

4,7-Substituted 1,10-phenanthroline-2,9-dicarboxamides: photophysics of ligands and their complexes with the Eu-Gd-Tb triad

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Supplementary Materials

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1. X-ray analysis

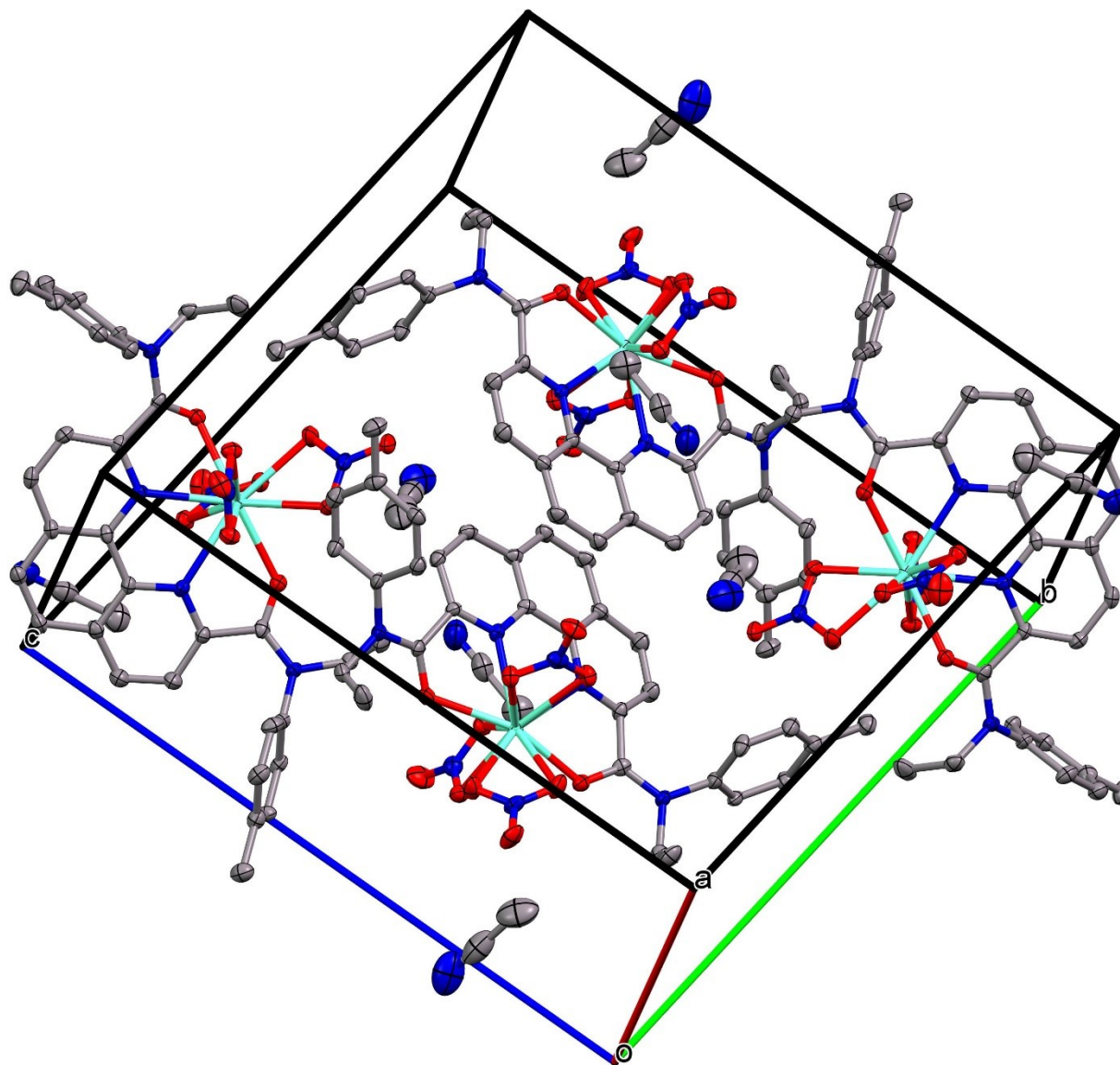


Figure S1. The crystal packing of LH•Eu(NO₃)₃. Hydrogen atoms are omitted for clarity and the non-hydrogen atoms are shown as thermal ellipsoids at 50% probability level.

