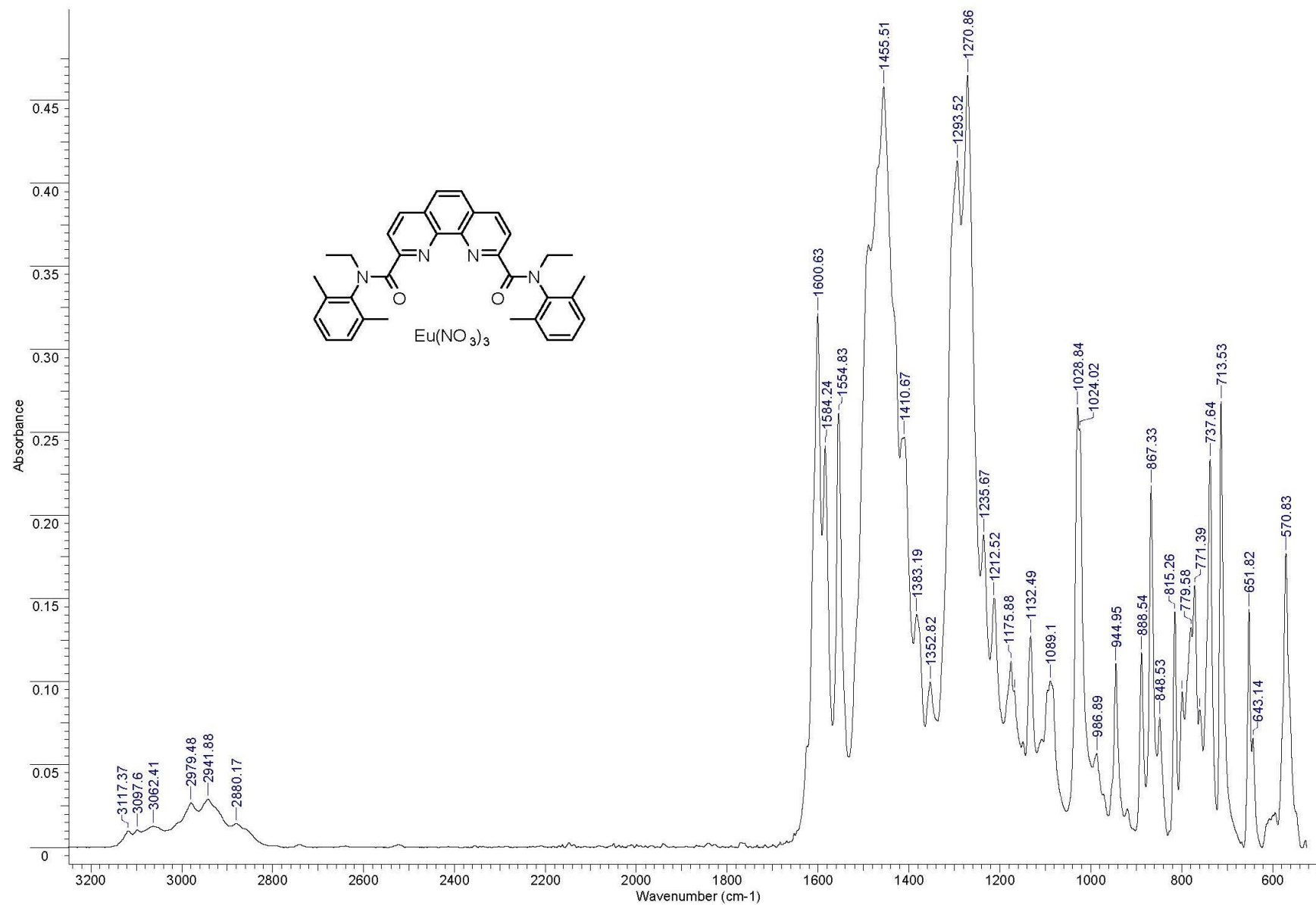


Figure S10. Solid-state IR spectrum at 25°C

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

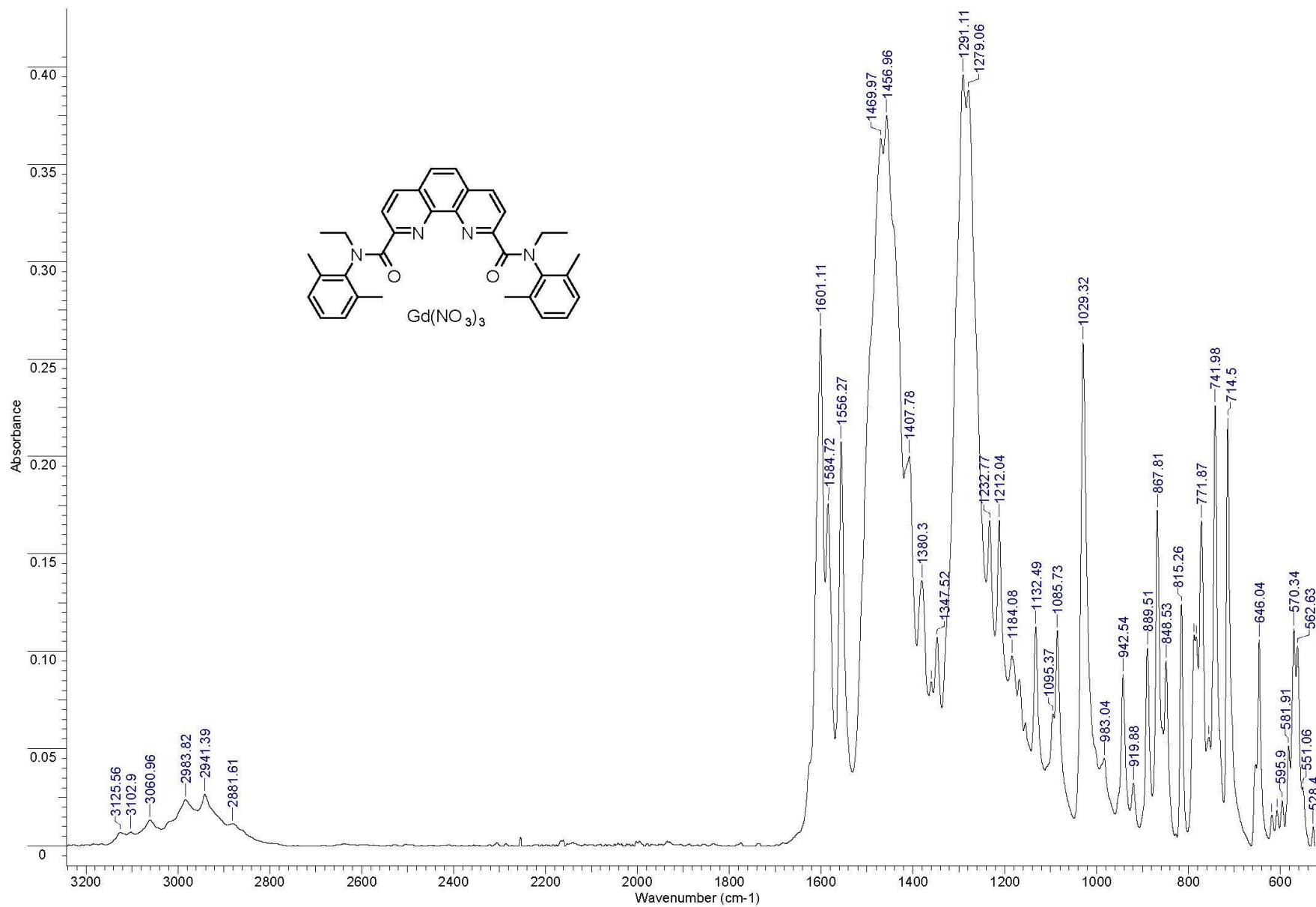


Figure S11. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,6-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide terbium trinitrate **L1**•**Tb(NO₃)₃**

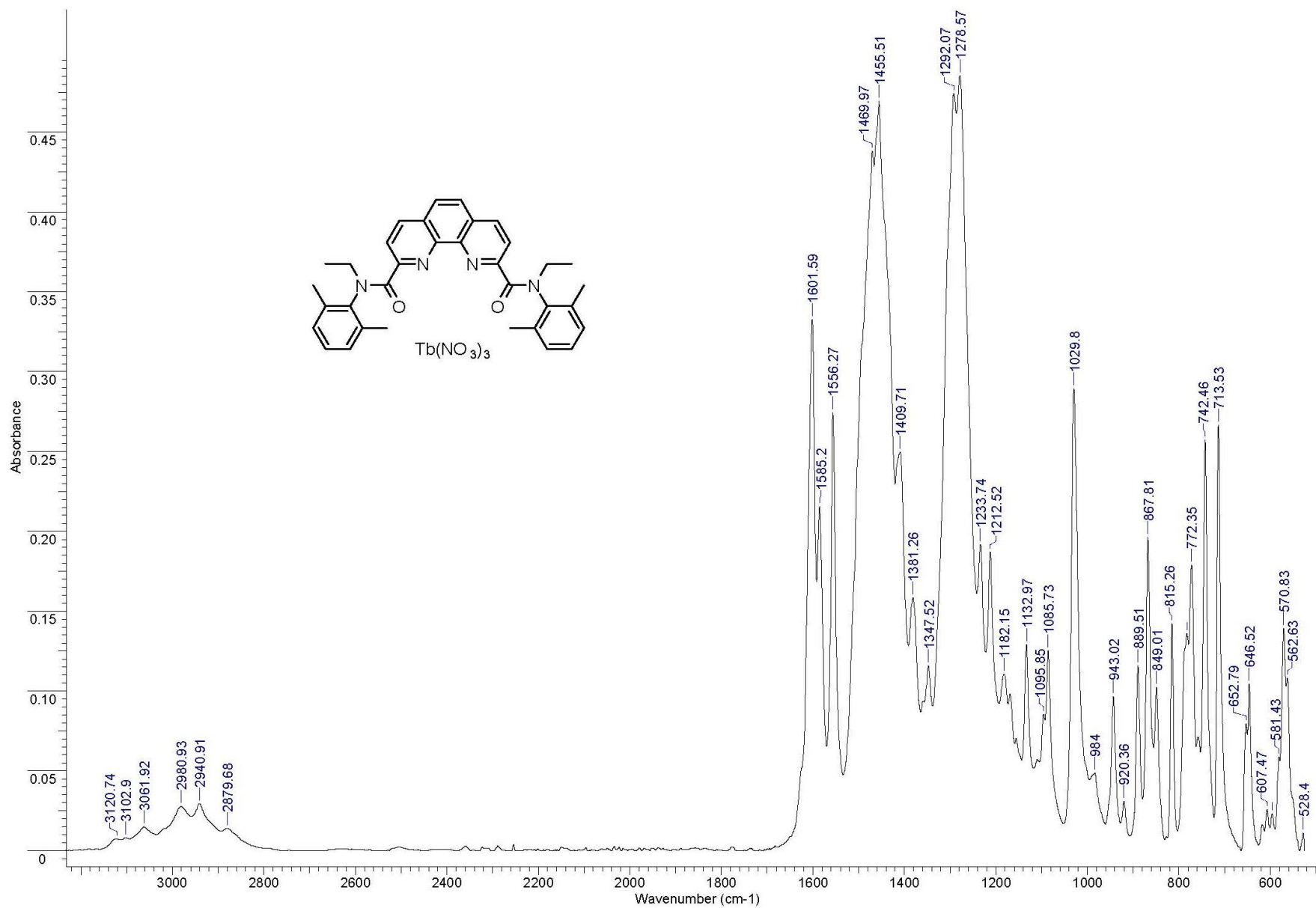


Figure S12. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,5-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide lanthanum trinitrate **L2**•**La(NO₃)₃**

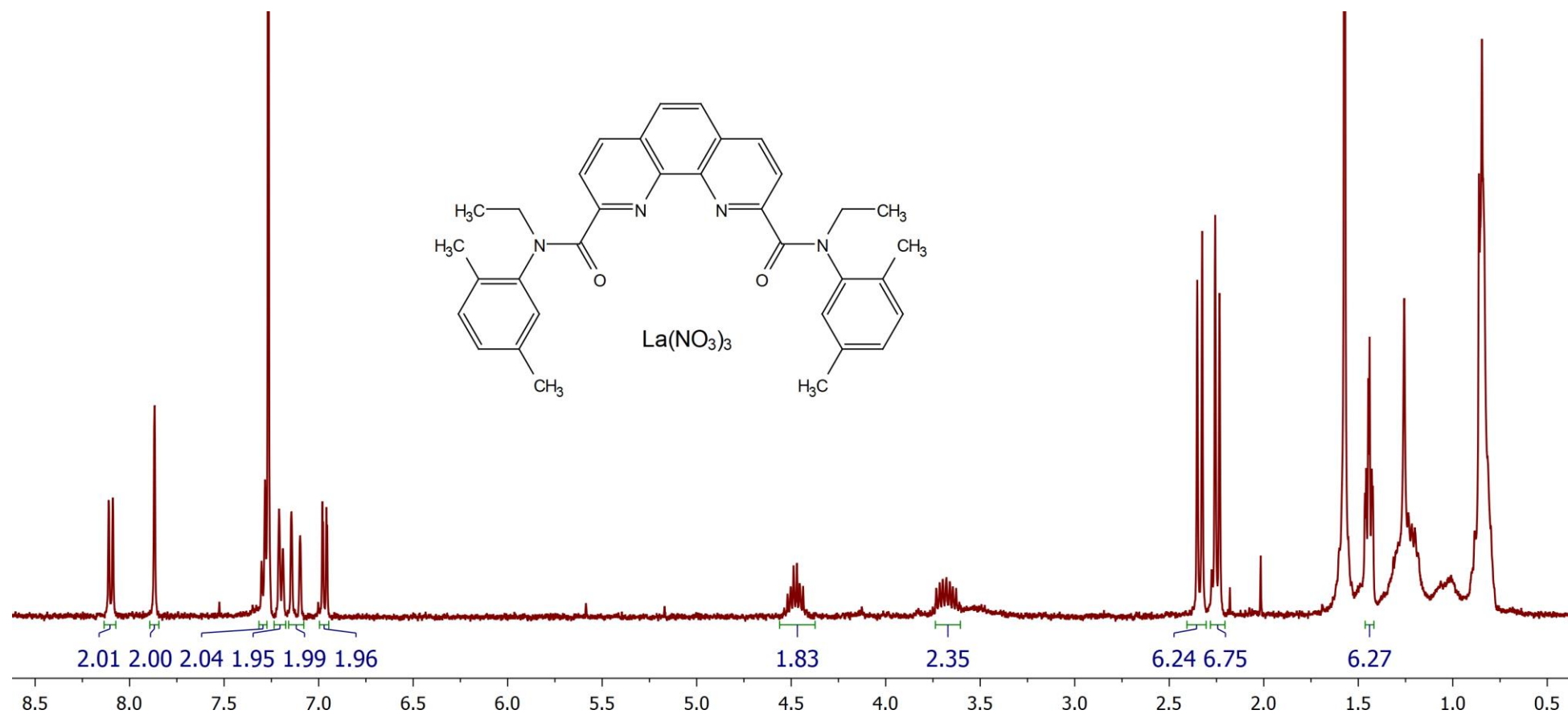


Figure S13. ^1H NMR spectrum in CDCl_3 at 25°C .

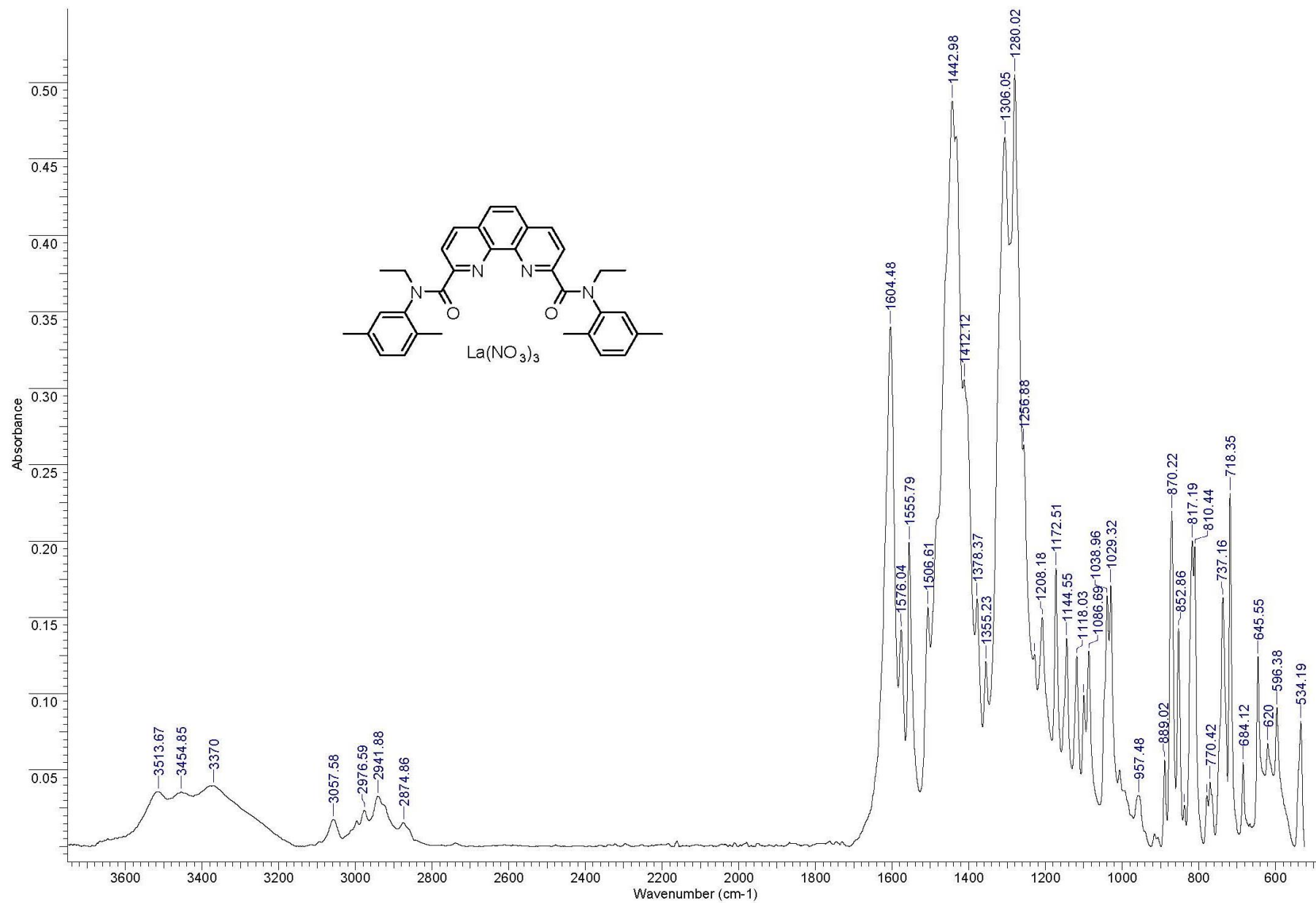


Figure S14. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,5-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide europium trinitrate **L2**• $\text{Eu}(\text{NO}_3)_3$

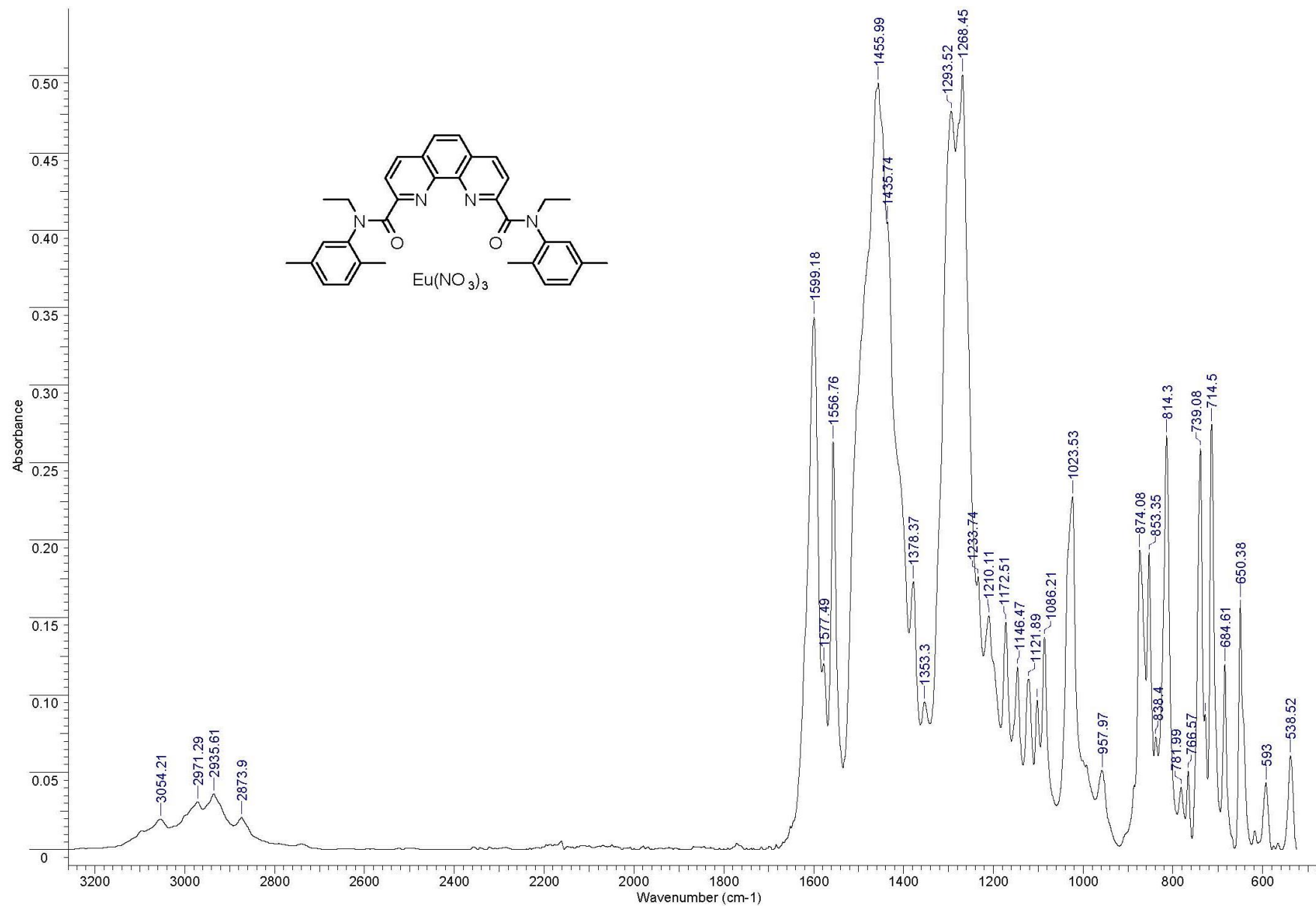


Figure S15. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,5-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide gadolinium trinitrate **L2**• $Gd(NO_3)_3$

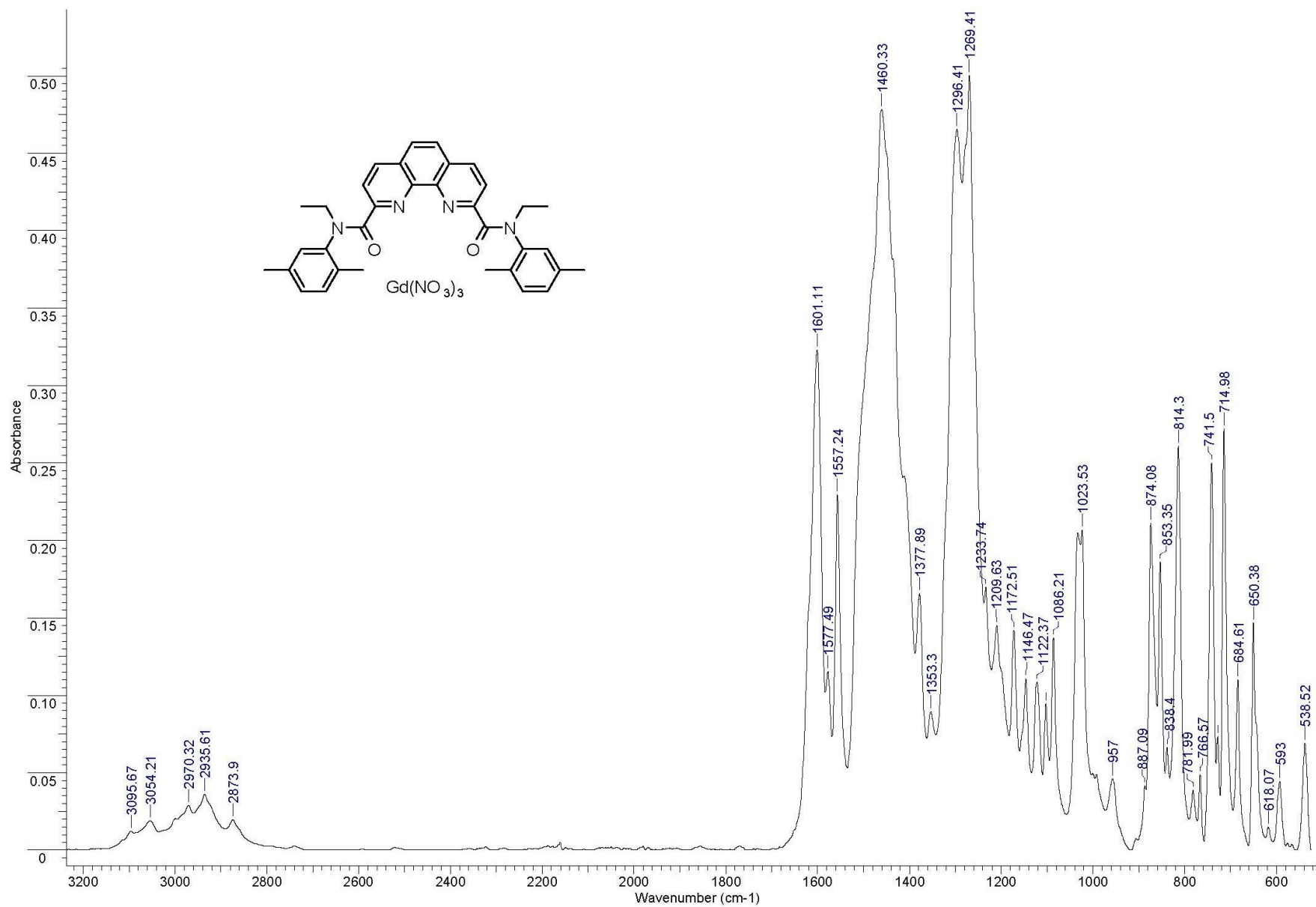


Figure S16. Solid-state IR spectrum at 25°C

N²,N⁹-bis(2,5-dimethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide terbium trinitrate **L2•Tb(NO₃)₃**

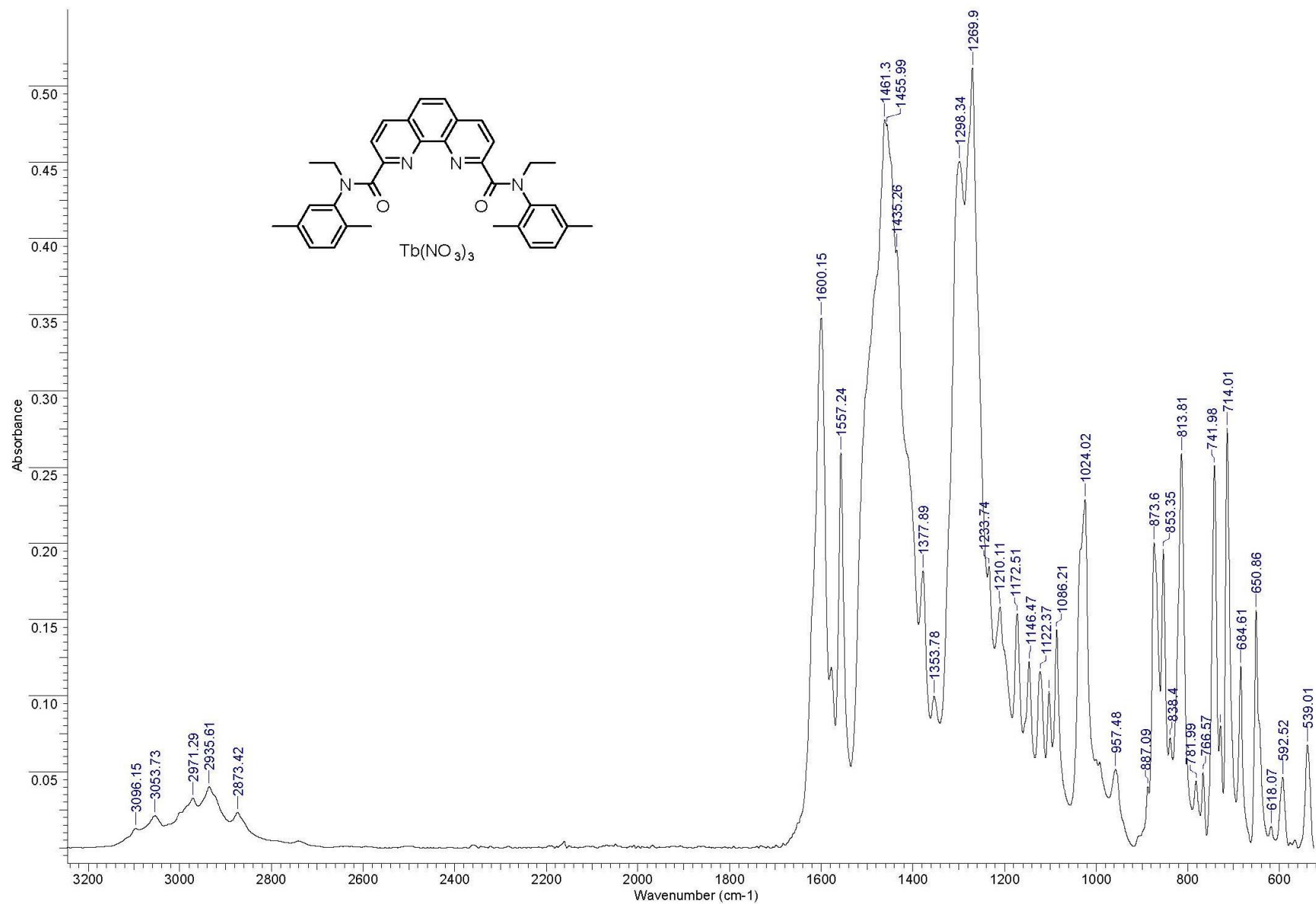


Figure S17. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,5-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide lutetium trinitrate **L2•Lu(NO₃)₃**

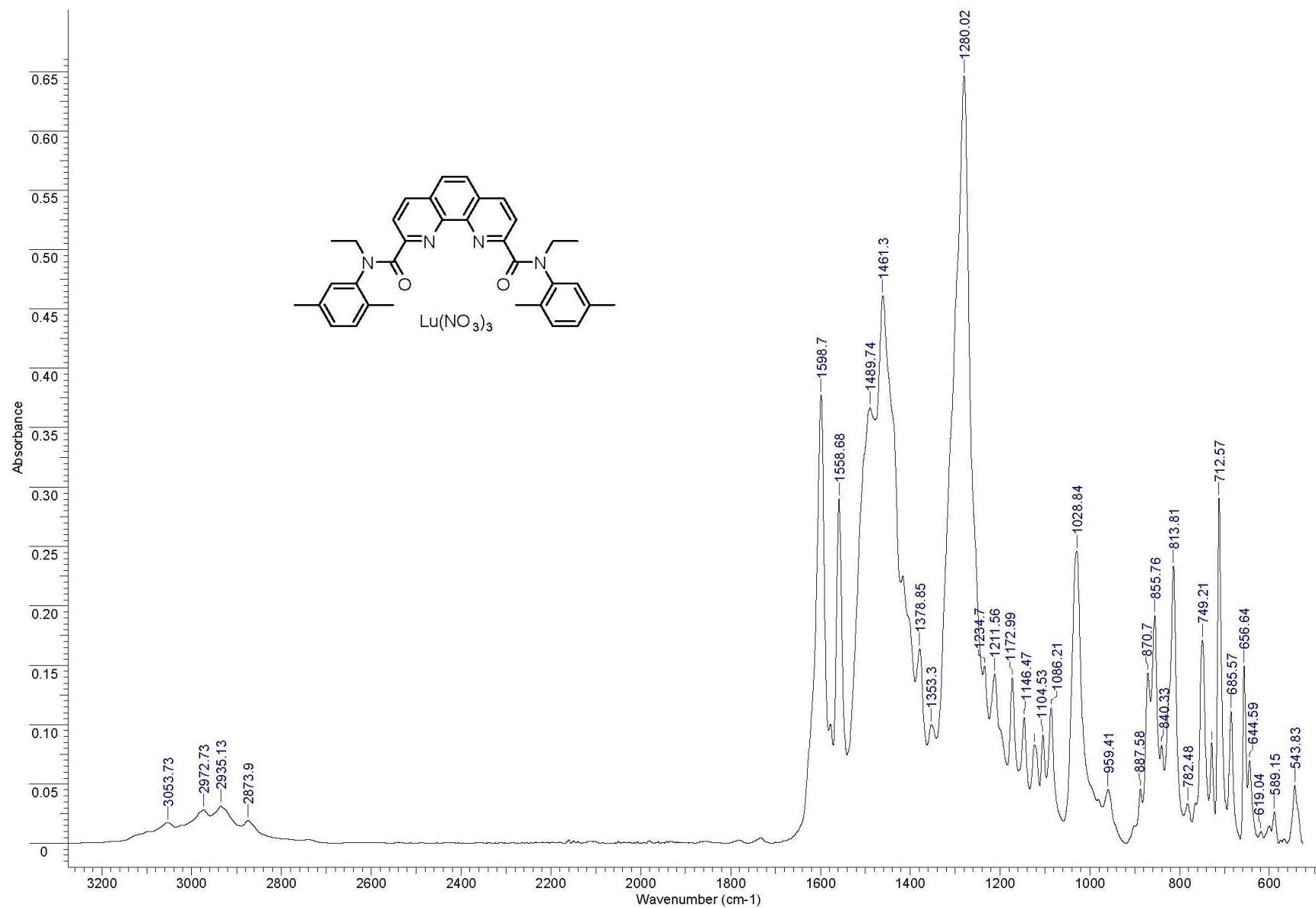


Figure S18. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,4-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide lanthanum trinitrate **L3**• $\text{La}(\text{NO}_3)_3$

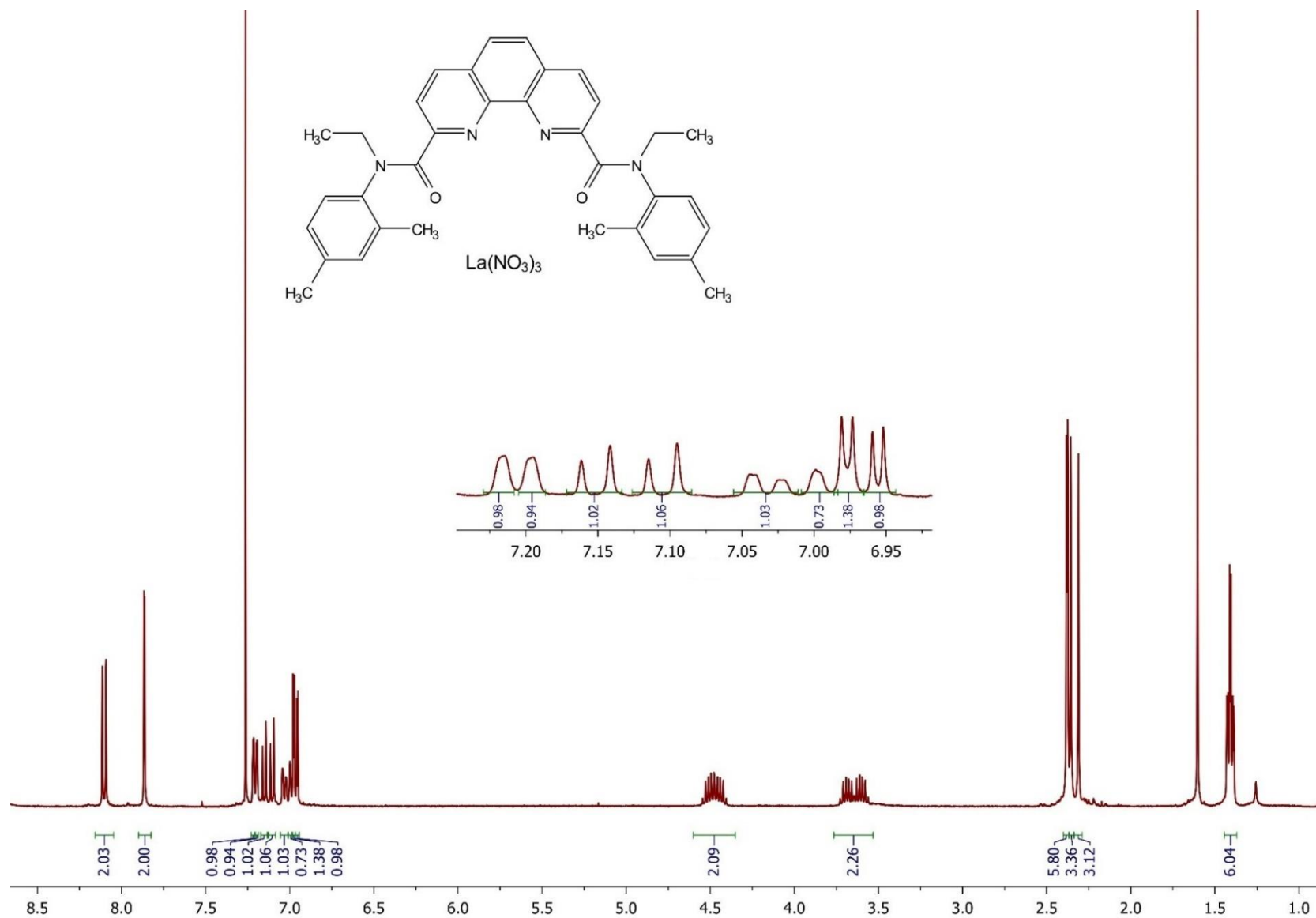


Figure S19. ^1H NMR spectrum in CDCl_3 at 25°C .

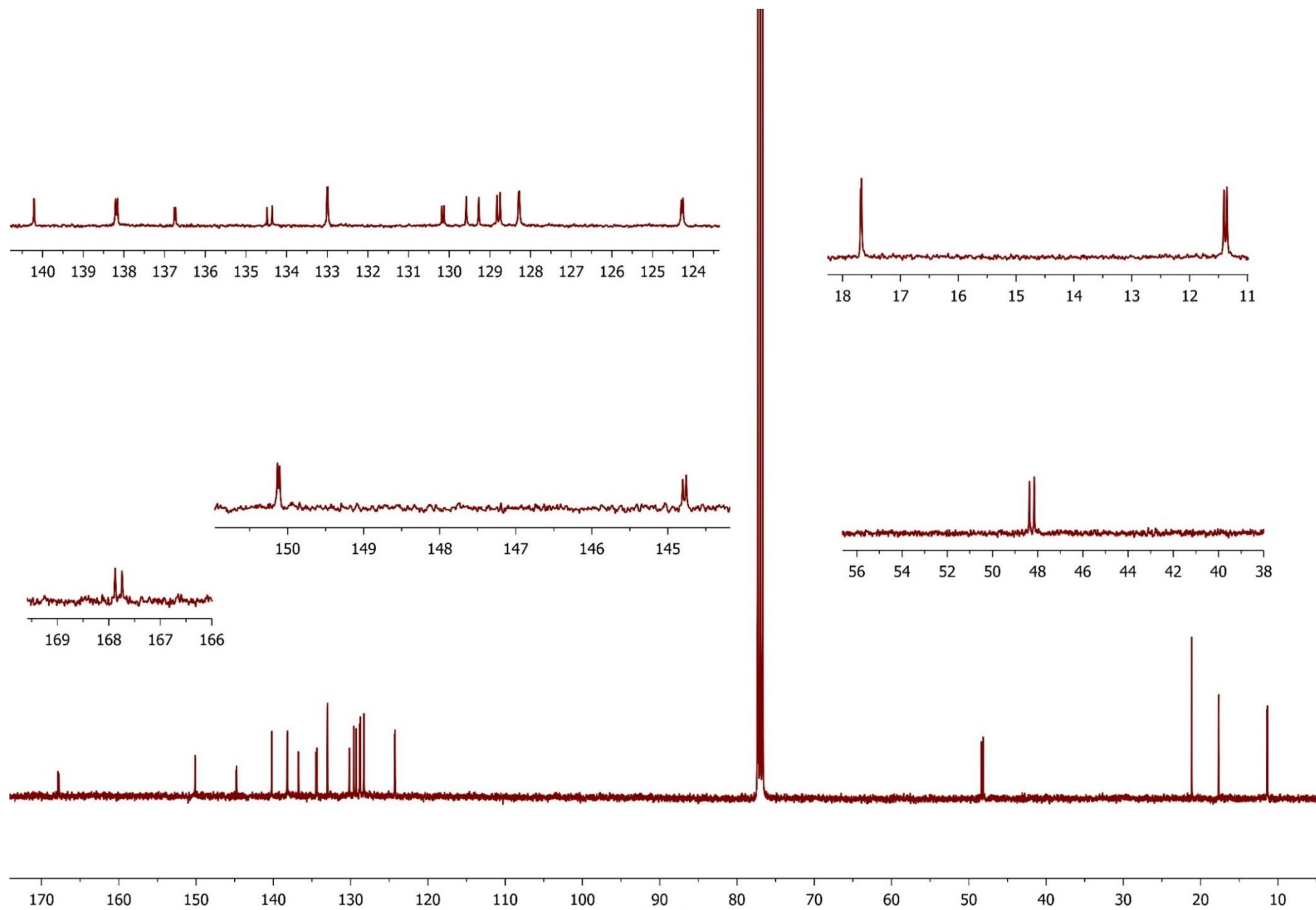


Figure S20. ^{13}C NMR spectrum in CDCl_3 at 25°C .

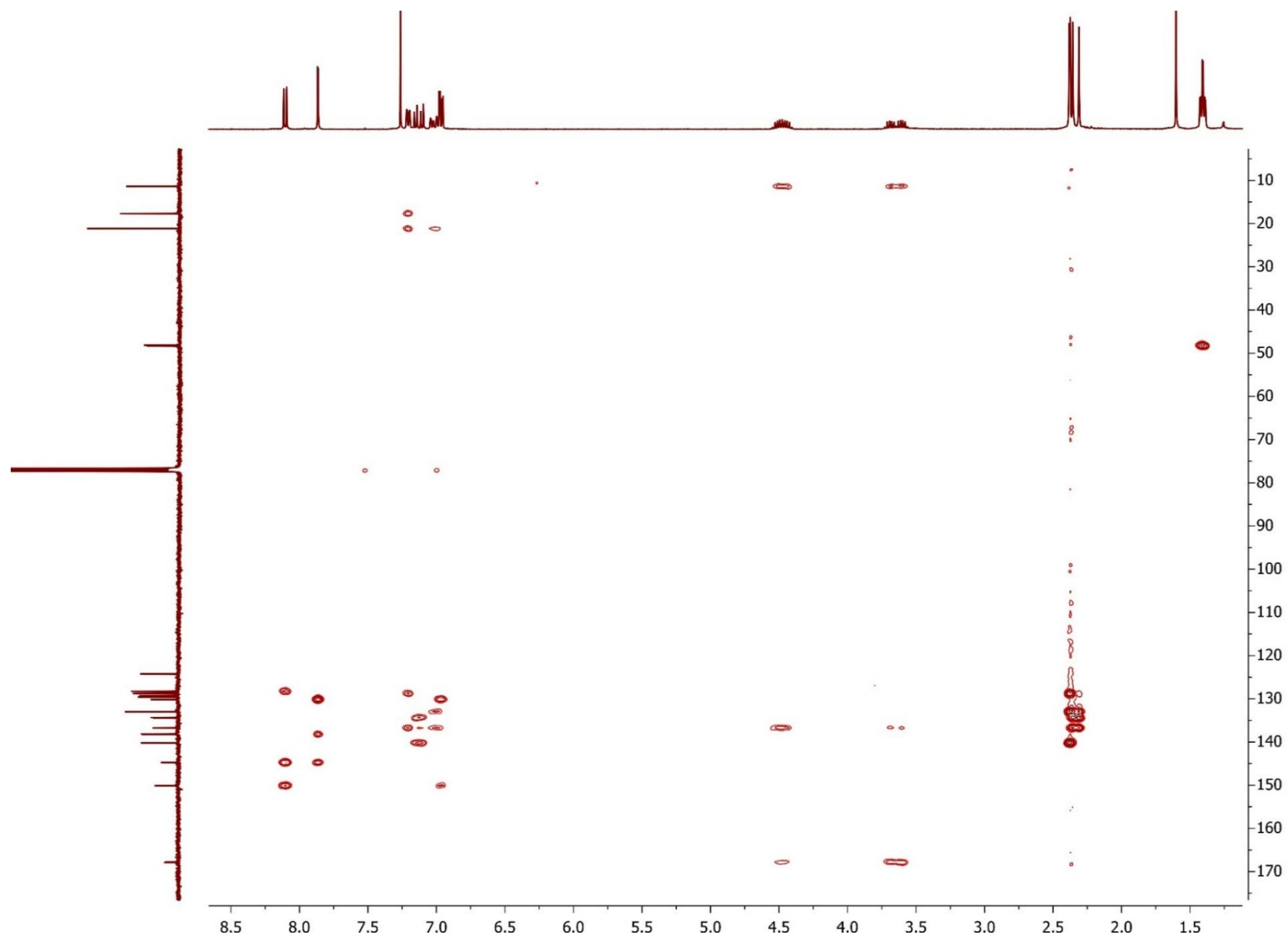


Figure S22. $^1\text{H}/^{13}\text{C}$ HMBC NMR spectrum in CDCl_3 at 25°C .

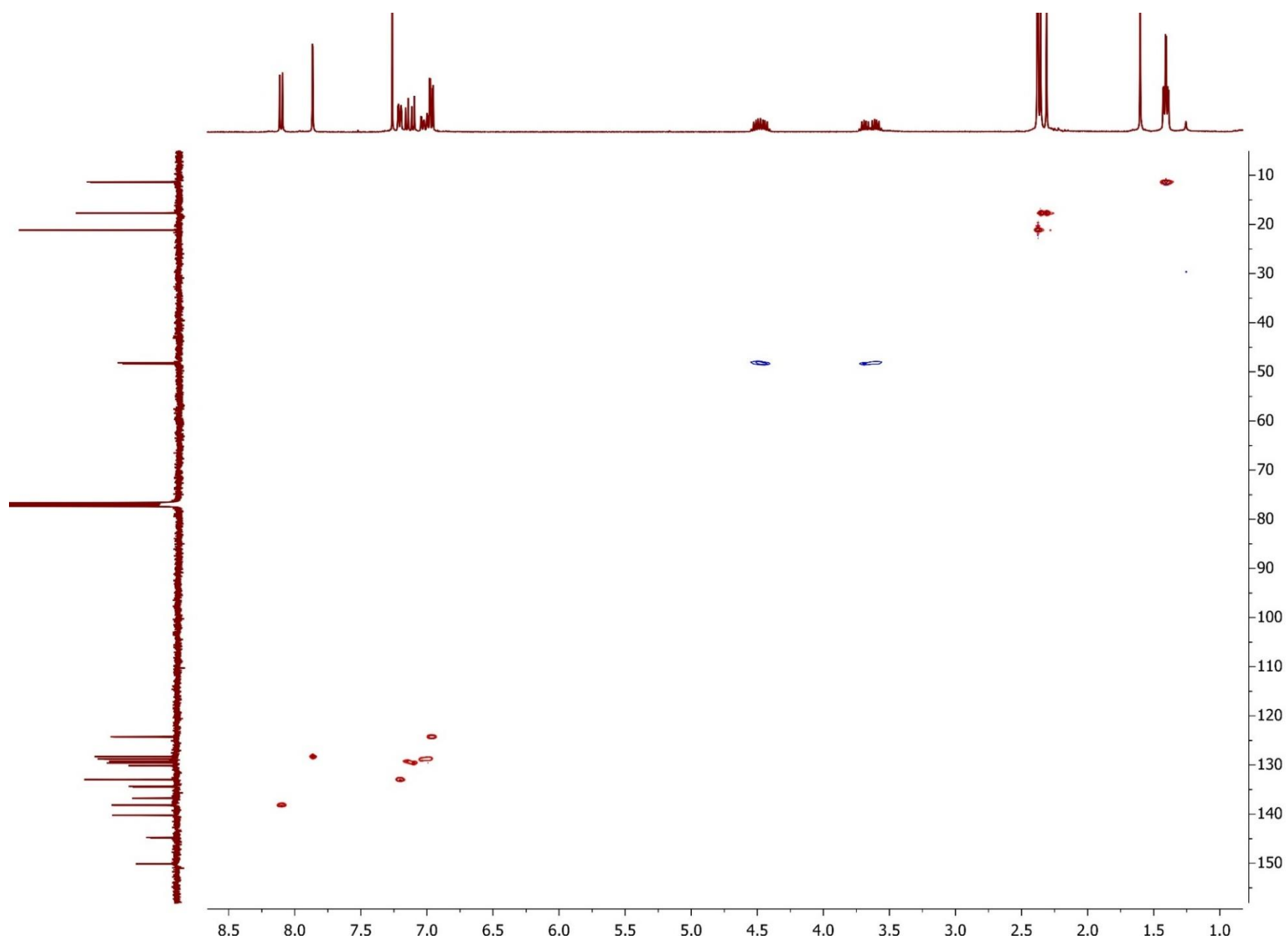


Figure S23. $^1\text{H}/^{13}\text{C}$ HSQC NMR spectrum in CDCl_3 at 25°C .