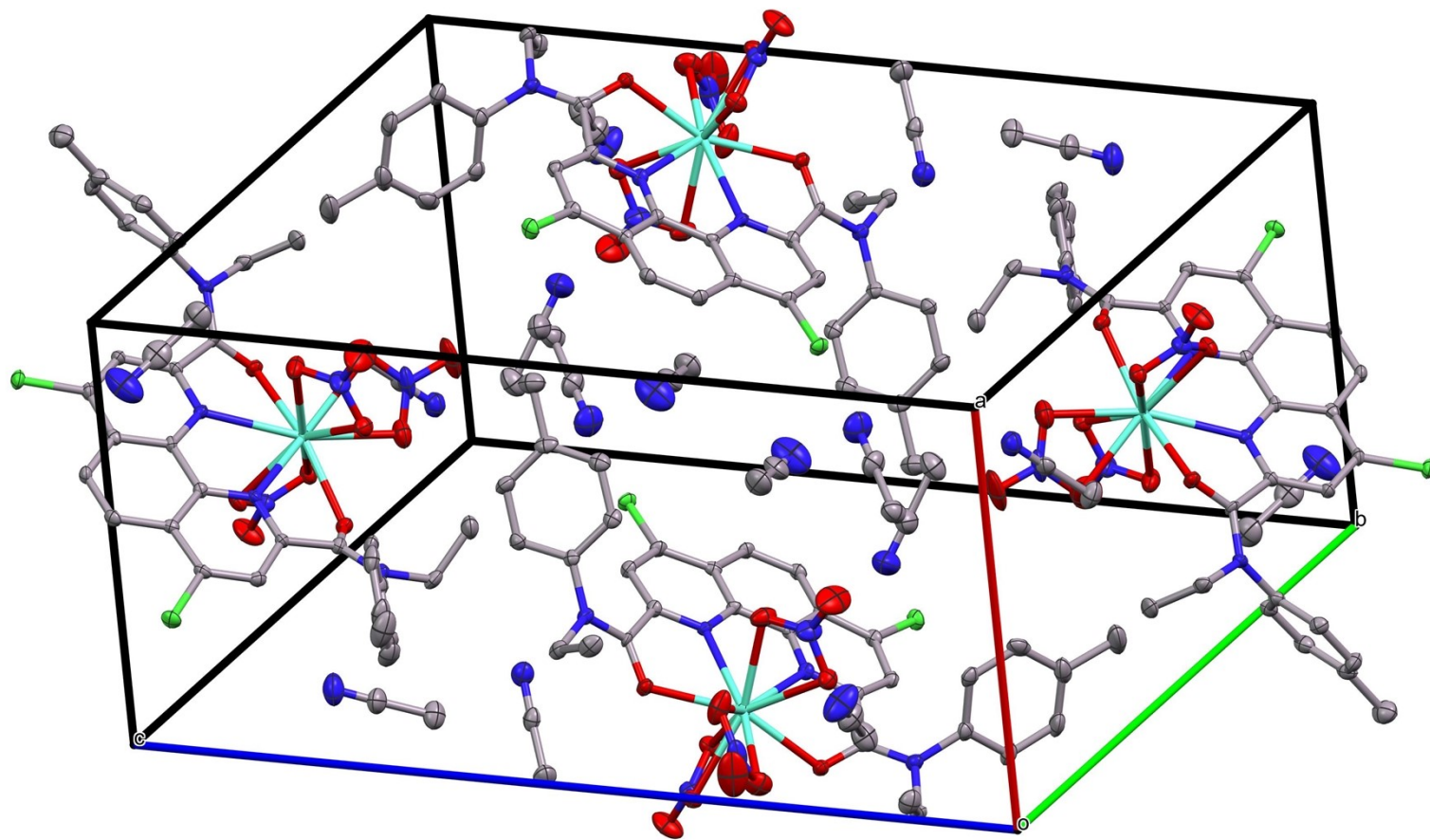


Figure S2. The crystal packing of $\text{LCl}\cdot\text{Eu}(\text{NO}_3)_3$. Hydrogen atoms are omitted for clarity and the non-hydrogen atoms are shown as thermal ellipsoids at 50% probability level.