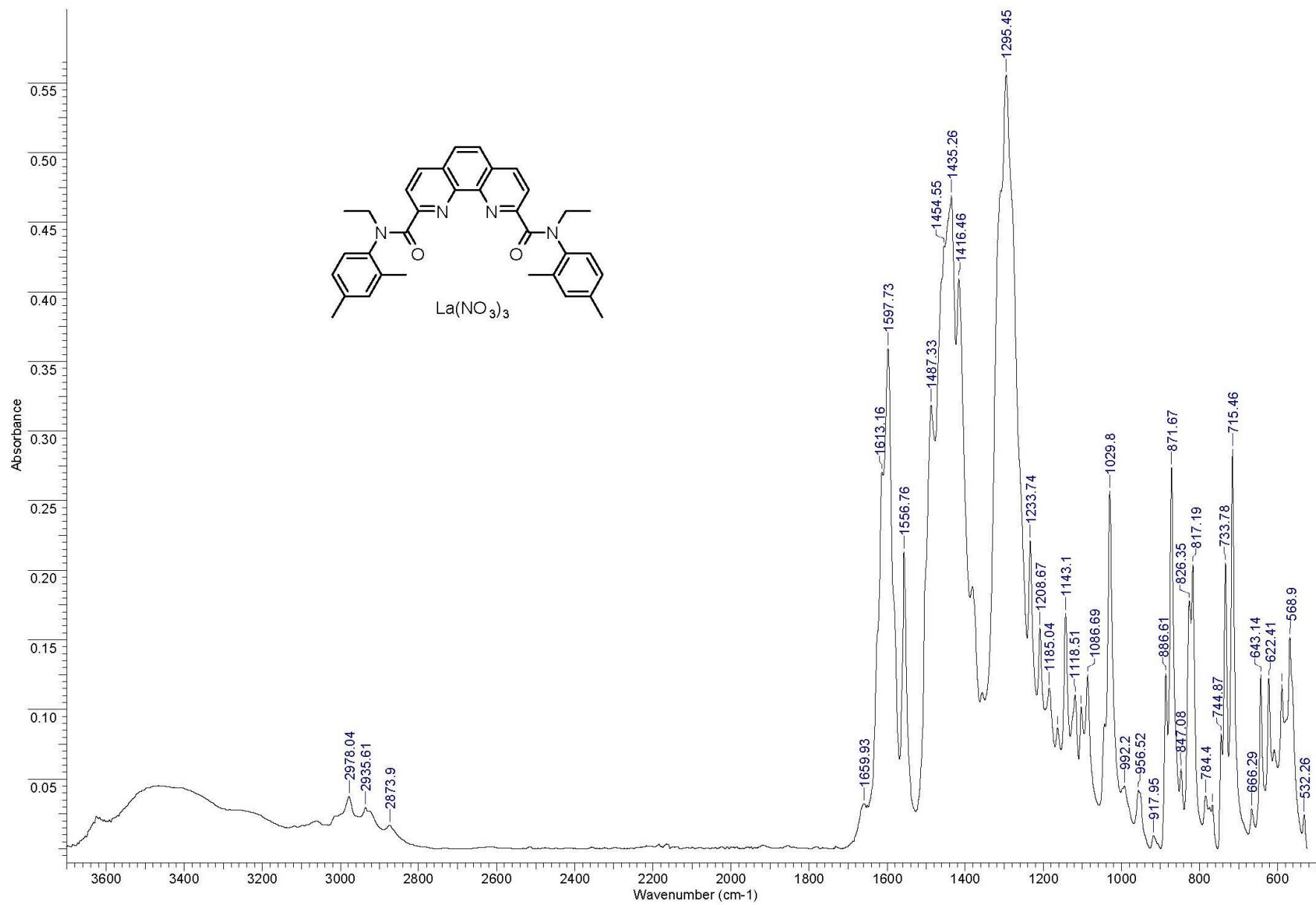


Figure S24. Solid-state IR spectrum at 25°C

N²,N⁹-bis(2,4-dimethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide europium trinitrate **L3•Eu(NO₃)₃**

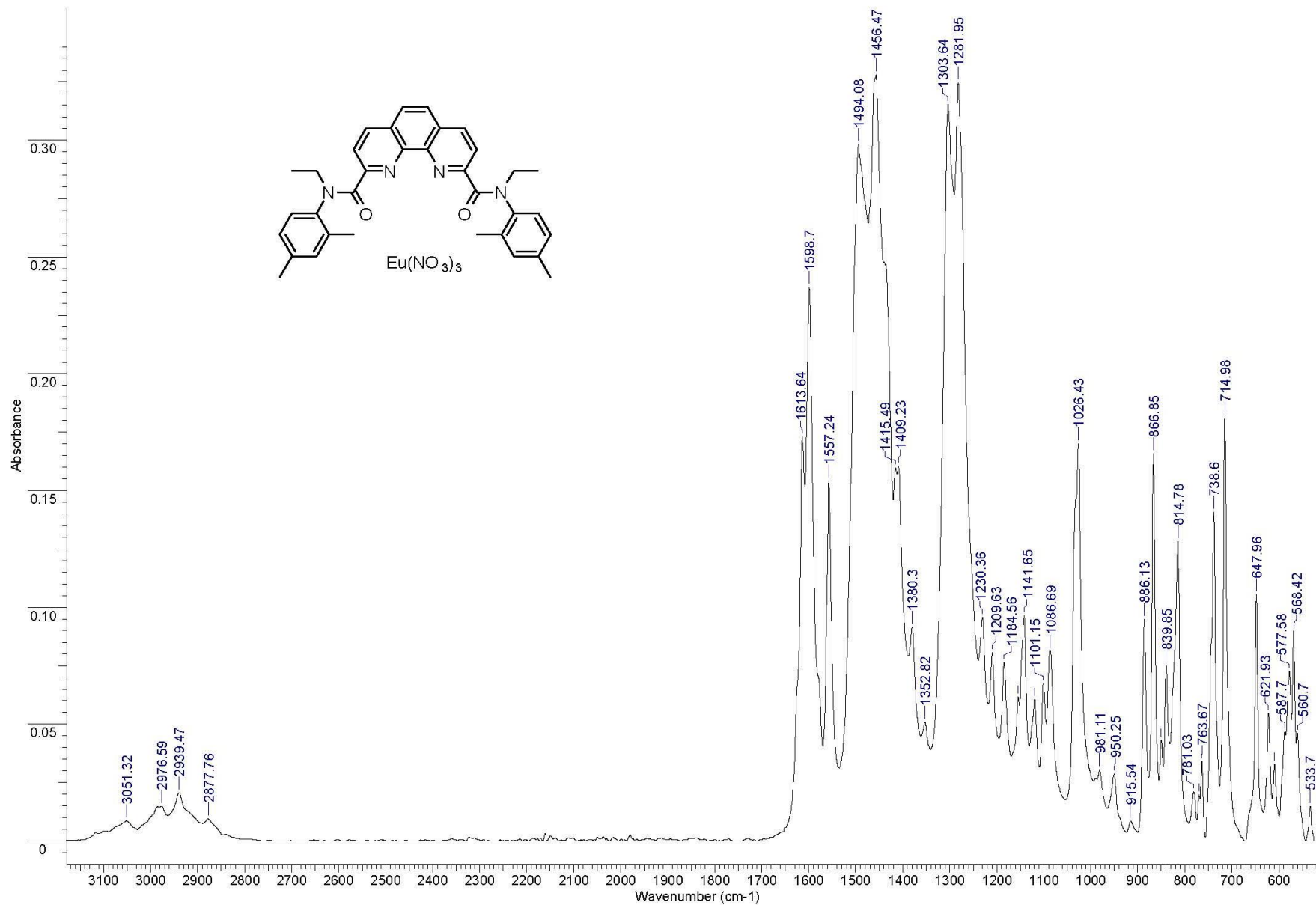


Figure S25. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,4-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide gadolinium trinitrate **L3**• $Gd(NO_3)_3$

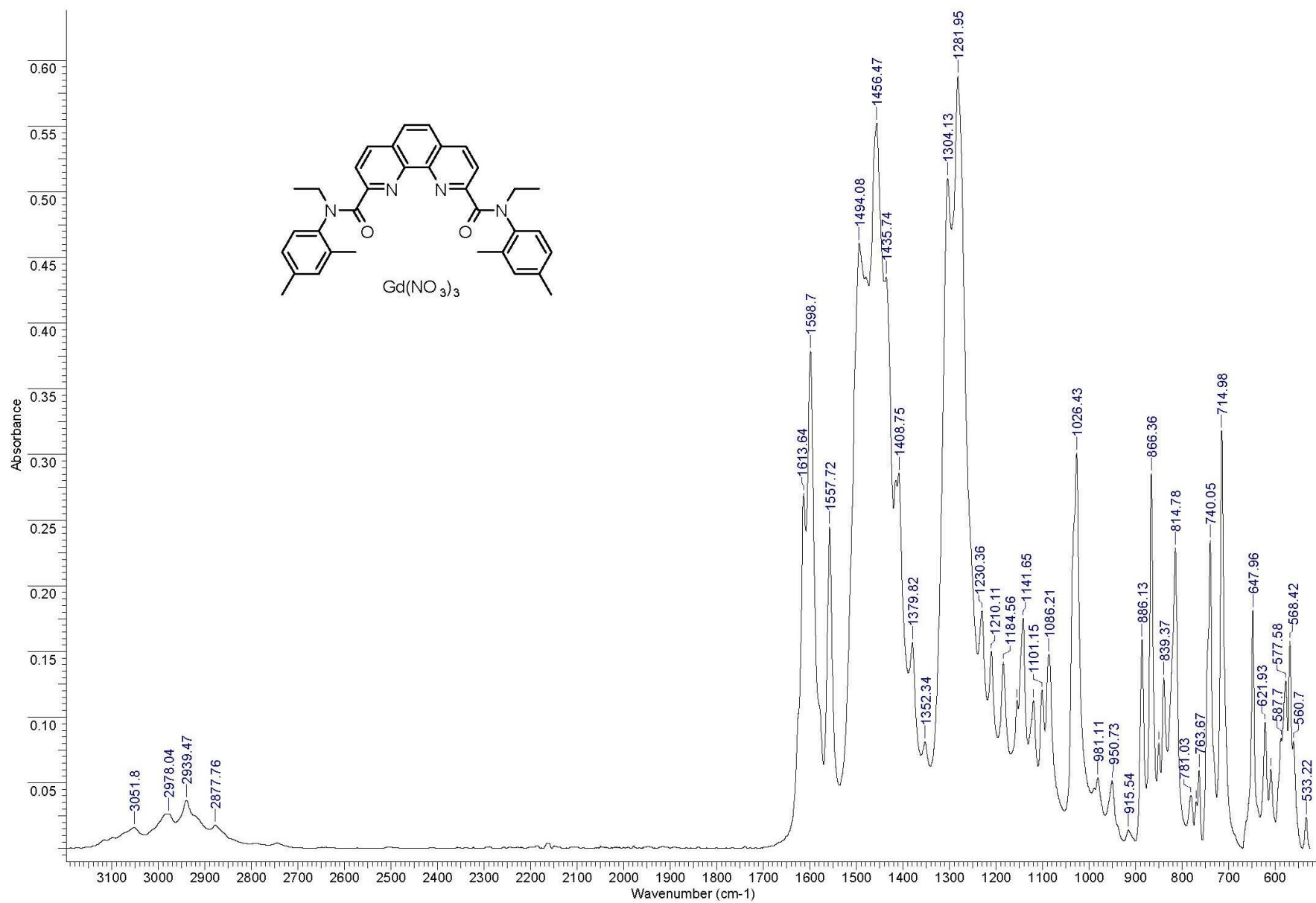


Figure S26. Solid-state IR spectrum at 25°C

N^2,N^9 -bis(2,4-dimethylphenyl)- N^2,N^9 -diethyl-1,10-phenanthroline-2,9-dicarboxamide terbium trinitrate **L3**•**Tb(NO₃)₃**

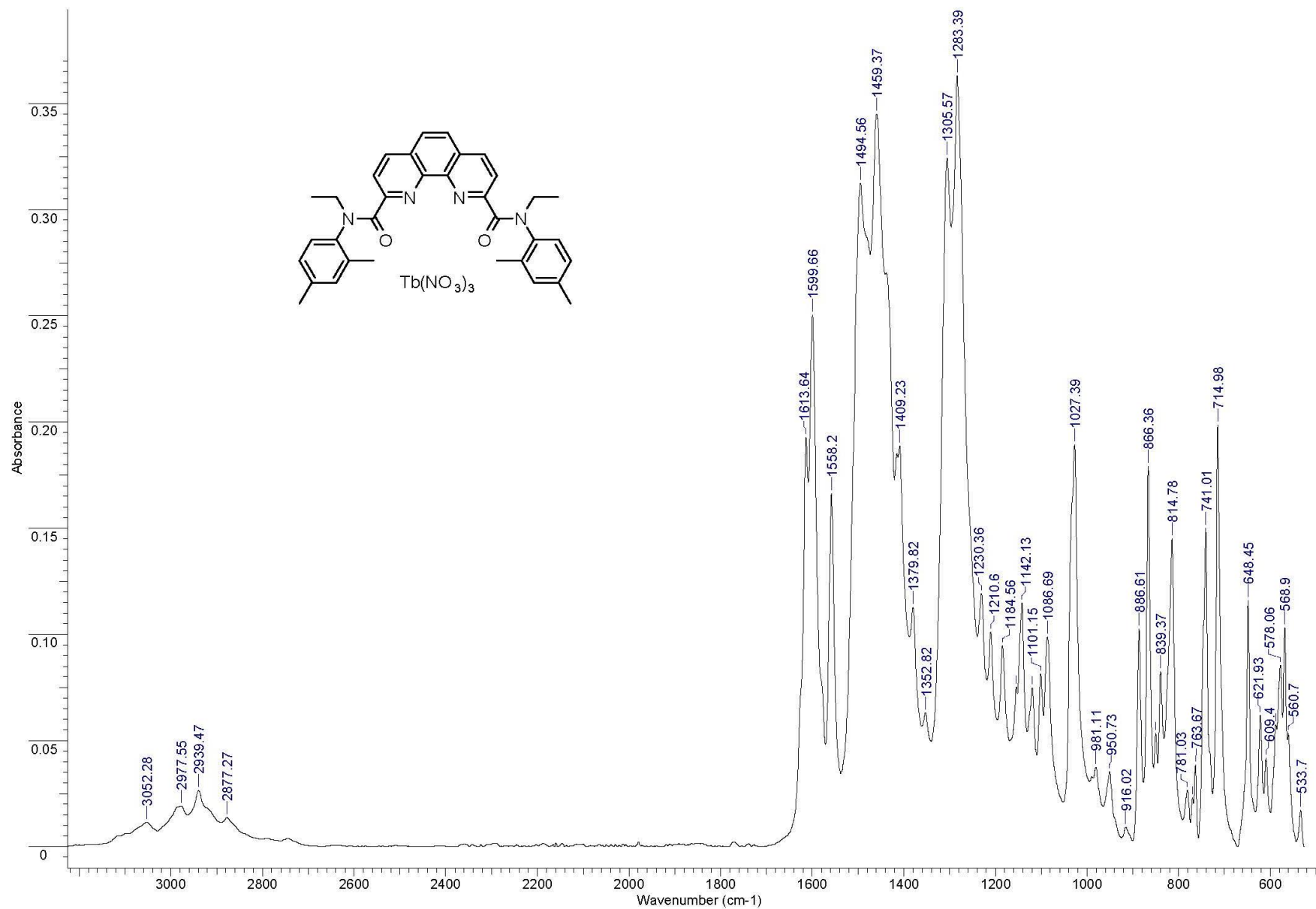


Figure S27. Solid-state IR spectrum at 25°C

N²,N⁹-bis(2,4-dimethylphenyl)-N²,N⁹-diethyl-1,10-phenanthroline-2,9-dicarboxamide lutetium trinitrate **L3•Lu(NO₃)₃**

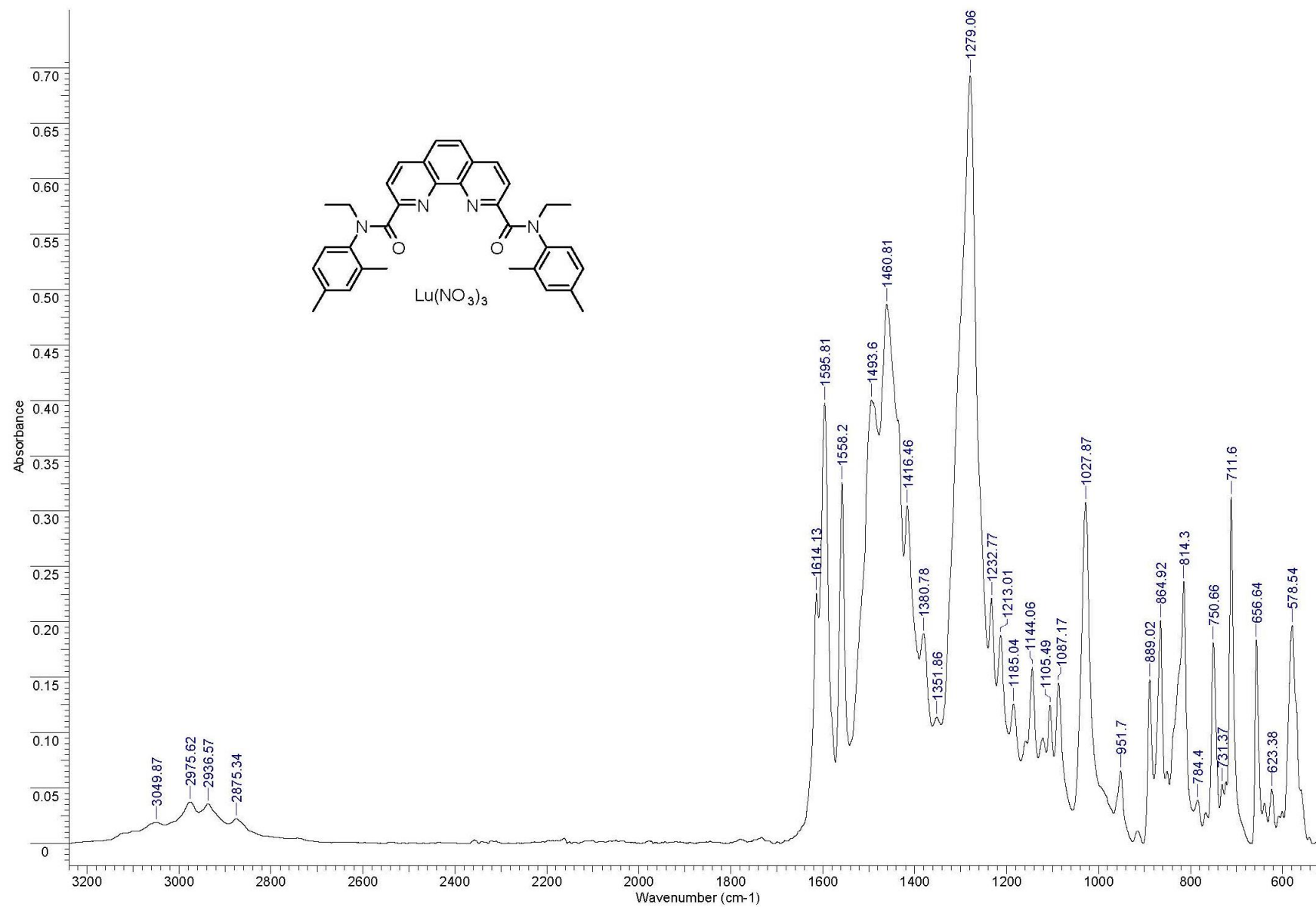


Figure S28. Solid-state IR spectrum at 25°C

2. NMR-titration

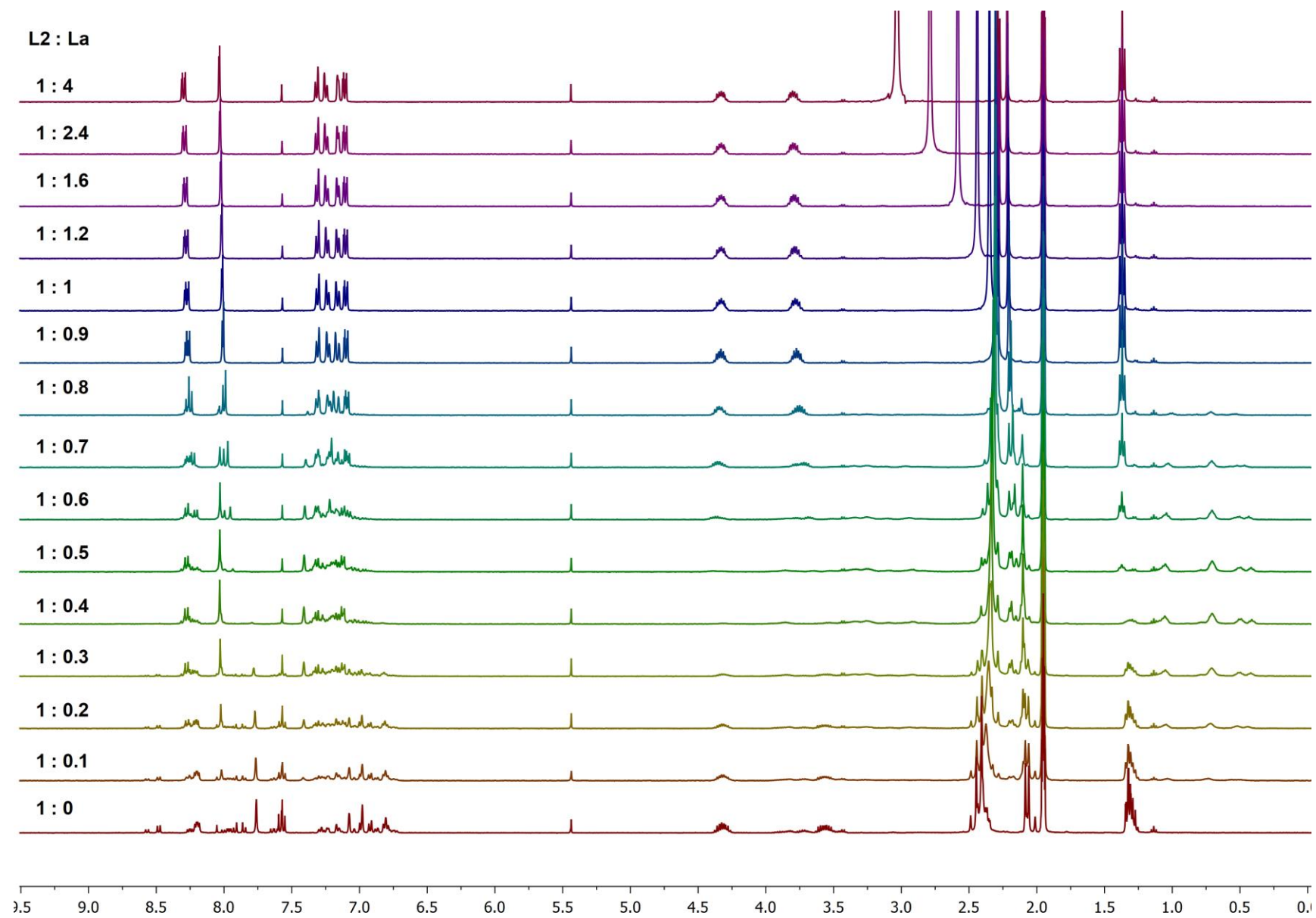


Figure S29. NMR titration of L2 with $\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ in CD_3CN

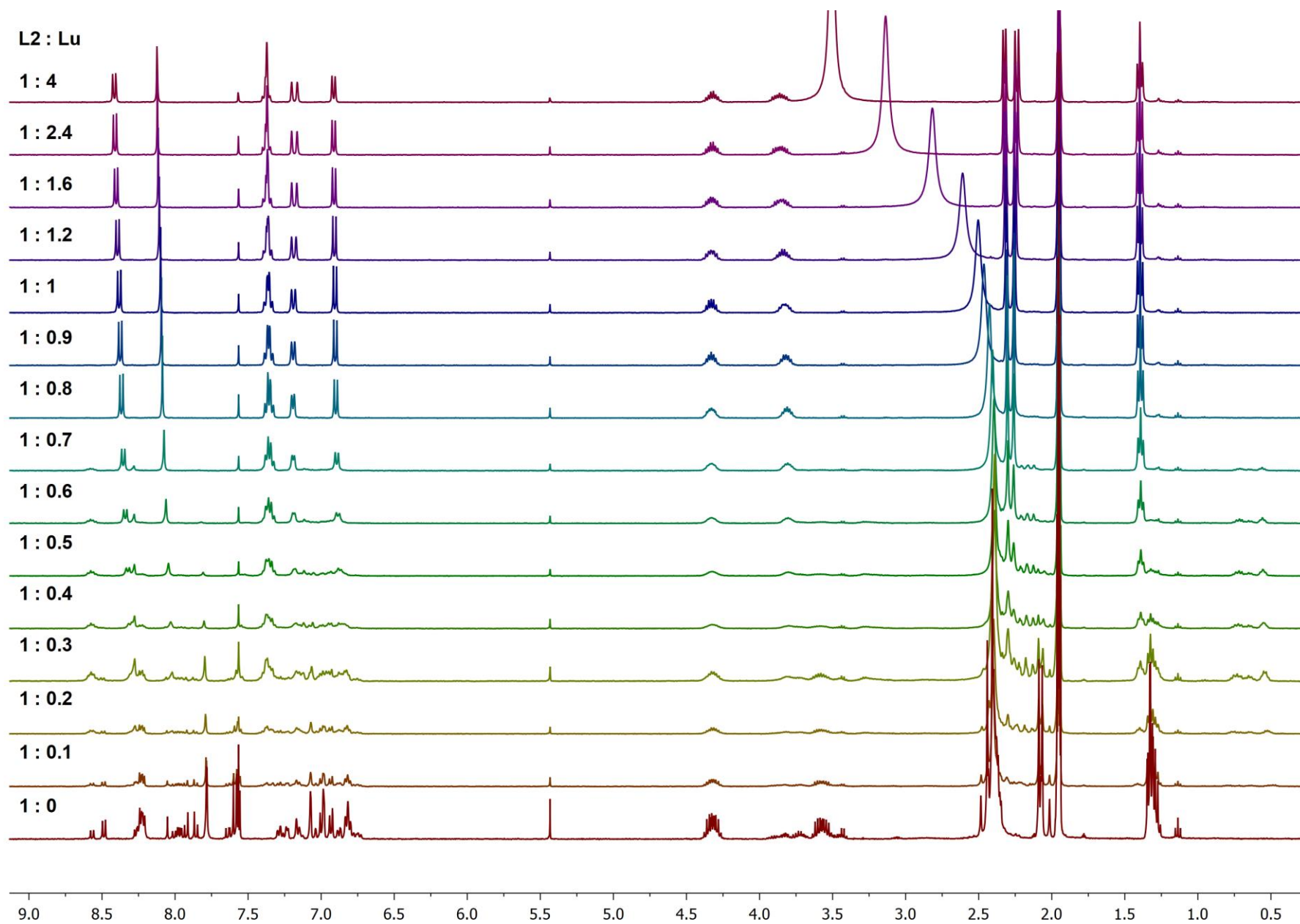


Figure S30. NMR titration of **L2** with $\text{Lu}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$ in CD_3CN

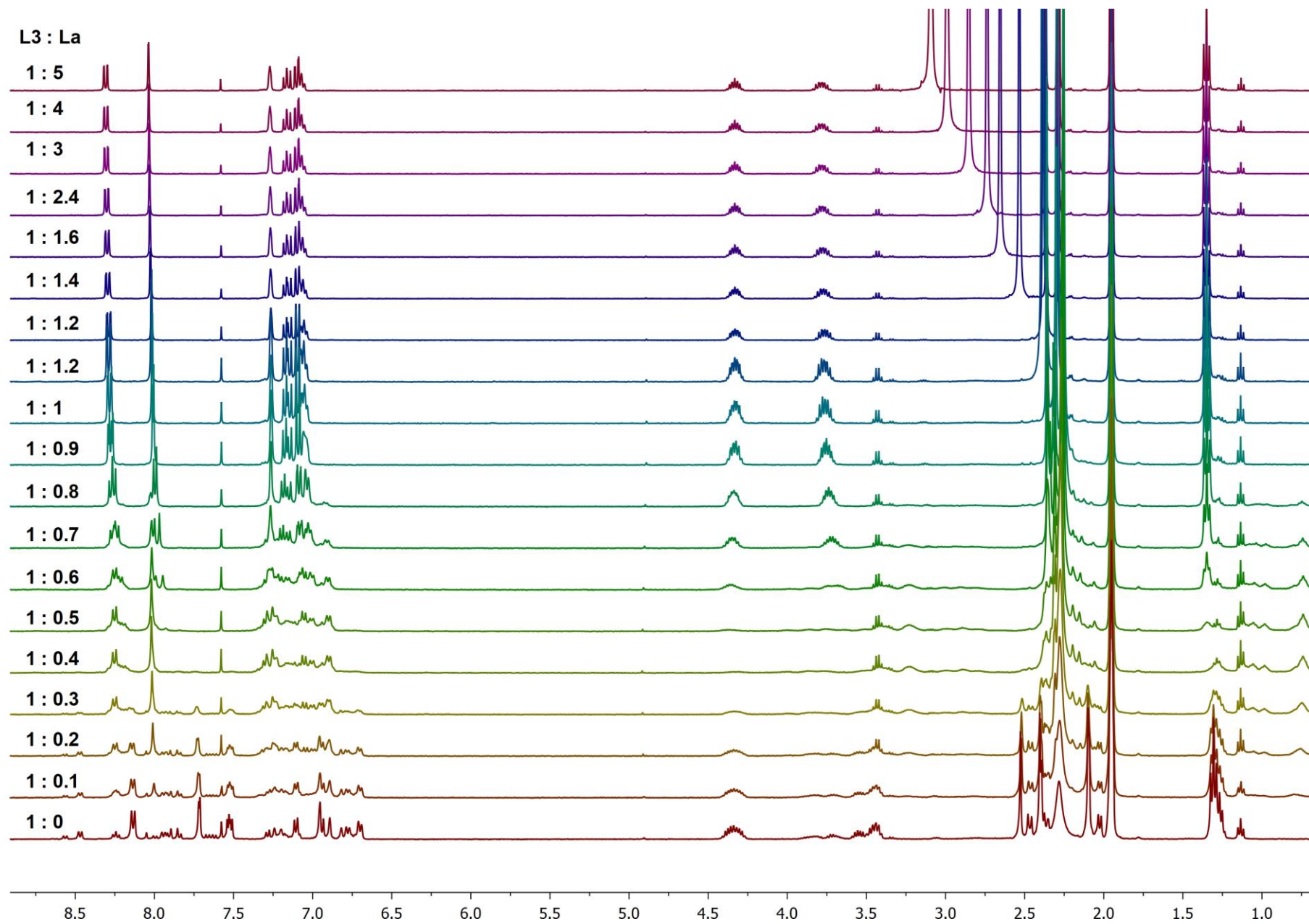


Figure S31. NMR titration of L3 with $\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ in CD_3CN

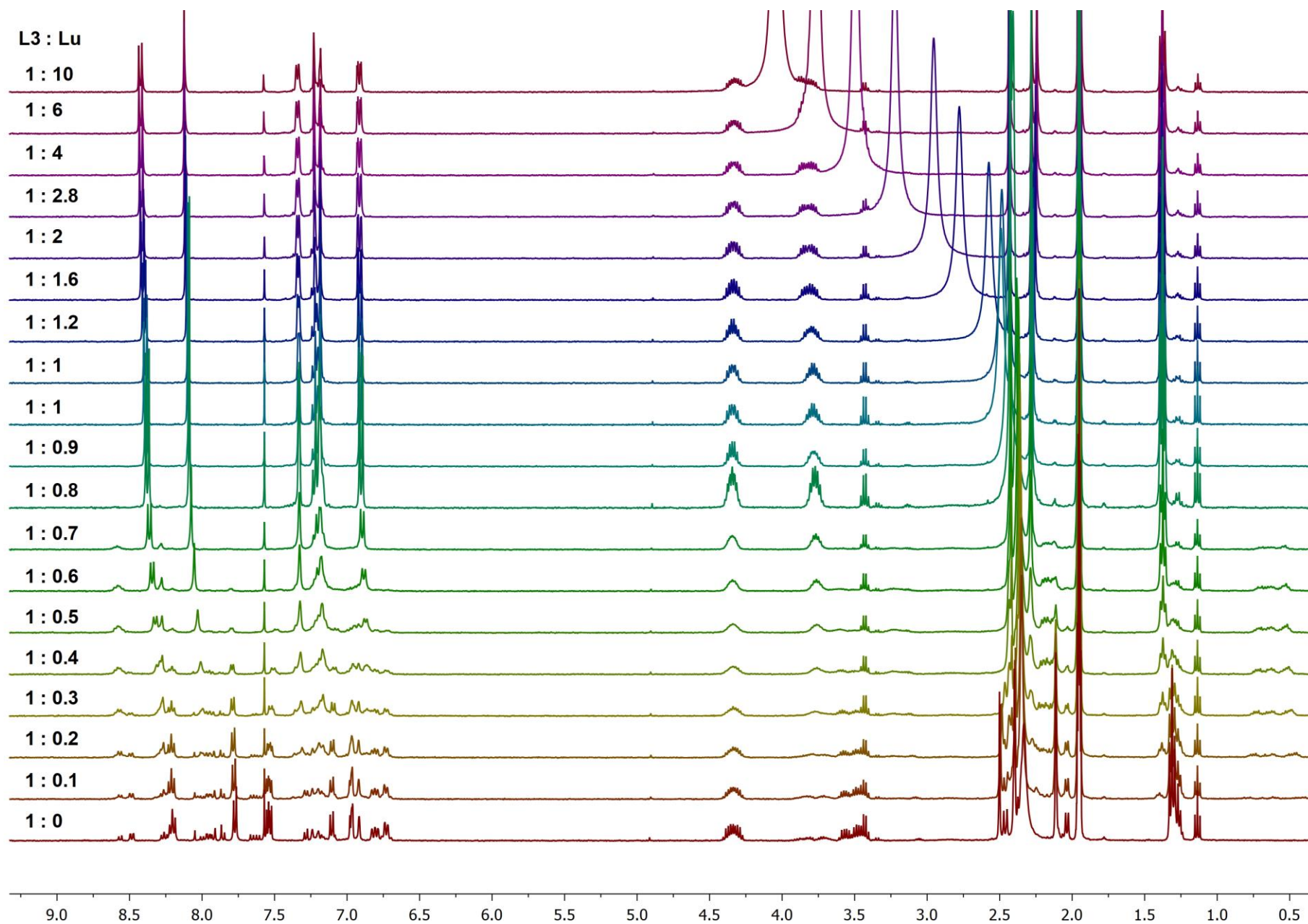


Figure S32. NMR titration of L3 with $\text{Lu}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$ in CD_3CN

3. Photophysical properties of complexes

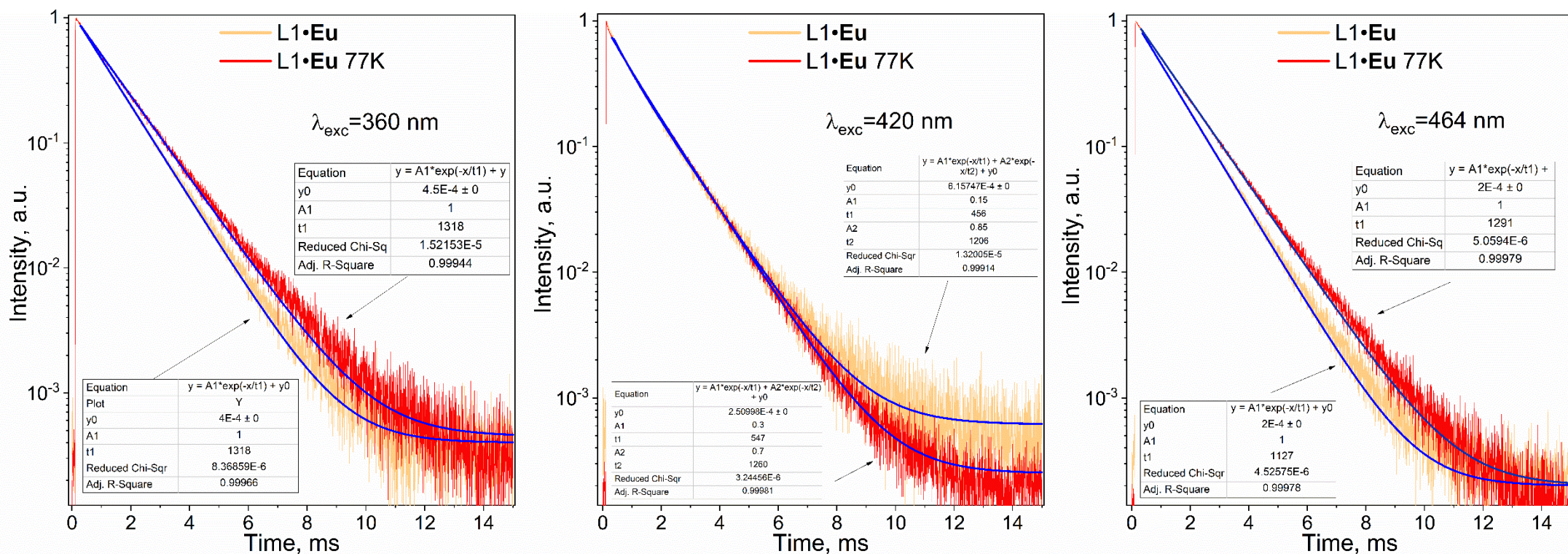


Figure S33. Photoluminescence decays of the investigated Eu^{3+} complexes at 300 and 77 K with excitation via ligand environment (360 nm), CT-related band (420 nm) and resonantly through ${}^7\text{F}_0 \rightarrow {}^5\text{D}_2$ transition (464 nm).

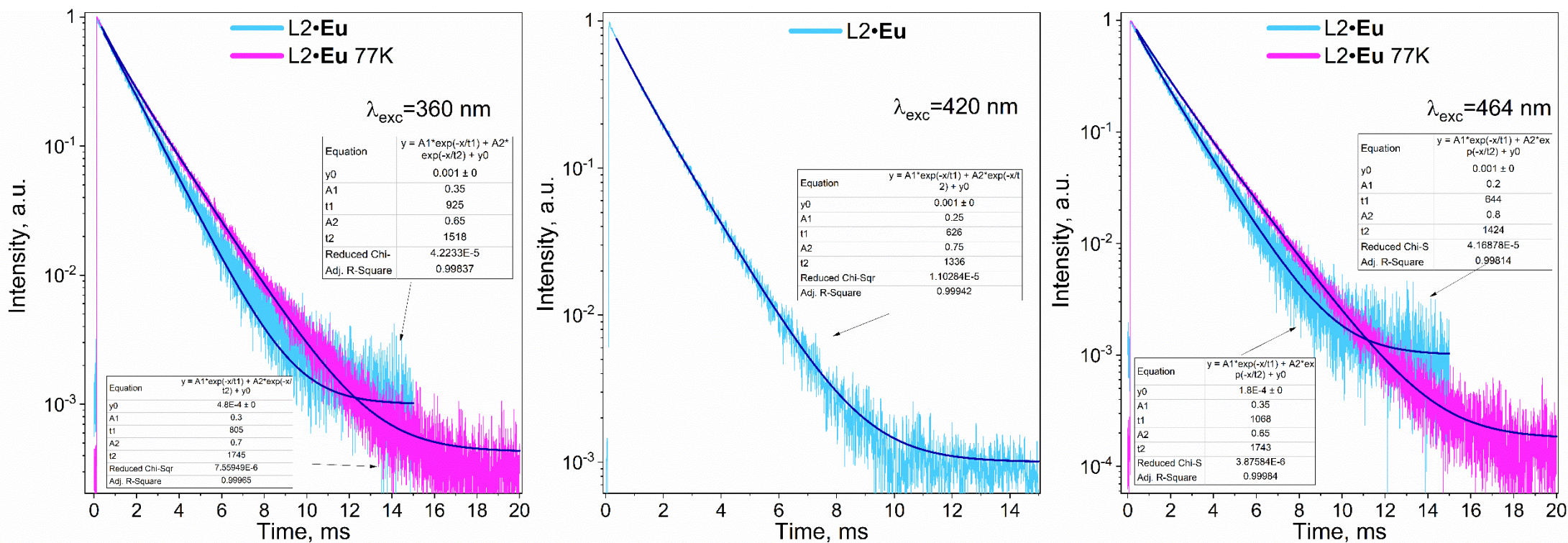


Figure S34. Photoluminescence decays of the investigated Eu^{3+} complexes at 300 and 77 K with excitation via ligand environment (360 nm), CT-related band (420 nm) and resonantly through ${}^7\text{F}_0 \rightarrow {}^5\text{D}_2$ transition (464 nm).

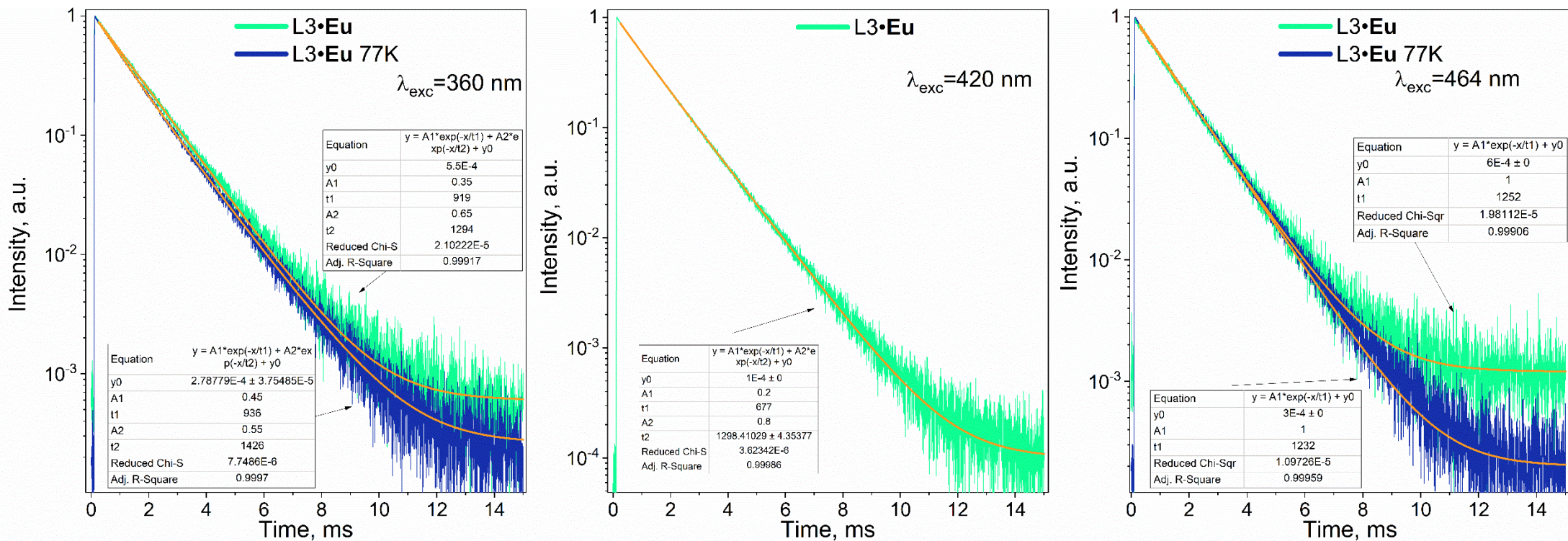


Figure S35. Photoluminescence decays of all the investigated Eu^{3+} complexes at 300 and 77 K with excitation via ligand environment (360 nm), CT-related band (420 nm) and resonantly through ${}^7\text{F}_0 \rightarrow {}^5\text{D}_2$ transition (464 nm).

Table S1. Stark components' energies (in cm^{-1}) of the Eu^{3+} complexes.

L1•Eu(NO₃)₃	L2•Eu(NO₃)₃	L3•Eu(NO₃)₃
$^5\text{D}_0 \rightarrow ^7\text{F}_0$		
17140	17140	17140
$^5\text{D}_0 \rightarrow ^7\text{F}_1$		
16820	16890	16820
16770	16760	16800
16710	16660	16690
$^5\text{D}_0 \rightarrow ^7\text{F}_2$		
16210	16210	16220
16190	16180	16200
16140	16140	16140
16110	16110	16060
16050	16080	16000
$^5\text{D}_0 \rightarrow ^7\text{F}_3$		
15340	15320	15310
15290	15280	15270
15210	15200	15210
$^5\text{D}_0 \rightarrow ^7\text{F}_4$		
14620	14600	14630
14520	14520	14560
14490	14430	14500
14360	14330	14350
14270	14240	14250
14160	14160	14150
14110	14070	14080
14030	14030	14070

4. X-ray

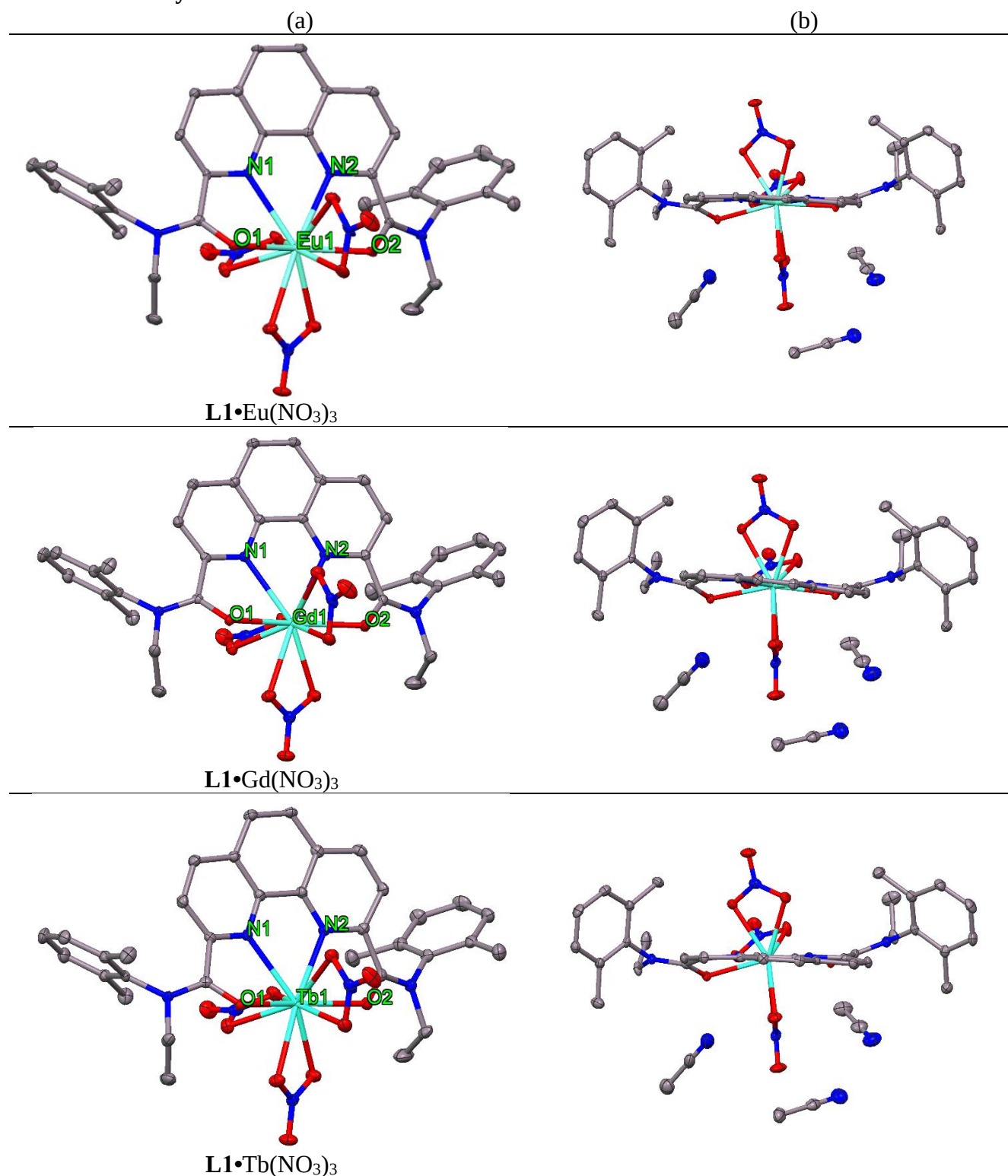


Figure S36. X-ray structures of the complexes **L1•Eu(NO₃)₃**, **L1•Gd(NO₃)₃** and **L1•Tb(NO₃)₃** in two projections. Hydrogen atoms and solvate acetonitrile molecules in (a) are omitted for clarity, and the non-hydrogen atoms are shown as thermal ellipsoids at 50% probability level.

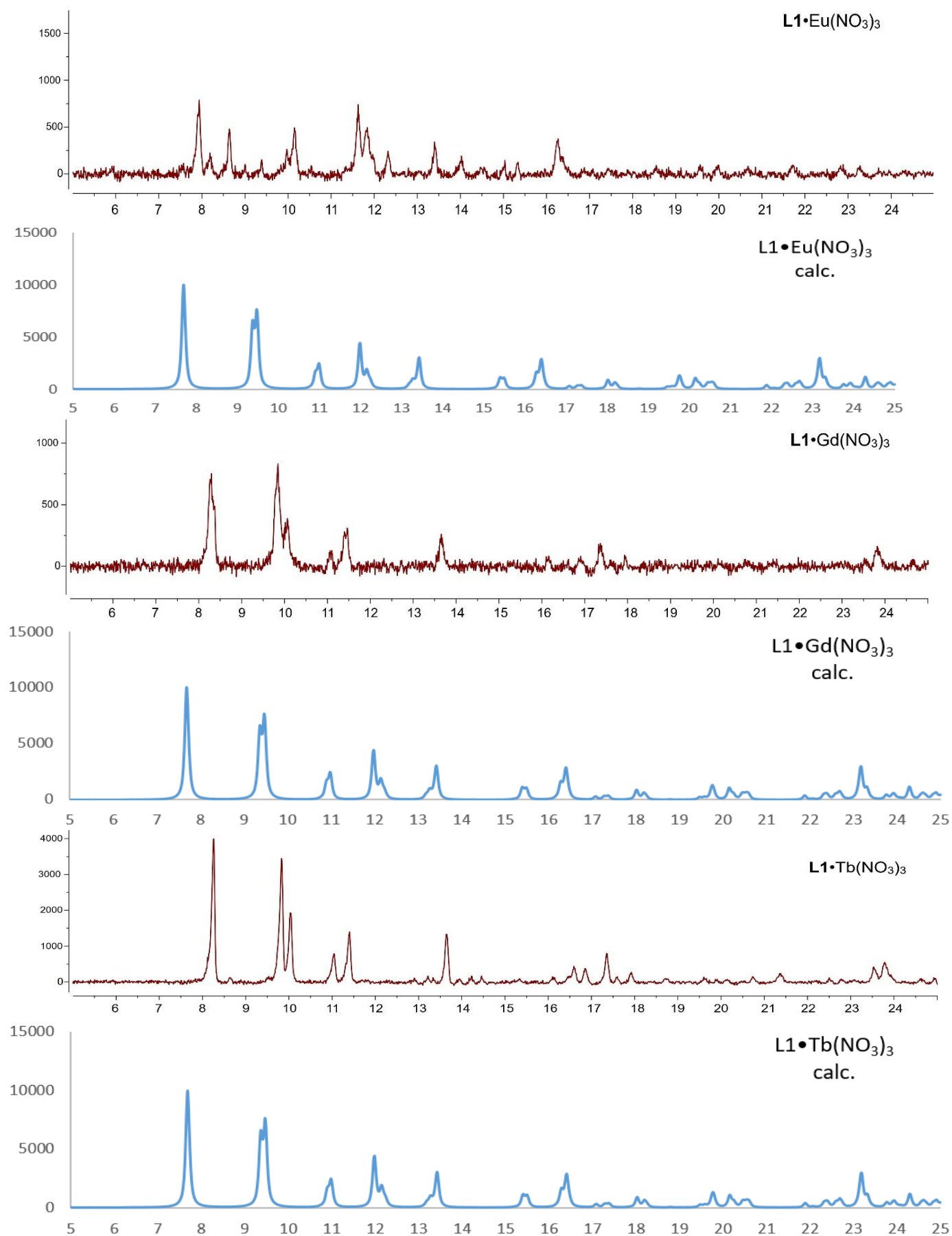
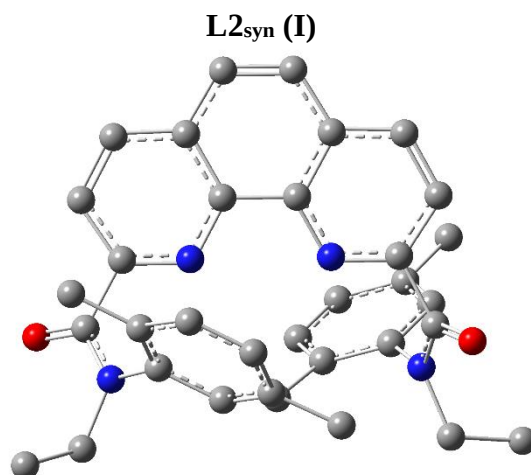


Figure S37. Experimental (red spectra) and calculated (blue spectra) powder X-ray diffraction patterns of the complexes $\text{L1}\cdot\text{Eu}(\text{NO}_3)_3$, $\text{L1}\cdot\text{Gd}(\text{NO}_3)_3$ and $\text{L1}\cdot\text{Tb}(\text{NO}_3)_3$.

5. DFT

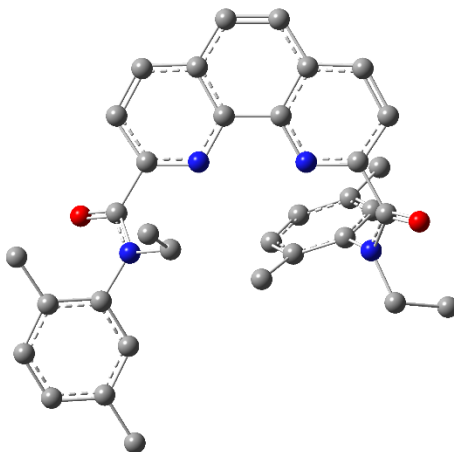
All structures were optimized at the DFT level in the gas phase (tolerance on gradient: 10^{-7} au) in Priroda-19 program¹. The generalized gradient approximation (GGA) functional PBE was used for the geometry optimization and frequency calculations of all structures. All stationary points on the potential energy surface (PES) were checked by vibrational analysis and none of them had imaginary frequencies. Full electron relativistic L1 basis set² of TZ quality including one polarization function was used for all the atoms to provide the most reliable result. All thermodynamic calculations are performed using the PBE/L1 theoretical level. The CREST 3.0 program was used to find the most stable conformations of the ligands³.



O	-4.40052486	-0.51119602	-1.47627167
O	3.54370830	-0.51728543	1.81453296
N	-1.62001825	1.04613761	-0.20305378
N	1.10679551	1.06501335	0.17227504
N	-3.36464898	-1.22170651	0.44421827
N	3.02657514	-1.15704616	-0.32780883
C	-2.91975117	1.03882668	-0.46615431
C	-3.65817158	2.20041686	-0.79553948
H	-4.71053145	2.10266305	-1.06860995
C	-3.01755393	3.42000471	-0.75321763
H	-3.55641739	4.34874230	-0.96346854
C	-1.64061973	3.47289097	-0.43311439
C	-0.92175985	4.70533170	-0.33149265
H	-1.46192964	5.64111509	-0.50396619
C	0.40575706	4.71913882	-0.00880041
H	0.94434545	5.66558829	0.08892714
C	1.12372576	3.49991357	0.20149060
C	2.49400698	3.47458600	0.55296692
H	3.03085807	4.41828478	0.68794784
C	3.12919894	2.26365519	0.72847621
H	4.17529402	2.19937878	1.03498054
C	2.39578751	1.08038615	0.48333164
C	0.45890279	2.24463017	0.06470798
C	-0.97269017	2.23173166	-0.20524341
C	3.05927850	-0.26333267	0.71341303
C	3.55552080	-2.51211036	-0.08617501

H	3.34991735	-2.74235574	0.97035949
H	2.98341190	-3.20690680	-0.72192345
C	5.05450512	-2.63864874	-0.36604019
H	5.62387603	-1.97281042	0.29955198
H	5.28655985	-2.38882523	-1.41278142
H	5.38124328	-3.67472824	-0.18061850
C	2.73928142	-0.77742972	-1.68621590
C	1.51792796	-1.13991960	-2.28651640
C	1.33991437	-0.78976648	-3.63165014
C	2.31456867	-0.09837240	-4.35008185
C	3.52011692	0.28112005	-3.74664744
C	3.71499541	-0.08070778	-2.40873227
C	-3.64006836	-0.29358940	-0.53581457
C	-3.89935898	-2.58361814	0.25677565
H	-4.04422389	-2.71051645	-0.82622554
H	-3.12958101	-3.29259999	0.60145229
C	-5.21637688	-2.82920746	0.99530992
H	-5.53585708	-3.87374835	0.84846743
H	-6.00642138	-2.17055567	0.60395602
H	-5.10401775	-2.65532451	2.07697960
C	-2.70590948	-0.92601840	1.68771626
C	-3.29830201	-0.07803196	2.64475188
C	-2.59813705	0.12070604	3.84530252
H	-3.04087001	0.77117464	4.60614612
C	-1.37795632	-0.49742886	4.10057725
C	-0.79534082	-1.35385264	3.15430506
C	-1.48439741	-1.55599502	1.95735788
H	-1.04974259	-2.19900163	1.18697951
C	-4.62426221	0.60557987	2.42548586
H	-5.07555823	0.88084973	3.39059019
H	-4.50758639	1.53208253	1.83732427
H	-5.33023350	-0.03905175	1.88164390
H	-0.86882230	-0.31880617	5.05259103
H	2.13236578	0.15576497	-5.39899943
C	0.54631508	-1.99656858	3.40250011
H	0.67348918	-2.25133202	4.46640075
H	0.66076363	-2.91874081	2.81187756
H	1.37072102	-1.31873403	3.12127356
H	0.39944035	-1.05860496	-4.12208482
H	4.64933394	0.18385344	-1.90413599
C	0.41381241	-1.79353926	-1.50239067
H	-0.39095833	-2.12975374	-2.17268209
H	0.77040830	-2.66026891	-0.92352357
H	0.00148784	-1.05559489	-0.79096281
C	4.56464533	1.06274820	-4.50495865
H	5.55333836	0.97694980	-4.02896905
H	4.65155745	0.70868891	-5.54430325
H	4.30484718	2.13467799	-4.54376997

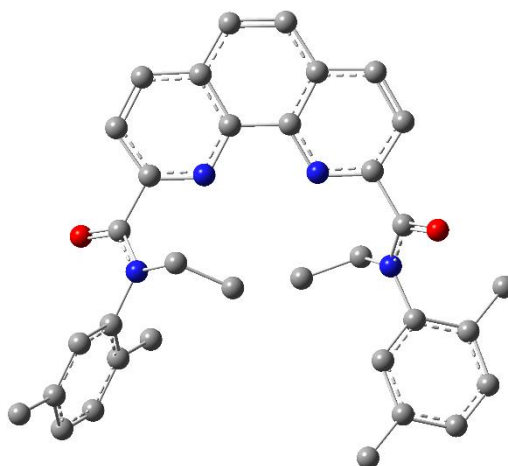
L2_{syn} (II)



O	4.75004365	0.70508352	1.06907382
O	-3.95081975	0.00002532	-0.24606989
N	1.76598417	1.76138370	-0.17911449
N	-0.98429065	1.70255435	0.06082777
N	3.52237865	-0.59605995	-0.36915218
N	-2.61986951	-0.33745519	1.59196870
C	3.09087942	1.82831032	-0.20088100
C	3.81194731	3.01520997	-0.46753101
H	4.90185719	3.00380163	-0.40726219
C	3.10666712	4.14970991	-0.80379461
H	3.62108319	5.08185578	-1.05557350
C	1.69243256	4.11295788	-0.81533960
C	0.90138058	5.25132678	-1.16618481
H	1.41364707	6.17597785	-1.44861020
C	-0.46288851	5.18804699	-1.15441043
H	-1.06398941	6.05834453	-1.43414412
C	-1.13798434	3.98947437	-0.76395241
C	-2.54888088	3.89284924	-0.72825102
H	-3.15305680	4.75440860	-1.02767126
C	-3.14053392	2.71664344	-0.32450194
H	-4.22292118	2.57961774	-0.32047998
C	-2.31053571	1.64972982	0.09721625
C	-0.39119102	2.83448644	-0.38400706
C	1.06383460	2.88326495	-0.45256662
C	-3.02186401	0.35717086	0.47457133
C	-1.56649020	0.11096004	2.53107417
H	-1.04252838	-0.79231460	2.88054986
H	-0.84359392	0.71211572	1.96532828
C	-2.12804565	0.88252316	3.72648193
H	-2.85646215	0.27568422	4.28712906
H	-2.62052740	1.81231083	3.40014875
H	-1.30781672	1.15223591	4.41150298
C	-3.29939966	-1.56617868	1.92566814
C	-2.55079023	-2.74931529	1.88655699
C	-3.10345035	-3.98498198	2.23204092
C	-4.45030548	-4.00739164	2.62022618
C	-5.19862646	-2.83432878	2.65795074
H	-6.24870073	-2.87615012	2.96322221

C	-4.65123074	-1.58745467	2.31824029
C	-5.50208120	-0.34780939	2.35692333
H	-4.97385517	0.49018357	2.83822926
C	3.87651155	0.59843062	0.21228646
C	4.20012608	-1.81189968	0.11991576
H	4.35614064	-1.67019305	1.20014827
H	3.50824681	-2.65565390	-0.03259325
C	5.53927496	-2.08485684	-0.56856366
H	5.41006081	-2.21022287	-1.65462237
H	5.98136996	-3.01110120	-0.16698572
H	6.23893945	-1.25738453	-0.37934415
C	2.81459456	-0.68463807	-1.61887719
C	1.50577826	-1.20216790	-1.66140070
C	0.90506979	-1.32136918	-2.92093703
C	1.56016132	-0.93306208	-4.08955827
C	2.85394106	-0.39961345	-4.04603803
C	3.46875219	-0.29326449	-2.79268907
H	-5.74283027	-0.03333312	1.32809936
H	-6.43695131	-0.53414131	2.90551985
H	-1.50823118	-2.69682579	1.55758940
H	1.05253868	-1.03984320	-5.05328913
H	-4.91951415	-4.95761659	2.89367529
C	-2.27960957	-5.24875270	2.19446123
H	-2.01375182	-5.57897895	3.21330487
H	-2.83529567	-6.07224458	1.71824252
H	-1.34346961	-5.09876935	1.63583573
H	4.48606520	0.10305375	-2.71710454
C	0.74497282	-1.51899942	-0.40382162
H	-0.21194078	-2.00529802	-0.644446060
H	1.31135933	-2.17352054	0.27759657
H	0.53918348	-0.57115122	0.12252509
C	3.55494720	0.06243759	-5.30003162
H	4.64851057	0.05425408	-5.17455779
H	3.30195401	-0.57983438	-6.15802870
H	3.25775327	1.09279694	-5.56129230
H	-0.11406306	-1.71504369	-2.98043727

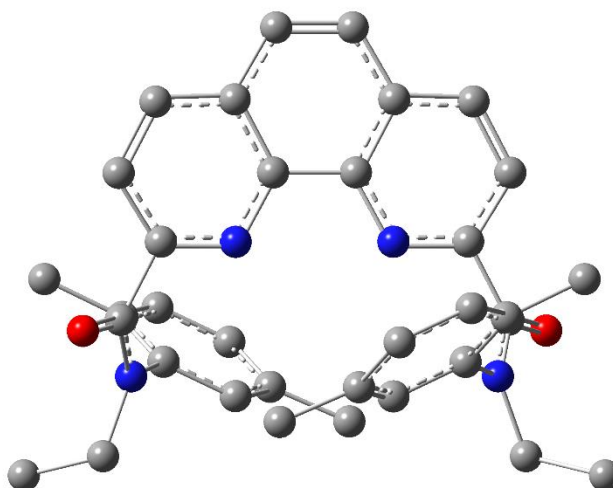
L2_{syn} (III)



O	-3.36448657	2.07898409	-2.20220276
O	4.08289807	-0.46304437	1.76656600
N	-0.16061465	2.49110426	-1.04977023
N	2.30555859	1.42768642	-0.41448216
N	-2.78894149	1.47491106	-0.06172754
N	2.91952406	-1.44891613	0.04669058
C	-1.33880246	2.98599435	-1.41076980
C	-1.49545920	4.23207829	-2.06471402
H	-2.49354863	4.54452350	-2.37632322
C	-0.37727433	5.00429844	-2.28559841
H	-0.45415993	5.98728502	-2.75971386
C	0.89426452	4.51888870	-1.89782511
C	2.09068132	5.27944826	-2.08302322
H	2.01403614	6.26933829	-2.54267476
C	3.30196256	4.78878771	-1.68578202
H	4.21284200	5.38072065	-1.81609819
C	3.40952086	3.49212550	-1.09298600
C	4.64653398	2.96115152	-0.65609974
H	5.55509762	3.56114509	-0.76326061
C	4.68547236	1.70503668	-0.09259126
H	5.60780898	1.27067660	0.29759970
C	3.48499029	0.95921752	-0.02250775
C	2.24711045	2.68239760	-0.91682943
C	0.94902086	3.22445983	-1.29859870
C	3.53066410	-0.38991680	0.67396412
C	2.55543427	-1.46983624	-1.38461180
H	3.09031182	-0.64450043	-1.87799165
H	2.95594300	-2.41086340	-1.80174593
C	1.05738113	-1.36476785	-1.66421217
H	0.68085308	-0.39112607	-1.31850204
H	0.50462636	-2.17688976	-1.16761029
H	0.88108443	-1.44982569	-2.74914353
C	2.80192071	-2.69421332	0.76545636
C	3.88233462	-3.59680546	0.80684345
C	3.68166509	-4.80625855	1.48076368
H	4.50639292	-5.52359574	1.53431338
C	2.46509006	-5.11082060	2.09430460
C	1.39785740	-4.20730732	2.06547378

C	1.59145942	-2.99325510	1.39147549
C	-2.58924637	2.13924256	-1.25187549
C	-2.01173153	1.71476906	1.17277326
H	-1.46903081	2.66207727	1.05663157
H	-2.73574778	1.85228675	1.99243332
C	-1.04159446	0.58367477	1.51217865
H	-1.56870417	-0.38337757	1.54381384
H	-0.59912511	0.76357297	2.50555940
H	-0.23156905	0.54938695	0.76986744
C	-3.92111830	0.59018041	0.04156420
C	-3.98599448	-0.59564876	-0.71674947
C	-5.10381830	-1.41969189	-0.52294533
C	-6.11626557	-1.09494297	0.37656342
C	-6.05684582	0.08958906	1.12253535
C	-4.94564350	0.91692456	0.93804627
H	0.79151227	-2.24755802	1.36163766
C	5.21450054	-3.25411249	0.19363034
H	5.65134658	-2.38299188	0.70900869
H	5.91226236	-4.09937671	0.28419814
H	5.12468964	-2.99695722	-0.87452345
H	-6.96659519	-1.77214128	0.50316203
H	2.34756659	-6.06608854	2.61515682
C	0.07863289	-4.51845893	2.72850925
H	-0.71321197	-4.68803897	1.97941639
H	0.15111804	-5.42209132	3.35223513
H	-0.25038786	-3.68457575	3.36919559
C	-2.92044421	-0.97023650	-1.70876807
H	-1.91207005	-0.80456921	-1.29977750
H	-3.01562327	-2.02583080	-2.00264480
H	-3.01114223	-0.33971870	-2.60906928
C	-7.17010577	0.47792002	2.06461076
H	-7.98990742	0.97894145	1.52142155
H	-7.59800219	-0.40685340	2.56143164
H	-6.81498534	1.17131929	2.84228237
H	-5.17070674	-2.34982147	-1.09552518
H	-4.87906527	1.85488070	1.49796055

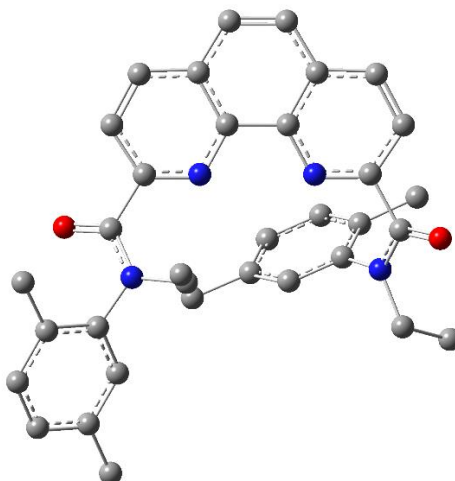
L2_{anti} (I)



O	-3.94816277	-0.31571103	1.88884755
O	3.95020322	-0.30992091	-1.88887487
N	-1.34553755	1.20387244	0.28278435
N	1.34612219	1.20498585	-0.28065644
N	-3.12667220	-1.09161995	-0.10890780
N	3.12774094	-1.09075852	0.10657928
C	-2.61876825	1.20758356	0.65144065
C	-3.33802031	2.38073696	0.98206810
H	-4.36472179	2.29503368	1.34315531
C	-2.71004963	3.59827600	0.82860686
H	-3.23590044	4.53541722	1.03449403
C	-1.36043866	3.63763953	0.40580049
C	-0.65313990	4.86499126	0.20649877
H	-1.18337741	5.80715773	0.37545029
C	0.65234008	4.86567513	-0.19643796
H	1.18229075	5.80840664	-0.36312263
C	1.36010090	3.63902966	-0.39843008
C	2.70986998	3.60111640	-0.82086194
H	3.23545732	4.53890654	-1.02445437
C	3.33839237	2.38416134	-0.97665487
H	4.36527654	2.29963957	-1.33750549
C	2.61947906	1.21000170	-0.64886086
C	0.70581592	2.38915201	-0.17896231
C	-0.70573525	2.38849867	0.18339775
C	3.30624776	-0.12482345	-0.85770705
C	3.60634641	-2.45330563	-0.19258641
H	2.83611006	-3.16076073	0.15583729
H	3.68338679	-2.51373552	-1.28830108
C	4.95514759	-2.78263077	0.44967211
H	5.22911216	-3.82614298	0.22502168
H	4.91290035	-2.66800634	1.54415515
H	5.74364206	-2.12694766	0.04996439
C	2.57518670	-0.84456181	1.41138130
C	3.27489376	-0.08131734	2.36625178
C	2.67634298	0.07216572	3.62700988
C	1.45149595	-0.51003106	3.93854739
C	0.75852200	-1.27679580	2.98962882

C	1.34634973	-1.43294771	1.73382685
C	-3.30483077	-0.12797947	0.85778562
C	-3.60506012	-2.45466268	0.18706647
H	-2.83610824	-3.16190278	-0.16459493
H	-3.68082926	-2.51848952	1.28269638
C	-4.95533131	-2.78177902	-0.45340338
H	-4.91584480	-2.66424318	-1.54767606
H	-5.74284162	-2.12695043	-0.05024537
H	-5.22980637	-3.82558290	-0.23070022
C	-2.57456911	-0.84207130	-1.41333024
C	-3.27534259	-0.07763805	-2.36645172
C	-2.67754345	0.07852958	-3.62723484
H	-3.20443313	0.66488585	-4.38645745
C	-1.45241323	-0.50221336	-3.94039372
C	-0.75827738	-1.26996789	-2.99312972
C	-1.34554485	-1.42911234	-1.73743424
H	-0.82243744	-1.99751465	-0.96364175
C	-4.60556689	0.56976270	-2.07544315
H	-4.47812693	1.50980395	-1.51126589
H	-5.12534027	0.81407102	-3.01387208
H	-5.25481090	-0.08407272	-1.47504118
H	-1.02496318	-0.36010710	-4.93771377
H	1.02334898	-0.36983293	4.93583705
C	0.59402546	-1.86060566	-3.30533800
H	1.39470079	-1.11630076	-3.15594403
H	0.81486581	-2.72012661	-2.65400539
H	0.64793224	-2.19855593	-4.35217855
H	0.82379110	-2.00000465	0.95867111
H	3.20226359	0.65790056	4.38738076
C	4.60460938	0.56782332	2.07699169
H	5.12325572	0.81242135	3.01596420
H	5.25538661	-0.08526826	1.47734743
H	4.47702704	1.50764692	1.51253027
C	-0.59345431	-1.86902428	3.30015675
H	-1.39445510	-1.12453882	3.15329027
H	-0.81431084	-2.72625624	2.64582057
H	-0.64721403	-2.21047413	4.34586119

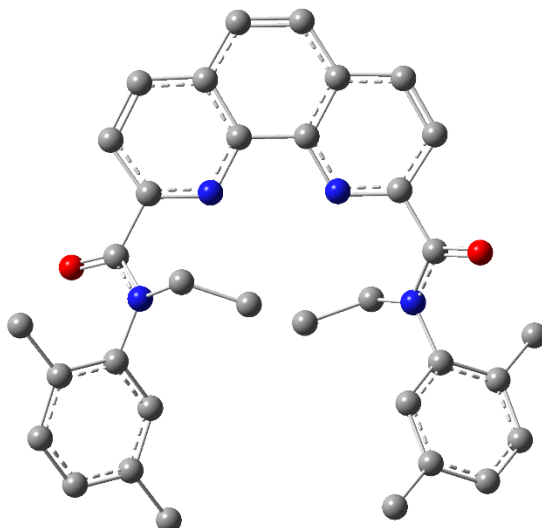
L2 anti (II)



O	4.79266874	1.03073798	1.15785161
O	-4.03751138	0.14039343	-0.27915617
N	1.78881728	1.93507578	-0.19521936
N	-0.95990188	1.78671369	-0.09033023
N	3.58506291	-0.38800368	-0.18240355
N	-2.47328452	-0.40817095	1.29906312
C	3.11081498	2.04100885	-0.17021313
C	3.80812691	3.24187805	-0.44318964
H	4.89452574	3.26368447	-0.33841422
C	3.08336543	4.34833929	-0.82908955
H	3.57960707	5.29085095	-1.07896656
C	1.67212005	4.26968608	-0.88902986
C	0.86015835	5.38072956	-1.27845608
H	1.35470450	6.31503192	-1.56087683
C	-0.50218033	5.28296424	-1.29573145
H	-1.11834580	6.13506989	-1.59794824
C	-1.15553160	4.07141246	-0.90820864
C	-2.56387041	3.93850960	-0.89595426
H	-3.18483924	4.78346591	-1.20827994
C	-3.13263829	2.75008317	-0.49569844
H	-4.21027373	2.58253026	-0.50105814
C	-2.28326978	1.69812929	-0.07050433
C	-0.38765791	2.93787342	-0.50768489
C	1.06695904	3.02846921	-0.52513109
C	-2.99187288	0.40278036	0.31266887
C	-1.24919561	-0.13604187	2.09114054
H	-0.78079307	-1.11225117	2.29343253
H	-0.56439626	0.44832620	1.46306394
C	-1.54489702	0.57822657	3.41110968
H	-2.24436700	-0.00116461	4.03428931
H	-1.97509730	1.57615374	3.23086120
H	-0.60836067	0.70881241	3.97731685
C	-3.21014457	-1.59673171	1.65797795
C	-2.59637786	-2.83427397	1.42725111
C	-3.20501521	-4.04045414	1.78258708
C	-4.46954615	-3.97626964	2.38390394
C	-5.08456665	-2.74895226	2.61409045

H	-6.07216659	-2.72266592	3.08481426
C	-4.47940133	-1.53200922	2.26454766
C	-5.19067838	-0.23115760	2.51651465
H	-4.51095179	0.52664702	2.93642800
C	3.91888305	0.85191687	0.31314135
C	4.19157165	-1.56720826	0.46292567
H	4.45938140	-1.25407961	1.48295431
H	3.41609784	-2.34824602	0.51982530
C	5.42797978	-2.09946541	-0.26388142
H	5.19209636	-2.37292181	-1.30424843
H	5.80128125	-3.00015246	0.24997229
H	6.23051324	-1.34642859	-0.26149869
C	2.78294581	-0.59964918	-1.35618915
C	1.54864453	-1.24113573	-1.21258274
C	0.73176713	-1.52470340	-2.31064832
C	1.19223458	-1.14213039	-3.57730415
C	2.42160170	-0.50467960	-3.72782525
H	2.76166926	-0.22242867	-4.72904856
C	3.25092962	-0.22313779	-2.63287669
C	4.57508436	0.46544347	-2.84692575
H	4.90475553	0.34347516	-3.88954195
H	-5.57566281	0.16948930	1.56428655
H	-6.02989555	-0.37451087	3.21280331
H	4.50114796	1.54825028	-2.64648169
H	5.35587922	0.06419816	-2.18464089
H	-1.61859904	-2.84877991	0.93606653
H	1.21026881	-1.49126303	-0.20276447
H	0.57645611	-1.34690035	-4.45825041
H	-4.97991803	-4.90029043	2.67291075
C	-2.52408906	-5.36400413	1.53381947
H	-2.13716734	-5.79414922	2.47351126
H	-3.22413618	-6.09711499	1.10229257
H	-1.67543819	-5.25304487	0.84192599
C	-0.60848071	-2.19150770	-2.12788726
H	-1.10524959	-2.35801966	-3.09530346
H	-0.50510345	-3.16935685	-1.62847009
H	-1.27724705	-1.57290137	-1.50743409

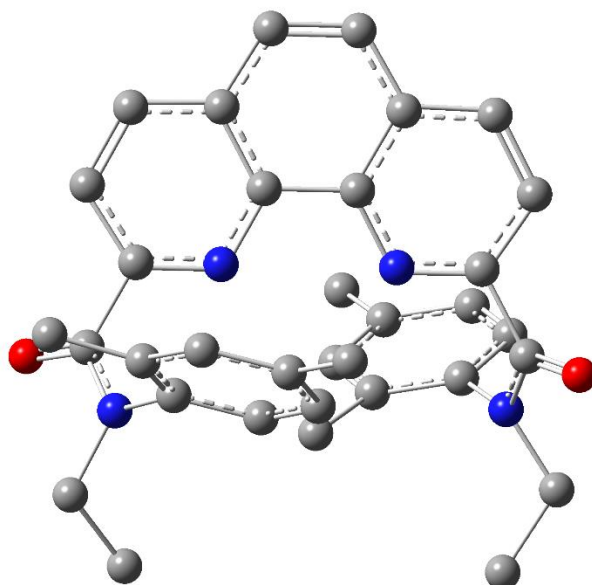
L2 anti (III)



O	-3.36522397	2.18652727	-2.02971910
O	4.20942919	-0.63144572	1.47532827
N	-0.14674468	2.58239053	-0.95447205
N	2.30494239	1.44484456	-0.46082535
N	-2.69924207	1.53207694	0.07048570
N	2.74626682	-1.44173702	-0.10122493
C	-1.32748181	3.10526414	-1.26239984
C	-1.48461195	4.37797725	-1.86086378
H	-2.48566073	4.71772590	-2.13271591
C	-0.36115223	5.14444935	-2.08216246
H	-0.43754048	6.14681136	-2.51392407
C	0.91439075	4.62506058	-1.75511546
C	2.12132138	5.36716932	-1.95102339
H	2.05175541	6.37793583	-2.36407303
C	3.33582939	4.83209236	-1.62525422
H	4.25419890	5.40936729	-1.76824881
C	3.43768189	3.50671310	-1.09727199
C	4.67685206	2.91934152	-0.74630609
H	5.59786360	3.49723503	-0.86781809
C	4.70383758	1.63448606	-0.24928382
H	5.62876298	1.15246865	0.07255010
C	3.48530590	0.92142164	-0.15245607
C	2.26258076	2.72078887	-0.90477717
C	0.96498915	3.30707762	-1.21112158
C	3.52261020	-0.46227919	0.47281765
C	2.21747346	-1.39258664	-1.48099064
H	2.73280621	-0.57665634	-2.00803576
H	2.51885791	-2.33643256	-1.96980106
C	0.70405305	-1.20893126	-1.58513395
H	0.41341480	-0.22744583	-1.18374063
H	0.17245168	-2.00886406	-1.04666228
H	0.40536213	-1.26030889	-2.64509491
C	2.61746599	-2.70164229	0.58983727
C	3.62212580	-3.68308292	0.48301255
C	3.40083249	-4.90044723	1.13607769

H	4.16825825	-5.67829905	1.07590997
C	2.23603840	-5.13991148	1.86779596
C	1.24517669	-4.15985300	1.98416444
C	1.46151278	-2.93610263	1.33526933
C	-2.56580606	2.24077193	-1.10061062
C	-1.98237498	1.84179354	1.32571324
H	-1.52875073	2.83734900	1.21509164
H	-2.74874259	1.92027754	2.11761605
C	-0.91657691	0.82303213	1.72744822
H	-1.35153184	-0.18378844	1.82528001
H	-0.49695707	1.10534700	2.70703263
H	-0.10504978	0.81184491	0.98569580
C	-3.76242512	0.56112796	0.16194143
C	-3.45126238	-0.78595470	-0.02525267
C	-4.42475986	-1.78649799	0.10505738
C	-5.72685985	-1.38728210	0.42242979
C	-6.04278072	-0.03814165	0.59513019
H	-7.07332580	0.24801533	0.82686867
C	-5.07654643	0.96554441	0.46819937
C	-5.43690177	2.42093949	0.60770642
H	-6.49067614	2.53366940	0.90162430
H	-4.81429298	2.93085299	1.36099741
H	-5.28329192	2.93731488	-0.35404658
H	-2.42411384	-1.04935005	-0.29421125
H	0.72462329	-2.13179131	1.41776576
C	4.90252482	-3.41708521	-0.26348868
H	5.46127868	-2.60583375	0.23133740
H	5.53465037	-4.31683292	-0.28342105
H	4.71711073	-3.10502245	-1.30433482
H	-6.51100293	-2.14319487	0.52874417
H	2.09957086	-6.10540302	2.36459329
C	-4.06687078	-3.23893432	-0.09384493
H	-3.35061471	-3.58127374	0.67237848
H	-4.95872251	-3.88045509	-0.03291350
H	-3.59509267	-3.40105811	-1.07675222
C	-0.01851975	-4.40011866	2.77317146
H	-0.89745949	-4.45858344	2.10836576
H	0.03818697	-5.34259529	3.33820893
H	-0.20342617	-3.58188252	3.48774602

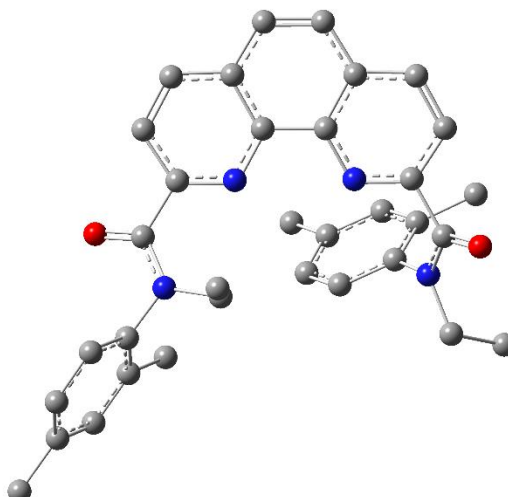
L3_{syn} (I)



O	1.08431747	-3.84872474	-1.55453036
O	-0.60317270	3.64818389	2.34637900
N	-0.43196121	-0.86205299	-1.45810629
N	-0.30391373	1.67765637	-0.40225452
N	-0.58391805	-3.52584482	0.00028930
N	1.35129045	2.51283829	1.92284464
C	-0.40710513	-2.07085844	-2.00004875
C	-0.70714921	-2.32641047	-3.35957967
H	-0.61585088	-3.34172934	-3.75040471
C	-1.11512552	-1.27504058	-4.15029178
H	-1.39147469	-1.42969838	-5.19750153
C	-1.16966857	0.02889934	-3.60353501
C	-1.58684875	1.16343271	-4.36801016
H	-1.89007409	1.00930888	-5.40798273
C	-1.61126804	2.41216946	-3.81487899
H	-1.94022937	3.27505259	-4.40170646
C	-1.19911061	2.62328160	-2.46187257
C	-1.20778482	3.90211573	-1.85713062
H	-1.56128377	4.76427595	-2.43048767
C	-0.77718878	4.04164217	-0.55547370
H	-0.79952774	5.00163439	-0.03586124
C	-0.29596538	2.89628280	0.12155590
C	-0.75969022	1.52316800	-1.66508324
C	-0.78063799	0.18471597	-2.23991766
C	0.13824697	3.05751372	1.56521352
C	1.75824375	2.60999140	3.33665402
H	2.79087006	2.99635058	3.37121189
H	1.08369282	3.35326356	3.79018310
C	1.66339483	1.27679204	4.08022145
H	0.62854855	0.90217546	4.07320128
H	1.97565312	1.41459414	5.12829218
H	2.31775932	0.51682737	3.62615732
C	2.34018326	2.06290506	0.97760570

C	2.47268253	0.70026593	0.69509449
C	3.45755812	0.24879016	-0.17914598
H	3.52938947	-0.81916452	-0.40484889
C	4.33708595	1.15277386	-0.79001326
C	4.18731065	2.51475602	-0.50218114
H	4.85849446	3.23610415	-0.98143955
C	3.20507364	2.99689039	0.37329723
C	3.07392132	4.47656744	0.63451273
H	3.12762333	4.71063396	1.71000476
C	0.09943789	-3.22987711	-1.16155166
C	-0.17156226	-4.74077565	0.73262468
H	-1.02370802	-5.44293416	0.73523884
H	0.64181201	-5.17746297	0.13219614
C	0.29337667	-4.48043647	2.16443151
H	1.18192755	-3.83070425	2.17849048
H	0.56180171	-5.43833995	2.63887115
H	-0.49903955	-4.01261988	2.76882758
C	-1.90750267	-3.01640316	0.26986138
C	-2.12699657	-1.92903874	1.13710305
C	-3.45712872	-1.54806167	1.37511930
H	-3.63747803	-0.69791253	2.04198222
C	-4.55258673	-2.19265961	0.79203337
C	-4.30159023	-3.26600934	-0.07467623
H	-5.13493986	-3.78579888	-0.55692247
C	-2.99452610	-3.67181680	-0.32425103
H	3.87445671	5.03072233	0.12297896
H	2.10773352	4.86356751	0.27003819
H	1.76410848	-0.00114311	1.13702225
C	5.42351138	0.67045583	-1.71920400
H	6.32235841	0.37220565	-1.15217779
H	5.09220975	-0.20721724	-2.29532252
H	5.72410808	1.45764803	-2.42745029
C	-5.96470887	-1.75851446	1.09875368
H	-6.59186825	-1.77315205	0.19333152
H	-6.43411269	-2.43510007	1.83362696
H	-5.98771851	-0.74178589	1.51878053
H	-2.79859806	-4.51161265	-0.99760209
C	-1.00294795	-1.13291914	1.74033248
H	-1.34394785	-0.60441421	2.64327353
H	-0.14741088	-1.77073248	2.00137605
H	-0.65086121	-0.38948597	1.00243219

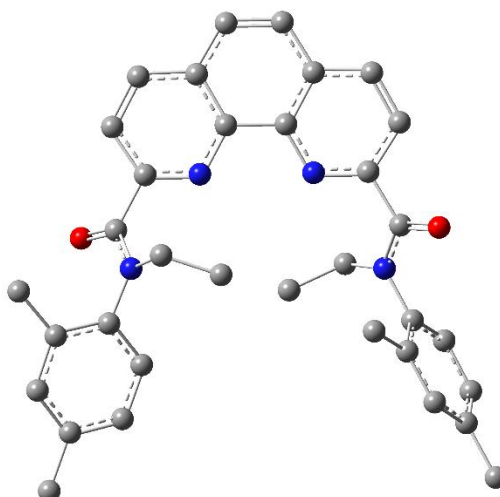
L3_{syn} (II)



O	4.68577110	1.22126762	1.34099609
O	-4.16836847	0.12514075	0.09596502
N	1.66763386	2.02794154	-0.02077101
N	-1.07777673	1.80728090	0.12340848
N	3.56904352	-0.23026274	-0.04286014
N	-2.48469606	-0.43020215	1.53110886
C	2.98607885	2.17538605	-0.00461947
C	3.64443373	3.39558608	-0.28828386
H	4.73002065	3.45272580	-0.18834061
C	2.88392816	4.47576410	-0.67926766
H	3.34949120	5.43063944	-0.94103008
C	1.47564601	4.35308521	-0.73041856
C	0.62937479	5.43522042	-1.12793488
H	1.09509232	6.37921767	-1.42668354
C	-0.72951728	5.29803108	-1.13330679
H	-1.37248999	6.12737518	-1.44300807
C	-1.34437948	4.07388398	-0.72341710
C	-2.74849706	3.90335367	-0.69283928
H	-3.39530339	4.72711205	-1.00957224
C	-3.28025189	2.70718321	-0.26679411
H	-4.35233919	2.50781078	-0.24963033
C	-2.39775446	1.68362377	0.16131829
C	-0.54149864	2.96688570	-0.31681196
C	0.91015706	3.09777297	-0.35048490
C	-3.07512904	0.38705029	0.59402408
C	-1.18226387	-0.21989427	2.20658447
H	-0.77518840	-1.22497998	2.40817135
H	-0.51808881	0.29463700	1.49944358
C	-1.28490980	0.57300616	3.51168820
H	-1.92116376	0.06382223	4.25158227
H	-1.69286379	1.57890257	3.32591074
H	-0.27932949	0.68885928	3.94795398
C	-3.24054356	-1.58815966	1.94612069
C	-3.12203898	-2.79720302	1.23760104
C	-3.82528244	-3.91168310	1.71093719
H	-3.73487378	-4.85697719	1.16448656

C	-4.63801242	-3.86180919	2.85016759
C	-4.74664622	-2.64107332	3.52840373
H	-5.38212082	-2.56629957	4.41600471
C	-4.05759949	-1.51669012	3.07753353
C	3.83475506	1.01529352	0.47971428
C	4.21741429	-1.39219686	0.59278961
H	4.48201396	-1.07363974	1.61197813
H	3.46905635	-2.19926711	0.65374629
C	5.46447997	-1.88055541	-0.14613362
H	5.23028311	-2.15283803	-1.18717676
H	5.86782184	-2.77384140	0.35781536
H	6.24484141	-1.10446082	-0.14290129
C	2.78399508	-0.45911626	-1.22293938
C	1.57509303	-1.15786333	-1.10347800
C	0.80177373	-1.44605896	-2.21975013
H	-0.14590009	-1.97896001	-2.09961796
C	1.21519732	-1.03651274	-3.49733371
C	2.42297811	-0.34340978	-3.60253904
H	2.76502562	-0.02403544	-4.59313220
C	3.23205834	-0.04769284	-2.49315628
C	4.52672222	0.69890633	-2.69504601
H	4.88010256	0.58045972	-3.73023388
H	4.39702575	1.77894782	-2.50917070
H	5.31227669	0.34236832	-2.01338122
H	1.23431092	-1.44709547	-0.10624907
C	-5.40113918	-5.07774875	3.31544528
H	-6.46773224	-5.00014728	3.04321662
H	-5.00595685	-5.99752817	2.85841288
H	-5.35001484	-5.18717051	4.41042189
C	0.37754147	-1.34224204	-4.71403027
H	-0.64115187	-0.93542503	-4.60431470
H	0.82125702	-0.91109229	-5.62387662
H	0.27960508	-2.43019508	-4.86578117
H	-4.16203668	-0.56151369	3.59714845
C	-2.28903903	-2.88068426	-0.01415131
H	-1.25111767	-2.55738525	0.16505419
H	-2.27068180	-3.90948237	-0.40278228
H	-2.70860264	-2.22114800	-0.79190322

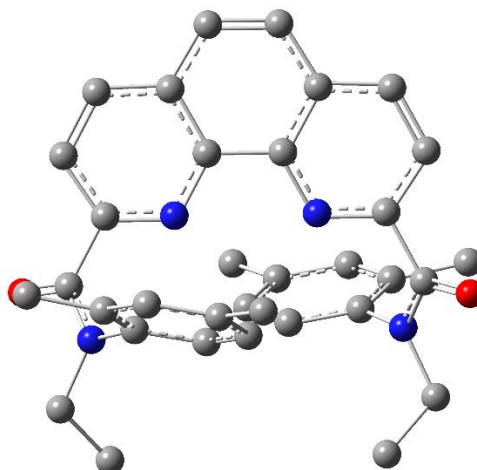
L3_{syn} (III)



O	-3.07022157	1.99035438	-2.46072243
O	4.36660117	-0.57766305	1.53191160
N	0.01853184	2.52396487	-1.15379789
N	2.46364797	1.42342301	-0.49841646
N	-2.64180341	1.55546767	-0.24446261
N	2.99755258	-1.48514428	-0.07516882
C	-1.14356091	3.02030360	-1.56268233
C	-1.27446924	4.26826361	-2.21691399
H	-2.25742524	4.58441738	-2.57103487
C	-0.14861658	5.04351994	-2.38442998
H	-0.20621220	6.03087143	-2.85217835
C	1.10732193	4.55200351	-1.95541795
C	2.31230849	5.30801703	-2.09913171
H	2.25264548	6.30643717	-2.54261096
C	3.51207419	4.79840240	-1.69101042
H	4.43052197	5.38382011	-1.79487277
C	3.59911569	3.48686149	-1.12852360
C	4.82865755	2.92434957	-0.71057198
H	5.74622444	3.51306128	-0.80250817
C	4.85072118	1.64945625	-0.19151008
H	5.76614934	1.18301187	0.17642261
C	3.63755546	0.92149221	-0.13325108
C	2.42510992	2.68962499	-0.97421920
C	1.13885193	3.25177237	-1.36679918
C	3.69912789	-0.45306562	0.50885045
C	2.39164225	-1.42676814	-1.42268587
H	2.82013508	-0.56615685	-1.95304122
H	2.71024224	-2.33322110	-1.96283347
C	0.86636803	-1.33529648	-1.40137716
H	0.55551367	-0.36036097	-0.99967393
H	0.43710386	-2.14946020	-0.79588711
H	0.47687878	-1.43103995	-2.42803019
C	2.97692974	-2.75875142	0.59515625
C	3.58429360	-3.85933717	-0.02174055
C	3.55764227	-5.11821339	0.57003674

H	4.04034220	-5.96236179	0.06848928
C	2.92579703	-5.30842400	1.80655551
C	2.32749835	-4.19888003	2.41221595
H	1.82200213	-4.32979833	3.37533782
C	2.33215310	-2.91988392	1.83780804
C	1.67876662	-1.76780425	2.54953834
H	2.45156490	-1.12381007	3.00146450
C	-2.38200016	2.14699511	-1.45754348
C	-2.05074063	1.99518218	1.03641206
H	-1.60658314	2.98893838	0.87640475
H	-2.88784697	2.12431818	1.74538711
C	-1.00832320	1.04227806	1.61790257
H	-1.43198357	0.03840152	1.77343089
H	-0.67006215	1.42316393	2.59562825
H	-0.14203799	0.98207632	0.94311527
C	-3.71174033	0.59219125	-0.16786686
C	-3.40076479	-0.76974607	-0.18922787
C	-4.40510963	-1.72828578	-0.06531518
H	-4.14580870	-2.79085868	-0.09035805
C	-5.74313742	-1.34073498	0.08019669
C	-6.03716656	0.02876722	0.08071536
H	-7.08165901	0.34698450	0.17011386
C	-5.04859416	1.01271751	-0.04257164
C	-5.41353456	2.47360464	-0.08574619
H	-6.49326089	2.61052823	0.07160820
H	1.10413426	-1.13886064	1.85267638
H	1.00665656	-2.12850746	3.34175465
H	-4.87810759	3.05507890	0.68258016
H	-5.14527607	2.89603109	-1.06790125
H	4.09816573	-3.72069510	-0.97664552
H	-2.35879577	-1.07039741	-0.32286875
C	2.91314235	-6.66199335	2.47279107
H	2.76368699	-7.46869481	1.73788990
H	3.87121327	-6.85765837	2.98476490
H	2.11402593	-6.72946122	3.22656319
C	-6.83469732	-2.36910201	0.24721477
H	-7.82234839	-1.94730075	0.00684452
H	-6.66390183	-3.24125307	-0.40325319
H	-6.87282800	-2.73716245	1.28702068

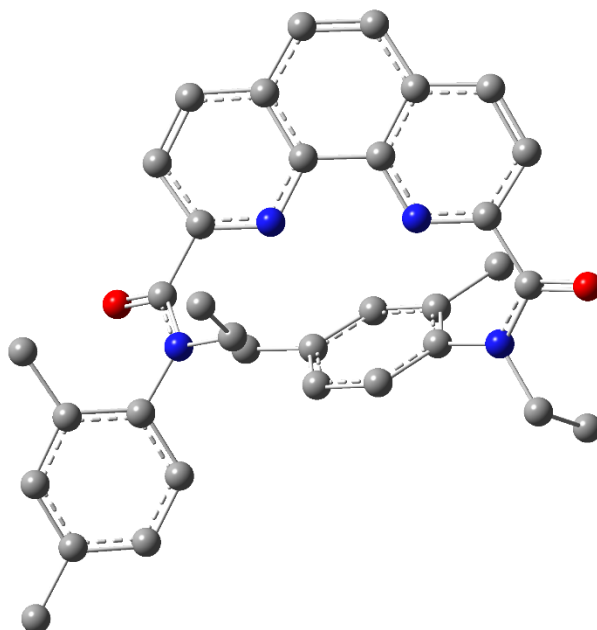
L3_{anti} (I)



O	1.05598396	-3.83493234	-1.82963564
O	-0.82586751	3.50707527	2.43556591
N	-0.42188013	-0.78974501	-1.56260241
N	-0.39243679	1.69559547	-0.39730687
N	-0.35804386	-3.34361143	-0.08444980
N	1.15542002	2.41957166	2.01405049
C	-0.38268491	-1.97996255	-2.14550503
C	-0.70064163	-2.19748598	-3.50690390
H	-0.58668958	-3.19682783	-3.93170530
C	-1.14089597	-1.12738957	-4.25621489
H	-1.42407606	-1.25115740	-5.30576289
C	-1.21693538	0.15507975	-3.66333763
C	-1.66679997	1.30853138	-4.38012298
H	-1.97358934	1.18832037	-5.42356797
C	-1.71640327	2.53435170	-3.77875106
H	-2.06857864	3.41081615	-4.33114337
C	-1.30666633	2.70370531	-2.41858904
C	-1.35691342	3.95437071	-1.75886643
H	-1.73079238	4.83055680	-2.29698356
C	-0.94518372	4.04756185	-0.44649960
H	-1.00451789	4.98159067	0.11586723
C	-0.43693817	2.88697320	0.18299189
C	-0.83297097	1.58539549	-1.66879740
C	-0.81315430	0.27192394	-2.29934941
C	-0.04942679	2.97562338	1.64555845
C	1.49449243	2.40332856	3.44877049
H	2.52554819	2.77774522	3.56294082
H	0.80075813	3.11172837	3.92811156
C	1.36046253	1.01377522	4.07437669
H	0.32473022	0.64985519	3.99230921
H	1.62568420	1.06042782	5.14330651
H	2.03126494	0.28874588	3.58810829
C	2.18988254	2.04564460	1.08498389
C	2.33029595	0.71462017	0.68187228
C	3.36287185	0.33613480	-0.17188130
H	3.44139941	-0.70648015	-0.49354020
C	4.28224160	1.28299768	-0.64273692

C	4.12113652	2.61440672	-0.24030765
H	4.81993527	3.37115167	-0.61382322
C	3.09196107	3.02273381	0.61843258
C	2.94736446	4.47424786	1.00222487
H	2.95455081	4.61415825	2.09529917
C	0.16388516	-3.14413344	-1.34345752
C	0.23897502	-4.40487749	0.74659451
H	-0.57803922	-5.02071079	1.15861396
H	0.83928386	-5.02097245	0.05888382
C	1.11204366	-3.85474566	1.87585542
H	1.94853457	-3.26674233	1.46776818
H	1.53081502	-4.68907448	2.46201633
H	0.52989039	-3.21662401	2.55849555
C	-1.57625822	-2.73974144	0.38934548
C	-1.53197597	-1.60570584	1.20481282
C	-2.70319859	-1.04953006	1.71270300
H	-2.64844381	-0.14822622	2.33019307
C	-3.94910538	-1.61743140	1.41636244
C	-3.97836104	-2.74646704	0.58820995
H	-4.94546823	-3.19292441	0.33137198
C	-2.81585966	-3.32679216	0.06437908
C	-2.90334073	-4.52735787	-0.84449961
H	-2.29103872	-5.36721635	-0.47852207
H	3.76796199	5.06955897	0.57585557
H	1.99644499	4.89282490	0.63262734
H	-3.94408420	-4.87300526	-0.92801155
H	-2.54335999	-4.28747903	-1.85899646
H	1.58751432	-0.01558375	1.00404637
H	-0.56962995	-1.13039840	1.39624706
C	5.42066297	0.87804193	-1.54614851
H	6.29817034	0.56248455	-0.95545663
H	5.13564167	0.03178144	-2.18985504
H	5.73823574	1.71268121	-2.18986686
C	-5.22247355	-1.03926600	1.98252806
H	-6.06790808	-1.17786896	1.29094850
H	-5.48951025	-1.53231487	2.93339273
H	-5.11390118	0.03666403	2.18717718

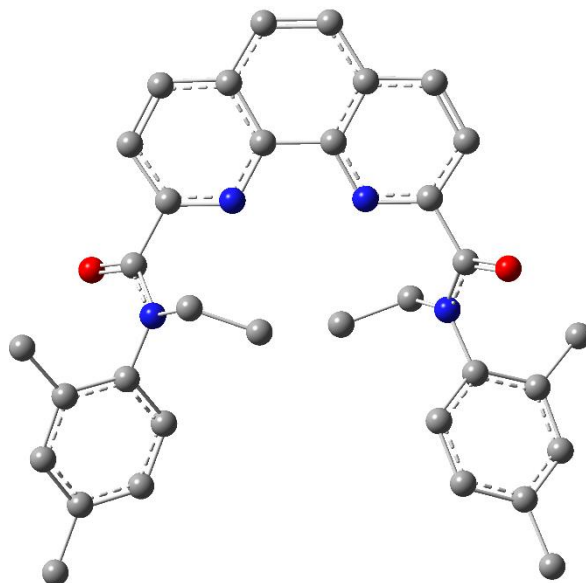
L3_{anti} (II)



O	5.42678837	0.91426955	0.82465975
O	-3.33298117	-0.06485920	-0.70896831
N	2.19773095	1.92392678	-0.04928803
N	-0.54717586	1.77331065	0.01096092
N	3.87040821	-0.45796899	-0.14530439
N	-2.24342714	-0.39772687	1.28460203
C	3.51994422	2.00521371	-0.06360519
C	4.22783592	3.21370078	-0.27590394
H	5.31716891	3.20059110	-0.21295626
C	3.50997615	4.35703462	-0.55019619
H	4.01406073	5.30863362	-0.74398987
C	2.09672718	4.29924898	-0.59015892
C	1.29024377	5.43581009	-0.91159931
H	1.78856852	6.38652551	-1.12398033
C	-0.07125721	5.33684582	-0.96925444
H	-0.68185059	6.20496136	-1.23533930
C	-0.73037146	4.09867379	-0.68922652
C	-2.13479824	3.94797069	-0.77450328
H	-2.74932387	4.80388322	-1.06914244
C	-2.70550630	2.72351658	-0.50384018
H	-3.77745071	2.54668145	-0.60660063
C	-1.86575821	1.66464811	-0.07942994
C	0.03007769	2.95020118	-0.31855249
C	1.48398498	3.04217595	-0.30173404
C	-2.53343879	0.31527764	0.14467908
C	-1.29498955	0.05815128	2.32839902
H	-0.84310075	-0.84672028	2.76256921
H	-0.49560958	0.62449906	1.83212977
C	-1.97479736	0.87699735	3.42673564
H	-2.77605575	0.30071199	3.91588827
H	-2.40692188	1.80399975	3.01759137
H	-1.23507939	1.15567809	4.19482718
C	-2.91645619	-1.65056882	1.51521142

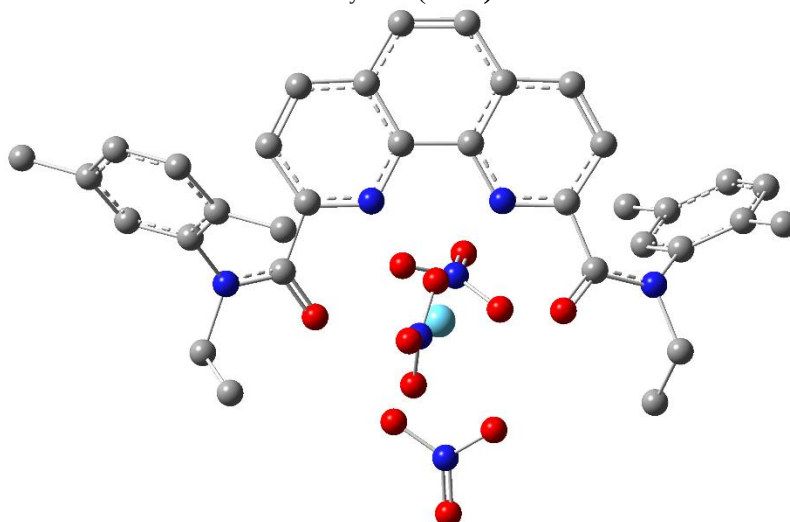
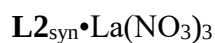
C	-2.14113236	-2.81393217	1.59389189
C	-2.72360646	-4.05028504	1.85691911
H	-2.09592449	-4.94475958	1.90982690
C	-4.10776134	-4.15580665	2.04621319
C	-4.86848123	-2.98414711	1.97268850
H	-5.95069596	-3.04522714	2.13212495
C	-4.31016193	-1.72426507	1.71405832
C	-5.19455446	-0.50924969	1.64967265
H	-4.75741661	0.33620193	2.20419930
C	4.35634012	0.77475477	0.23504111
C	4.63065325	-1.64095264	0.30383233
H	5.16718116	-1.33827278	1.21492676
H	3.90075641	-2.42546916	0.55924988
C	5.62033296	-2.15599317	-0.74270978
H	5.10520809	-2.42393331	-1.67850392
H	6.13010987	-3.05612746	-0.36244454
H	6.38445111	-1.39343243	-0.95657552
C	2.74704213	-0.68573407	-1.01247523
C	1.63149612	-1.35791024	-0.49574171
C	0.52309195	-1.62041073	-1.28845658
H	-0.34934246	-2.12217301	-0.85981868
C	0.49413546	-1.21144280	-2.63049459
C	1.62449895	-0.56699400	-3.13973940
H	1.62636229	-0.25440717	-4.18993565
C	2.76634710	-0.30185644	-2.36657193
C	3.94342534	0.40447564	-2.99097854
H	3.93196032	0.27592397	-4.08368127
H	-5.30483676	-0.18809732	0.60086906
H	-6.18828257	-0.72736490	2.06713347
H	3.91798713	1.48841406	-2.78379118
H	4.89933759	0.02226563	-2.60354395
H	-1.06108204	-2.74271859	1.43969931
H	1.63215235	-1.63799857	0.56108838
C	-4.76084370	-5.49239141	2.29677841
H	-5.00519316	-5.99457644	1.34467959
H	-4.09595718	-6.16371818	2.86206816
H	-5.69944564	-5.37999672	2.86090937
C	-0.72696013	-1.45996762	-3.48014278
H	-1.63452869	-1.09077542	-2.97436125
H	-0.64362601	-0.95867289	-4.45618903
H	-0.87020209	-2.53827060	-3.66439481

L3_{anti} (III)



O	-3.34204233	2.26617988	-2.06039780
O	4.27042904	-0.56449340	1.44362995
N	-0.11950017	2.63899590	-0.97726599
N	2.33680431	1.50074276	-0.48495088
N	-2.68565066	1.58757182	0.03449422
N	2.79090858	-1.38910415	-0.10908363
C	-1.29959135	3.16360449	-1.28524713
C	-1.45583790	4.43774413	-1.88124927
H	-2.45681666	4.77791176	-2.15257735
C	-0.33223800	5.20353713	-2.10164215
H	-0.40754702	6.20672882	-2.53167043
C	0.94275831	4.68200560	-1.77653757
C	2.14880455	5.42461058	-1.97437667
H	2.07797882	6.43523175	-2.38757176
C	3.36367414	4.88968926	-1.65079438
H	4.28205089	5.46656319	-1.79534235
C	3.46589848	3.56440571	-1.12325304
C	4.70662288	2.97916264	-0.77494410
H	5.62644859	3.55838779	-0.89909860
C	4.73621308	1.69506095	-0.27720435
H	5.66187963	1.21420591	0.04401731
C	3.51881835	0.98025331	-0.17735186
C	2.29164536	2.77696626	-0.92910409
C	0.99316641	3.36317070	-1.23377736
C	3.56780214	-0.40175305	0.45085447
C	2.24084898	-1.34858151	-1.48084469
H	2.73914137	-0.52846645	-2.01765714
H	2.54315456	-2.29079613	-1.97197234
C	0.72434625	-1.17924111	-1.56089646
H	0.43274648	-0.19503376	-1.16731812
H	0.20863336	-1.97624047	-1.00297887
H	0.40745144	-1.24637375	-2.61468522
C	2.69138527	-2.64787349	0.58707836
C	3.70064493	-3.62182178	0.46107250

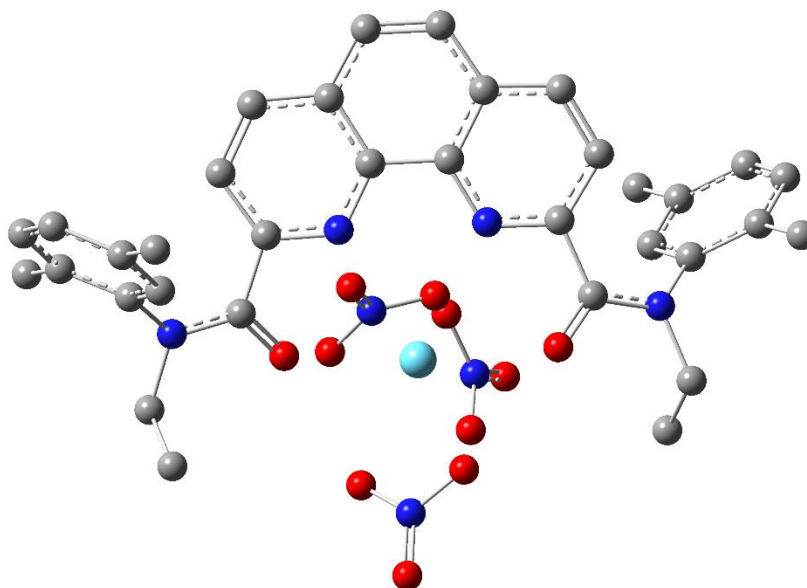
C	3.51804553	-4.84429526	1.11678706
H	4.29856186	-5.60762579	1.02314440
C	2.38393286	-5.12386724	1.89160795
C	1.40378847	-4.13166963	2.00759302
H	0.51082481	-4.31757283	2.61157175
C	1.55873545	-2.90502648	1.36180731
C	-2.54288352	2.30513444	-1.13006157
C	-1.96480663	1.87622452	1.29258489
H	-1.49809613	2.86683254	1.19247927
H	-2.73013403	1.95525435	2.08533405
C	-0.91242233	0.83905801	1.68206531
H	-1.35822540	-0.16481158	1.75914526
H	-0.49481869	1.09932234	2.66860055
H	-0.09694629	0.83304025	0.94477849
C	-3.76764175	0.63810200	0.11716688
C	-3.49741804	-0.71630433	-0.09270430
C	-4.50921087	-1.66812280	0.02457082
H	-4.28307402	-2.72402475	-0.15111762
C	-5.81404958	-1.28075734	0.35386916
C	-6.06964619	0.08370407	0.54210949
H	-7.09054128	0.40482033	0.77660004
C	-5.07331624	1.06069002	0.42852735
C	-5.40275114	2.52208276	0.58698322
H	-6.45360737	2.65484260	0.88266755
H	-4.76813518	3.00801546	1.34589338
H	-5.23728569	3.04612202	-0.36859034
H	-2.48307628	-1.01360825	-0.36964202
C	2.24653302	-6.44497003	2.60774185
H	2.66477386	-7.27002420	2.01020764
H	2.78767597	-6.42787482	3.56952816
H	1.19207777	-6.67456799	2.82404822
C	-6.91120446	-2.30420815	0.51428090
H	-7.90369432	-1.85468262	0.35829459
H	-6.79103278	-3.13286727	-0.20083585
H	-6.89881985	-2.73960307	1.52848719
H	0.80179250	-2.12351121	1.46329042
C	4.95752192	-3.34495826	-0.32164579
H	5.52169949	-2.52864278	0.15831096
H	5.59676578	-4.23895769	-0.36070479
H	4.73907668	-3.03364263	-1.35612806



La	0.67923417	-0.60770120	1.45547415
O	-0.72177672	-2.69751613	0.97603654
O	1.33602583	1.85074998	2.06030048
O	-0.90031760	-0.88755744	3.48648513
O	-1.63306486	0.41849050	1.87852519
O	-2.90542090	0.01217690	3.63139488
O	3.03429862	-0.13807531	0.45411950
O	1.78103400	-1.51128299	-0.70960059
O	3.74442073	-0.89325158	-1.49115496
O	1.88460483	-2.56063140	2.51026231
O	2.24895997	-0.60426754	3.43948409
O	3.25482294	-2.39937137	4.22974748
N	-1.05537441	-0.76188046	-0.78999901
N	0.52633781	1.43584233	-0.43161683
N	-2.71859694	-3.66641512	0.54087432
N	2.98428671	3.29311693	1.43348121
N	-1.85257818	-0.14406649	3.03191741
N	2.88812586	-0.85684224	-0.61854449
N	2.49918818	-1.88015825	3.43203595
C	-1.82462671	-1.84117138	-0.93715933
C	-2.53516916	-2.09873855	-2.13026933
H	-3.12224989	-3.00920995	-2.24187228
C	-2.47336438	-1.17402963	-3.15521052
H	-3.01278602	-1.34765923	-4.09023515
C	-1.71655549	0.00555790	-2.99757472
C	-1.64610878	1.03160754	-3.99290492
H	-2.20585121	0.89698849	-4.92254816
C	-0.90841312	2.16220623	-3.78429922
H	-0.87163186	2.94927572	-4.54251217
C	-0.16308715	2.34344117	-2.57570986
C	0.60046570	3.49886033	-2.30495874
H	0.62277640	4.31236006	-3.03509220
C	1.31077753	3.59716390	-1.12478004
H	1.90743311	4.48261425	-0.90812316
C	1.26410524	2.52488666	-0.20812985
C	-0.17872785	1.33099058	-1.57580665
C	-0.99756573	0.15085795	-1.77706505

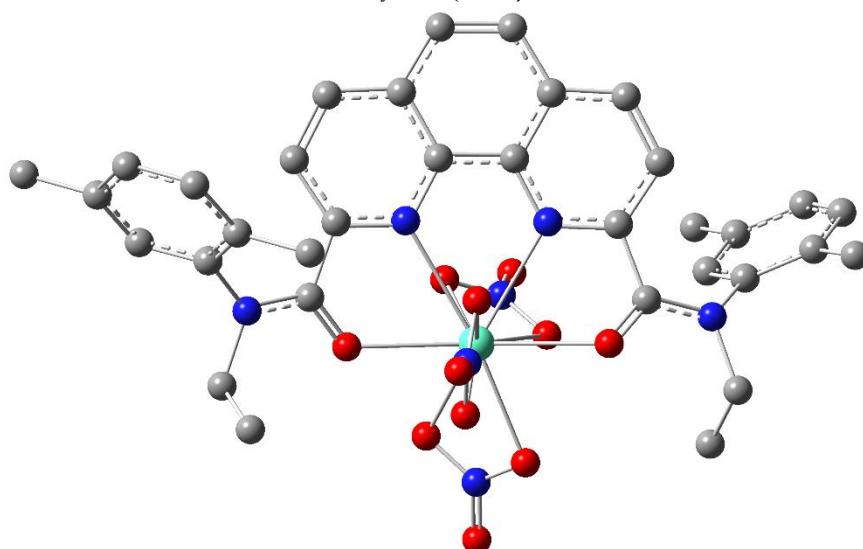
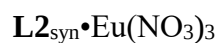
C	1.89304154	2.52467084	1.17589054
C	3.48354110	3.31668751	2.83521327
H	3.99853927	4.28080120	2.96355432
H	2.59792191	3.29933411	3.48766023
C	4.41437324	2.15129358	3.16405789
H	3.87985699	1.19054227	3.11707855
H	4.79209683	2.27878839	4.19115534
H	5.27728762	2.12473739	2.48097576
C	3.90218378	3.70865865	0.40384903
C	4.49541342	2.71643652	-0.38620242
C	5.39737576	3.04609844	-1.40363376
C	5.69349114	4.40297137	-1.59723886
C	5.11026271	5.38741977	-0.79997049
H	5.35270814	6.43945073	-0.98049233
C	4.20313722	5.07283943	0.22186545
C	3.56538676	6.16079324	1.04866336
H	4.14029229	6.35972164	1.97009365
C	-1.73931099	-2.76675150	0.26261587
C	-2.46103283	-4.62151643	1.65359805
H	-3.01364745	-5.54019054	1.40380300
H	-1.38266414	-4.83632938	1.64551825
C	-2.88409472	-4.08902620	3.02160486
H	-2.32548707	-3.17632832	3.28246867
H	-2.65547560	-4.84990293	3.78523198
H	-3.96502759	-3.88408372	3.05849185
C	-4.02664329	-3.68382258	-0.06005166
C	-4.94079580	-2.63194803	0.15436191
C	-6.19317002	-2.75543799	-0.46717937
H	-6.92763883	-1.95848235	-0.31797371
C	-6.53481752	-3.86316302	-1.23991738
C	-5.63065285	-4.91748658	-1.42968233
C	-4.37541308	-4.80524499	-0.82376361
H	3.52317501	7.10388431	0.48305301
H	2.54385944	5.88915002	1.35806019
H	4.23750591	1.66779346	-0.19158861
H	-3.63406111	-5.60041874	-0.95513677
C	-4.62728847	-1.43182933	1.00748702
H	-5.54621628	-0.86916274	1.22657197
H	-4.16760270	-1.71104955	1.96690323
H	-3.92661902	-0.73361907	0.51821426
H	6.39138800	4.69564102	-2.38798386
H	-7.52919741	-3.91872517	-1.69318096
C	6.03757004	1.96518930	-2.23747775
H	6.07913119	2.25449155	-3.29965761
H	7.07438662	1.78183227	-1.90670024
H	5.48333273	1.01851650	-2.14825443
C	-5.98288424	-6.11689296	-2.27395983
H	-7.07348968	-6.24344266	-2.34720693
H	-5.59185414	-6.00894451	-3.30034750
H	-5.55580453	-7.04130537	-1.85541250

L2_{anti}•La(NO₃)₃



La	0.29717038	-0.47065580	1.58396701
O	-0.30282267	-2.80814796	0.57548355
O	1.47791018	1.78094209	2.03249952
O	-2.23253244	-0.90228409	1.99074046
O	-1.68243489	1.19121302	1.63810858
O	-3.80303582	0.63843295	1.85166983
O	2.79974803	-1.04845072	2.02046308
O	2.25776305	-0.66424751	-0.07232236
O	4.37564643	-0.88985830	0.48804137
O	0.21592769	-2.20336686	3.42630407
O	0.27207868	-0.10682911	4.07838512
O	0.15786713	-1.72044478	5.57625221
N	-1.03498310	-0.70851832	-0.85227377
N	0.43503985	1.53436274	-0.39578562
N	-2.22728876	-3.95322787	0.15873940
N	3.12237196	3.18269905	1.32758238
N	-2.62049987	0.32842407	1.83244363
N	3.19304923	-0.87937433	0.80500799
N	0.21291574	-1.36123116	4.41685521
C	-1.69811907	-1.84416236	-1.07600354
C	-2.47008703	-2.03973714	-2.24167792
H	-2.99397389	-2.98080995	-2.40559672
C	-2.55829191	-1.01626237	-3.16548971
H	-3.14981931	-1.14279939	-4.07624795
C	-1.87497104	0.19825815	-2.94293983
C	-1.91032630	1.30138399	-3.85467565
H	-2.52077849	1.21257157	-4.75753675
C	-1.19458332	2.43973023	-3.61068277
H	-1.22578997	3.27604146	-4.31449816
C	-0.37538425	2.55882771	-2.44293154
C	0.41432980	3.69386019	-2.15954458
H	0.39065446	4.55082392	-2.83804325
C	1.22134081	3.71006609	-1.03847272
H	1.85344095	4.57089386	-0.82286432
C	1.21658955	2.59003398	-0.17882222

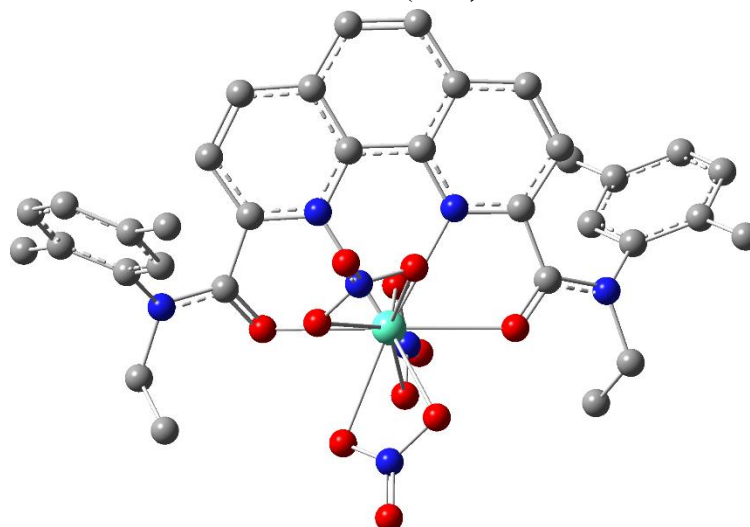
C	-0.32692673	1.49097402	-1.50371078
C	-1.10460916	0.29364792	-1.75071163
C	1.97047538	2.48564745	1.13334710
C	3.73921065	3.11519210	2.68056304
H	4.29059684	4.05798072	2.81738102
H	2.91054232	3.08179941	3.40294421
C	4.66311069	1.91330959	2.86615356
H	4.11214121	0.96494648	2.77200932
H	5.09623997	1.95226726	3.87867880
H	5.48908509	1.92409863	2.13922234
C	3.96467126	3.61588940	0.24330205
C	4.47751246	2.64508834	-0.62643274
C	5.31519775	2.99744466	-1.69028096
C	5.62866605	4.35419900	-1.85163687
C	5.12720975	5.31703892	-0.97697360
H	5.38205011	6.37002009	-1.13229548
C	4.28854343	4.97884875	0.09399777
C	3.74404516	6.04326070	1.01267407
H	4.39448952	6.18805961	1.89302132
C	-1.38311201	-2.90611667	-0.03434536
C	-1.79976563	-5.00496942	1.12062081
H	-2.29905459	-5.93363925	0.80504959
H	-0.71366909	-5.12702647	0.99507186
C	-2.13682707	-4.66844395	2.57178137
H	-1.57412732	-3.78746339	2.91570587
H	-1.85273655	-5.52158004	3.20839525
H	-3.21524561	-4.48788356	2.69948211
C	-3.63038620	-3.88999559	-0.16181187
C	-4.39234911	-2.87350446	0.42514341
C	-5.76021663	-2.74854082	0.15545665
C	-6.34081891	-3.68327195	-0.71258450
C	-5.58070788	-4.70423298	-1.28409282
H	-6.05940197	-5.41351513	-1.96665380
C	-4.20990972	-4.84066441	-1.02602588
C	-3.40609944	-5.93478203	-1.68238623
H	-3.34793991	-6.83390258	-1.04415909
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H	-3.87001377	-6.24076384	-2.63222404
H	-2.37173278	-5.61371971	-1.88252863
H	4.22861080	1.59070023	-0.46029245
H	-3.89282766	-2.16729595	1.10027467
H	6.27715814	4.66299077	-2.67735706
H	-7.40691356	-3.61024772	-0.94916109
C	5.88812513	1.94256922	-2.60241289
H	6.91589328	1.68153696	-2.29697835
H	5.29016806	1.01960401	-2.57042863
H	5.93292301	2.29745065	-3.64400313
C	-6.56921264	-1.65900736	0.81195389
H	-7.38703486	-1.31910233	0.15777027
H	-7.02515866	-2.02673532	1.74760861
H	-5.93400895	-0.79851526	1.07235248



Eu	0.66765104	-0.61081033	1.28339894
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O	1.31812252	1.75493934	2.02675046
O	-0.69822623	-0.59490111	3.34488478
O	-1.56712320	0.48730157	1.65648351
O	-2.71037737	0.27840640	3.52616932
O	3.00725594	-0.12379905	0.42015412
O	1.74878856	-1.39984945	-0.83149220
O	3.76932061	-0.85634630	-1.51379878
O	2.01697007	-2.55849367	1.95731215
O	2.20135924	-0.77997889	3.20639615
O	3.40134262	-2.56474245	3.66843097
N	-1.01779543	-0.80274952	-0.81289553
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C	-1.81264870	-1.86643967	-0.92875742
C	-2.53344806	-2.13224190	-2.11437566
H	-3.13934082	-3.03251802	-2.20623966
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H	-3.00657821	-1.41163729	-4.08684424
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H	-2.17073497	0.82740107	-4.95532897
C	-0.86896018	2.09501125	-3.82446861
H	-0.83165901	2.87649198	-4.58850914
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H	0.65552339	4.26109484	-3.06118952
C	1.32107058	3.54782395	-1.14214227
H	1.90666487	4.43870801	-0.91671245
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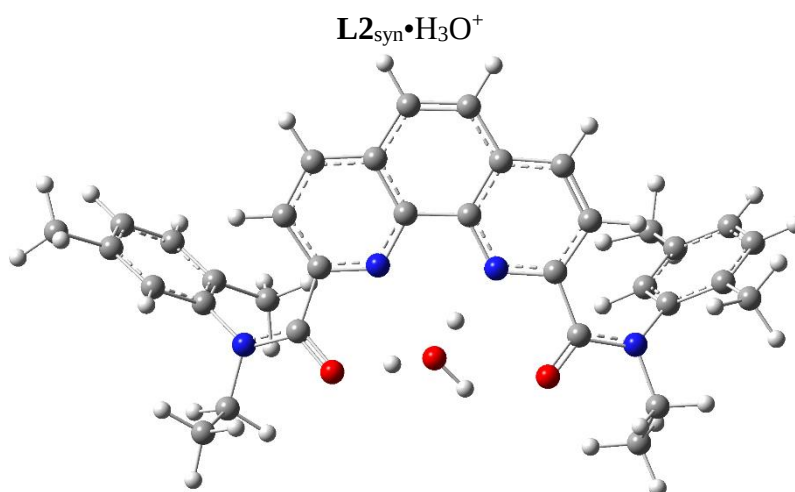
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H	3.90550575	4.22592924	3.04016562
H	2.50635575	3.21456988	3.50909058
C	4.34332157	2.09652977	3.20111599
H	3.82330879	1.13214088	3.09813381
H	4.68302469	2.19209537	4.24479880
H	5.22924835	2.10450459	2.54780694
C	3.87303657	3.70145562	0.46456731
C	4.49756568	2.73097268	-0.32828739
C	5.41320078	3.08932590	-1.32370223
C	5.69324356	4.45297498	-1.49061538
C	5.08046104	5.41630235	-0.68929068
H	5.31107672	6.47441658	-0.84868382
C	4.15747748	5.07265595	0.30856748
C	3.48565498	6.13733183	1.13849362
H	4.03233725	6.32349842	2.07954931
C	-1.75174665	-2.74164761	0.30809669
C	-2.47784964	-4.57226209	1.72920266
H	-3.01129258	-5.50566163	1.49209772
H	-1.39671857	-4.77162327	1.74832600
C	-2.93743911	-4.01527902	3.07566210
H	-2.39299311	-3.09180800	3.32653573
H	-2.72035995	-4.75662160	3.86147922
H	-4.02057426	-3.81879045	3.08287020
C	-4.03124420	-3.67474746	-0.01364361
C	-4.93695667	-2.61012589	0.17413338
C	-6.19180832	-2.74011785	-0.44100754
H	-6.91999006	-1.93399948	-0.31145097
C	-6.54366139	-3.86525197	-1.18334505
C	-5.64755232	-4.93083880	-1.34782658
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H	3.44844055	7.09099540	0.59059634
H	2.45941134	5.84732002	1.41339822
H	4.24923780	1.67610916	-0.15666153
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H	-5.52813720	-0.82155226	1.21104070
H	-4.13811374	-1.64641701	1.95266465
H	-3.91727198	-0.70383609	0.47809978
H	6.40118879	4.76811844	-2.26361157
H	-7.53960223	-3.92506965	-1.63262670
C	6.08352689	2.02981595	-2.16161474
H	6.18020270	2.35326211	-3.21006135
H	7.10098700	1.82453318	-1.78627702
H	5.51827070	1.08600857	-2.12875539
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H	-7.10094635	-6.29638699	-2.18772441
H	-5.66612213	-6.04406084	-3.20537150
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L2_{anti}•Eu (NO₃)₃



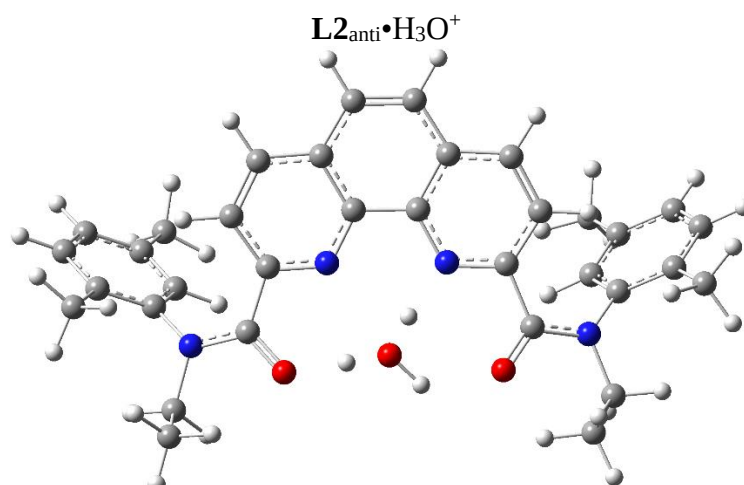
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O	-3.83326728	0.66989468	1.75344891
O	2.47558921	-1.28177670	1.94805000
O	2.09601566	-0.69711181	-0.12373757
O	4.10526687	-1.37149662	0.47059149
O	0.07483063	-1.88730590	3.45763656
O	-0.15403632	0.23926167	3.88407137
O	-0.32090677	-1.22598050	5.51787131
N	-1.02672162	-0.67955027	-0.80640047
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N	-2.17153214	-3.93573708	0.21684698
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N	2.93933936	-1.13406847	0.75269662
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C	-1.66945086	-1.82574990	-1.02977196
C	-2.42395152	-2.03681903	-2.20506582
H	-2.93136862	-2.98666016	-2.37167413
C	-2.51952649	-1.01750642	-3.13406258
H	-3.10142171	-1.15679810	-4.04916237
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H	-2.49281361	1.22313407	-4.72814401
C	-1.18186758	2.45634108	-3.57063741
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H	0.40955208	4.57013763	-2.78221442
C	1.24532961	3.70990526	-0.99420172
H	1.88839992	4.56315641	-0.78009685
C	1.23879469	2.58394739	-0.14171290
C	-0.32694213	1.51080656	-1.46191035

C	-1.09888993	0.31401465	-1.71188115
C	2.02918280	2.42314156	1.14116331
C	3.86026888	2.93585949	2.65387940
H	4.46669215	3.84028942	2.81284918
H	3.06346039	2.90613859	3.41151189
C	4.72721693	1.68047014	2.73560512
H	4.11948343	0.76902029	2.62992558
H	5.21589972	1.64695860	3.72255937
H	5.51254714	1.68356200	1.96454745
C	3.99902736	3.60119571	0.25215549
C	4.46152655	2.69077958	-0.70633062
C	5.26005756	3.10775621	-1.77681086
C	5.58687079	4.46873213	-1.85310996
C	5.13433870	5.37215425	-0.89246365
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C	4.33366473	4.96819210	0.18471750
C	3.83481001	5.97017054	1.19452980
H	4.50856651	6.03530914	2.06674839
C	-1.34995424	-2.86543837	0.03353304
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C	-4.36109509	-2.89050356	0.41944384
C	-5.72522332	-2.79643847	0.12232514
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H	-3.88697394	-2.15978358	1.08648881
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H	-7.33601797	-3.71405765	-0.99143586
C	5.77434674	2.11645275	-2.78972313
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C	-6.56480397	-1.70161271	0.73081081
H	-7.31328268	-1.32839017	0.01424548
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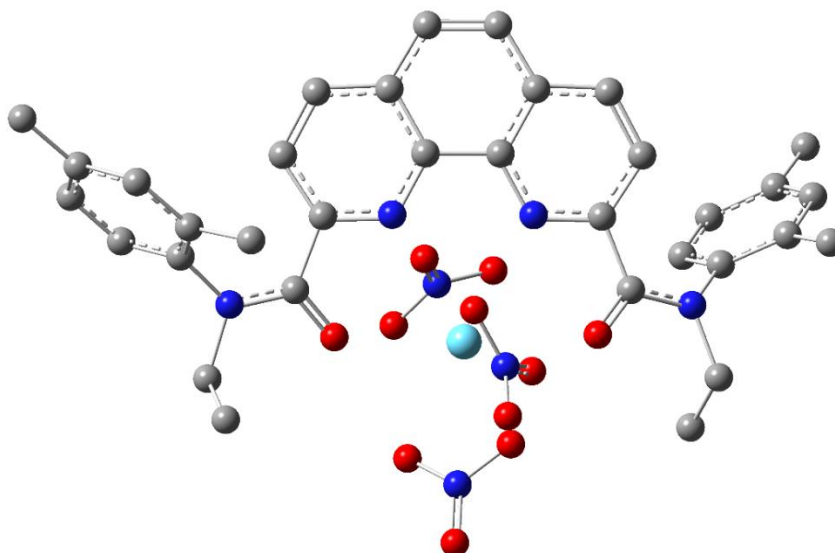
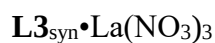
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C	-1.55323771	-2.38034379	-0.70023856
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H	-3.21165437	-3.33753959	-1.73333023
C	-2.26772118	-1.83568756	-2.94374439
H	-2.91929775	-2.00638645	-3.80502167
C	-1.26462990	-0.84387038	-3.01057183
C	-1.02582907	-0.01650794	-4.15678732
H	-1.67465281	-0.13454028	-5.02878733
C	-0.00015434	0.89009753	-4.17813503
H	0.17780357	1.49856050	-5.06907095
C	0.85883474	1.05753838	-3.04423144
C	1.96175702	1.94196379	-2.99630047
H	2.20527163	2.54940714	-3.87216334
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H	3.59440693	2.70216338	-1.82181506
C	2.39368909	1.23066998	-0.73483139
C	0.62686530	0.28230527	-1.87626541
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C	5.90676961	0.73217162	2.04480327
H	5.46725930	-0.23647600	1.77324765
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H	1.19521227	-2.50400850	1.27904961
H	0.73476378	-1.62132879	0.05944810
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H	-7.55049697	-2.00902622	-0.43251931
H	5.58841134	5.99536641	-0.89481925
H	1.89410896	3.54531511	1.31671892
C	6.29383068	3.43003613	-0.35678408
H	6.93821452	3.39551529	0.53845561
H	6.15067032	2.39193316	-0.69449402
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C	1.19907181	6.13952623	0.74052793
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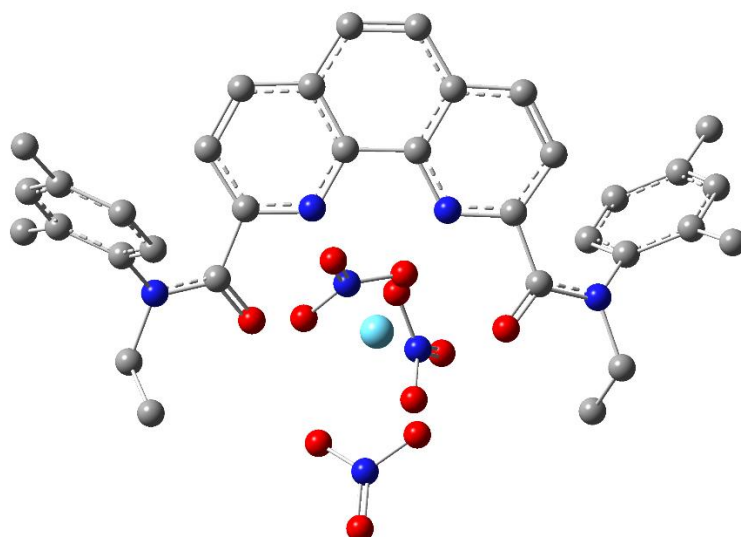
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C	-1.59528132	-2.39909079	-0.72927782
C	-2.47995961	-2.58504567	-1.81528738
H	-3.24451031	-3.35955893	-1.77455225
C	-2.36362285	-1.78275621	-2.93600856
H	-3.02589684	-1.93521330	-3.79252605
C	-1.38956647	-0.76121897	-2.97741897
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H	-3.44458018	-5.46168804	2.07336588
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C	-2.70766962	-3.96348175	3.46489330
H	-1.86960126	-3.25777828	3.55668912
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C	-4.04220032	-3.44022200	0.56678373
C	-4.45232589	-2.13305915	0.86158305
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C	-6.59341061	-2.57485501	-0.11494127
C	-6.19092304	-3.87819314	-0.39826871
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C	-4.91345340	-4.35079534	-0.06456093
C	-4.50565983	-5.76166450	-0.40541158
H	-4.71280379	-6.45384512	0.42924500
H	0.92290832	4.88045035	1.75948336
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H	-5.07116675	-6.12841640	-1.27465523
H	-3.43000791	-5.83388551	-0.62804892
H	2.10793260	-1.05476766	0.86819045
O	1.58710406	-1.92132675	0.52567254
H	1.19373461	-2.52162344	1.20723051
H	0.69649719	-1.60979654	0.02964453
H	-3.75059010	-1.46385001	1.36859908
H	5.81757105	3.16605899	-0.23539394
C	6.41163943	5.62854640	-1.30004744
H	7.06506336	6.19817176	-0.61793493
H	6.98519789	4.76611532	-1.67077652
H	6.18046915	6.28389202	-2.15386994
C	-6.17427180	-0.27465454	0.86589451
H	-6.72749973	0.18010607	0.02948621
H	-6.84748944	-0.27959520	1.73947115
H	-5.31741231	0.37207878	1.10601784
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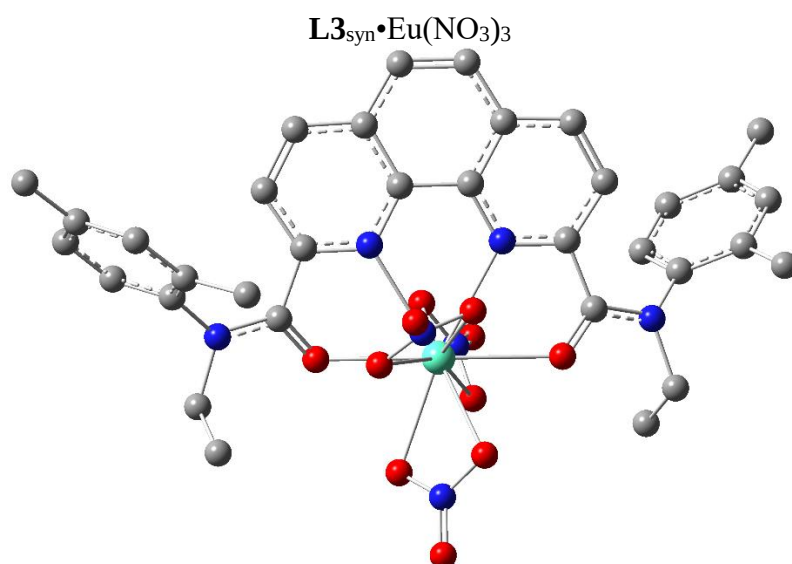
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O	-1.39038533	1.24776155	1.98443993
O	-3.47949099	0.86315045	2.56895107
O	2.94681593	-1.21748831	1.85686500
O	2.10952148	-0.99400582	-0.16128402
O	4.29137457	-1.12922249	0.11309986
O	0.45831662	-2.33774343	3.54456938
O	0.77320083	-0.27002327	4.21428887
O	0.75191700	-1.91058582	5.68681536
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C	-1.85234259	-1.79765106	-0.84219728
C	-2.66111941	-1.94313510	-1.99032006
H	-3.21110544	-2.86555998	-2.16913206
C	-2.74342301	-0.89528008	-2.88712039
H	-3.36865881	-0.98042759	-3.78012770
C	-2.00660125	0.28550916	-2.66542413
C	-2.04403566	1.40650381	-3.55431550
H	-2.70534781	1.36083128	-4.42394637
C	-1.26751819	2.50666472	-3.32840019
H	-1.29958052	3.35978695	-4.01173857
C	-0.37504836	2.55945737	-2.21103866
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H	0.45322899	4.52104211	-2.62735115
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C	2.23760064	2.29545572	1.16308830
C	4.17818166	2.76925190	2.55107985
H	4.78393222	3.68045409	2.67228491
H	3.41977101	2.73916575	3.34692844
C	5.05686459	1.52101108	2.59673829
H	4.45549845	0.60307872	2.50631777
H	5.57846039	1.49079007	3.56704887
H	5.81629076	1.53450161	1.80035779
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H	5.59818200	6.13332348	-1.25115822
C	4.56727848	4.71750686	-0.00529333
C	4.14534157	5.76124855	0.99846243
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H	-1.94317372	-3.62054098	3.17274955
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H	-3.53353996	-4.42601343	2.93657660
C	-3.75279913	-4.05556175	-0.16100743
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C	-6.07125455	-3.50116418	-0.44506374
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C	-6.26360236	-4.55688056	-1.33822369
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H	-5.27408129	-6.21115323	-2.33469404
C	-3.92756591	-5.12881843	-1.05056655
H	4.07179747	6.75103472	0.52350659
H	3.17527161	5.51469997	1.45738960
H	4.33262915	1.36471649	-0.69653035
C	6.56918609	4.58435928	-3.27368269
H	7.64254944	4.45782720	-3.04992608
H	6.34682840	3.98060349	-4.16681568
H	6.40550384	5.64464784	-3.51975506
C	-7.61673713	-4.83231251	-1.94404536
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H	-3.06683994	-5.75955183	-1.29090854
C	-4.73623880	-2.04775213	1.10630352
H	-5.59938522	-2.02999077	1.79027383
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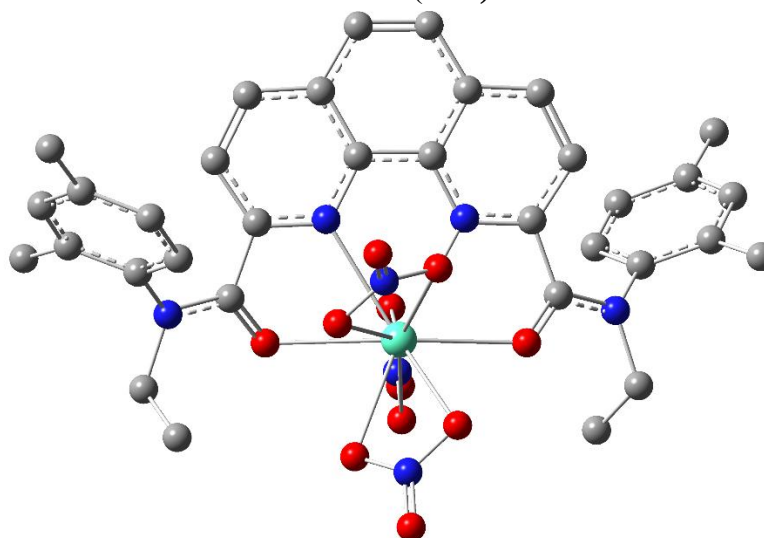
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O	-2.18996951	-0.95713612	2.07777969
O	-1.63450023	1.13935950	1.74529909
O	-3.75670664	0.58650691	1.95552007
O	2.83821059	-1.10344715	2.10656036
O	2.28430680	-0.73362428	0.01391066
O	4.40578618	-0.94850594	0.56556467
O	0.25808263	-2.25366182	3.52515696
O	0.33215768	-0.15650673	4.17331138
O	0.23068683	-1.76740200	5.67495204
N	-1.00285592	-0.75546172	-0.75992444
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N	-2.23061284	-3.97540928	0.27761504
N	3.17083289	3.12670753	1.41130386
N	-2.57656639	0.27669402	1.93253913
N	3.22519818	-0.94039409	0.88777993
N	0.27200223	-1.41004679	4.51420939
C	-1.67087363	-1.88846583	-0.98219304
C	-2.43947526	-2.08458378	-2.14988967
H	-2.96315213	-3.02549954	-2.31488084
C	-2.52256516	-1.06254478	-3.07575912
H	-3.11123572	-1.18904820	-3.98836071
C	-1.83848479	0.15128546	-2.85225499
C	-1.87348095	1.25478172	-3.76344253
H	-2.48325943	1.16633065	-4.66680506
C	-1.15817614	2.39306679	-3.51824348
H	-1.18975570	3.23020445	-4.22106853
C	-0.33933715	2.51130549	-2.35021331
C	0.44750517	3.64768233	-2.06472228
H	0.42044228	4.50646984	-2.74077907
C	1.25594267	3.66283214	-0.94476934
H	1.88551293	4.52505020	-0.72777796
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C	-0.28858321	1.44191910	-1.41275714

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C	3.79811097	3.04387710	2.75904875
H	4.35550436	3.98258440	2.89916453
H	2.97558918	3.00795894	3.48836035
C	4.71807087	1.83617783	2.92485529
H	4.16092002	0.89127202	2.83327435
H	5.16630979	1.86725876	3.93105559
H	5.53336529	1.84686826	2.18585079
C	4.00053164	3.58368133	0.32907016
C	4.51765182	2.64346707	-0.57058951
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H	5.72874809	2.30978358	-2.31712030
C	5.66677549	4.40697246	-1.78169460
C	5.14243152	5.32975773	-0.86596662
H	5.37846328	6.39259417	-0.98961620
C	4.31424937	4.95239290	0.19773746
C	3.76269055	5.99286517	1.14021545
H	4.41478712	6.12320457	2.02137978
C	-1.36960974	-2.94559883	0.06832489
C	-1.82245675	-5.01409923	1.26249252
H	-2.32917765	-5.94315757	0.96031487
H	-0.73667270	-5.14996649	1.14959788
C	-2.16931057	-4.64603906	2.70355832
H	-1.59716483	-3.76719162	3.03672856
H	-1.90326743	-5.49122253	3.35839515
H	-3.24623649	-4.44807514	2.81736644
C	-3.62645306	-3.91415122	-0.06679760
C	-4.41119515	-2.89440362	0.48321798
C	-5.76846098	-2.81680767	0.17615140
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H	-6.01159018	-5.50870214	-1.88145340
C	-4.19438133	-4.88181304	-0.92253855
C	-3.37164424	-5.98060455	-1.54825838
H	-3.32032735	-6.86849140	-0.89423660
H	3.69131290	6.97078844	0.64107236
H	2.76614282	5.71297815	1.51581334
H	-3.81610780	-6.30412016	-2.50142921
H	-2.33568028	-5.65598840	-1.73290114
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C	6.58183435	4.85800908	-2.89221801
H	7.62449418	4.92134324	-2.53587509
H	6.56338817	4.15278706	-3.73666456
H	6.30096976	5.85545576	-3.26441743
C	-7.84113511	-3.70313332	-0.98388152
H	-8.02979269	-3.88330044	-2.05423495
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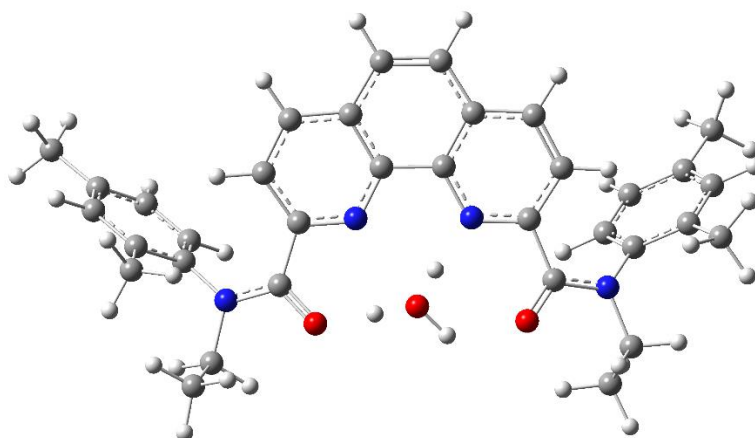
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O	-1.93780840	-0.78443178	2.37668059
O	-1.32422123	1.24714858	1.84637164
O	-3.37116961	0.87874225	2.57504948
O	2.83482883	-1.12760409	1.51404329
O	1.78503896	-1.24669379	-0.39747044
O	3.98411696	-1.35042302	-0.35068837
O	0.71953136	-2.15630574	3.41689163
O	0.43617277	-0.08145764	4.02356794
O	0.69831756	-1.63926091	5.55505531
N	-1.10518853	-0.73538684	-0.61782795
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N	-2.25760426	0.47242325	2.28336692
N	2.91070159	-1.25432503	0.23211352
N	0.62176945	-1.30520389	4.38530205
C	-1.82585445	-1.84275382	-0.81467285
C	-2.60846637	-2.02385963	-1.97639710
H	-3.15517593	-2.95157153	-2.13799981
C	-2.67381328	-1.00339136	-2.90630367
H	-3.28370932	-1.11509033	-3.80694217
C	-1.93903326	0.18307062	-2.70669226
C	-1.95891019	1.28432202	-3.62100939
H	-2.60462090	1.22032654	-4.50120344
C	-1.18880484	2.39148772	-3.40382278
H	-1.21309273	3.23125129	-4.10380467
C	-0.31323531	2.46877760	-2.27404465
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C	-1.12928421	0.24787330	-1.53778632

C	2.25452108	2.23591227	1.13650387
C	4.16956540	2.69285691	2.56037632
H	4.76002245	3.60580507	2.73264497
H	3.40444816	2.61126497	3.34580619
C	5.06540037	1.45520403	2.54871490
H	4.47531197	0.54304453	2.36763644
H	5.55666682	1.35900102	3.53023368
H	5.84889604	1.53556876	1.77966051
C	4.20600913	3.39126796	0.16749615
C	4.64045389	2.49719913	-0.81925279
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C	5.74262111	4.30647257	-2.00486269
C	5.30357857	5.18263161	-1.00338788
H	5.55470796	6.24621018	-1.08210911
C	4.54114136	4.75875338	0.09234586
C	4.07762130	5.75096474	1.12909463
H	4.78141450	5.80328556	1.97794357
C	-1.57720839	-2.87610707	0.27120514
C	-2.05739629	-4.88003560	1.54916411
H	-2.49596286	-5.84465558	1.25045855
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C	-2.53089499	-4.47086935	2.94235253
H	-2.08503666	-3.50827375	3.23492225
H	-2.20885228	-5.23222957	3.67046095
H	-3.62806308	-4.39068226	2.98685124
C	-3.74706976	-4.06497712	-0.08907552
C	-4.82416709	-3.20357324	0.19528646
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H	-5.27753081	-6.28926111	-2.18667799
C	-3.92851244	-5.17118131	-0.93594913
H	4.01113471	6.76111808	0.69837029
H	3.09504262	5.47510631	1.54207088
H	4.39017050	1.43478027	-0.73459443
C	6.58887372	4.80239396	-3.15028224
H	7.66210043	4.70747160	-2.91090125
H	6.40368230	4.21988567	-4.06557906
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C	-4.71631105	-1.99263974	1.08310286
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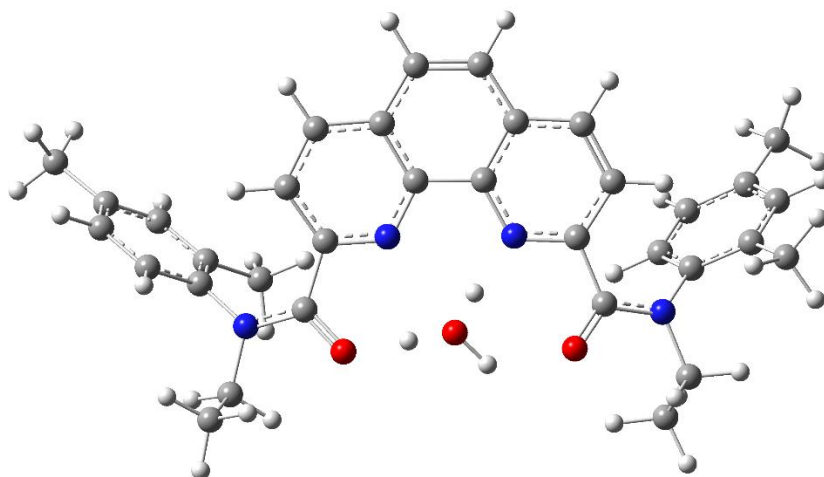
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O	-2.20145474	-0.88181760	2.01788660
O	-1.64470666	1.17895309	1.54484625
O	-3.76365841	0.66053748	1.84107783
O	2.49436468	-1.41017953	2.01206212
O	2.11492903	-0.83190078	-0.06190589
O	4.09423308	-1.60545006	0.51263094
O	0.10307239	-1.92964931	3.55267545
O	-0.08363930	0.20652724	3.95135856
O	-0.26315174	-1.23292421	5.60678580
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C	-1.65624740	-1.88166491	-0.94028360
C	-2.41218459	-2.09289726	-2.11441010
H	-2.93227899	-3.03697743	-2.27380463
C	-2.49374659	-1.08014691	-3.05191268
H	-3.07742367	-1.21885270	-3.96595835
C	-1.81488030	0.13871242	-2.83691512
C	-1.84234096	1.23924421	-3.75286883
H	-2.44807452	1.14938289	-4.65889979
C	-1.12569895	2.37817901	-3.50971098
H	-1.15380516	3.21168629	-4.21698131
C	-0.30721374	2.49947977	-2.34108361
C	0.49155117	3.62775771	-2.05554803
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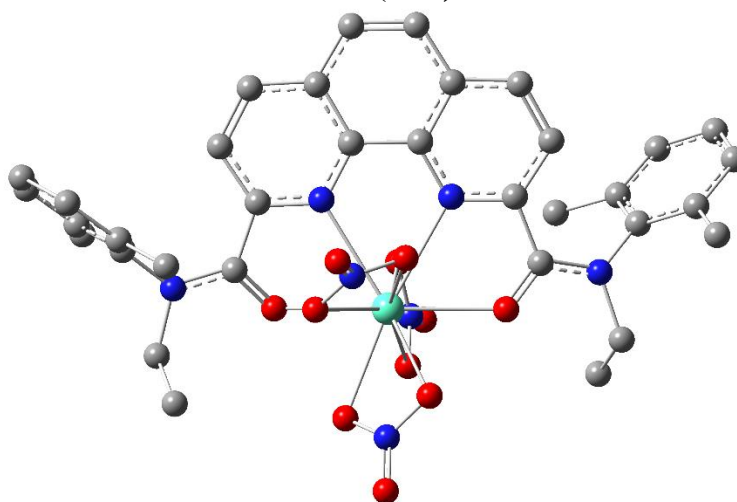
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H	-2.97198079	-6.25290020	-2.47793061
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