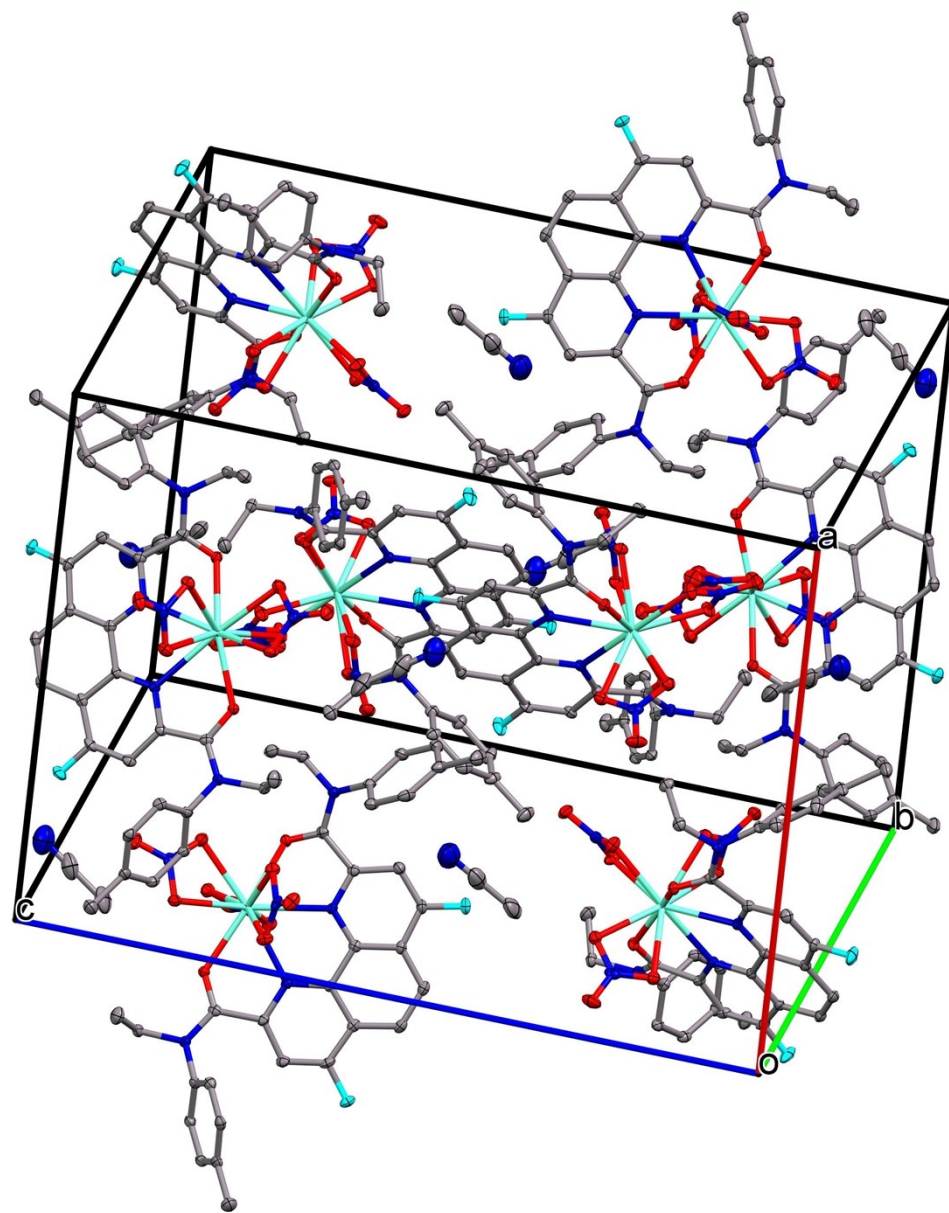


Figure S3. The crystal packing of LF•Eu(NO₃)₃. Hydrogen atoms are omitted for clarity and the non-hydrogen atoms are shown as thermal ellipsoids at 50% probability level.

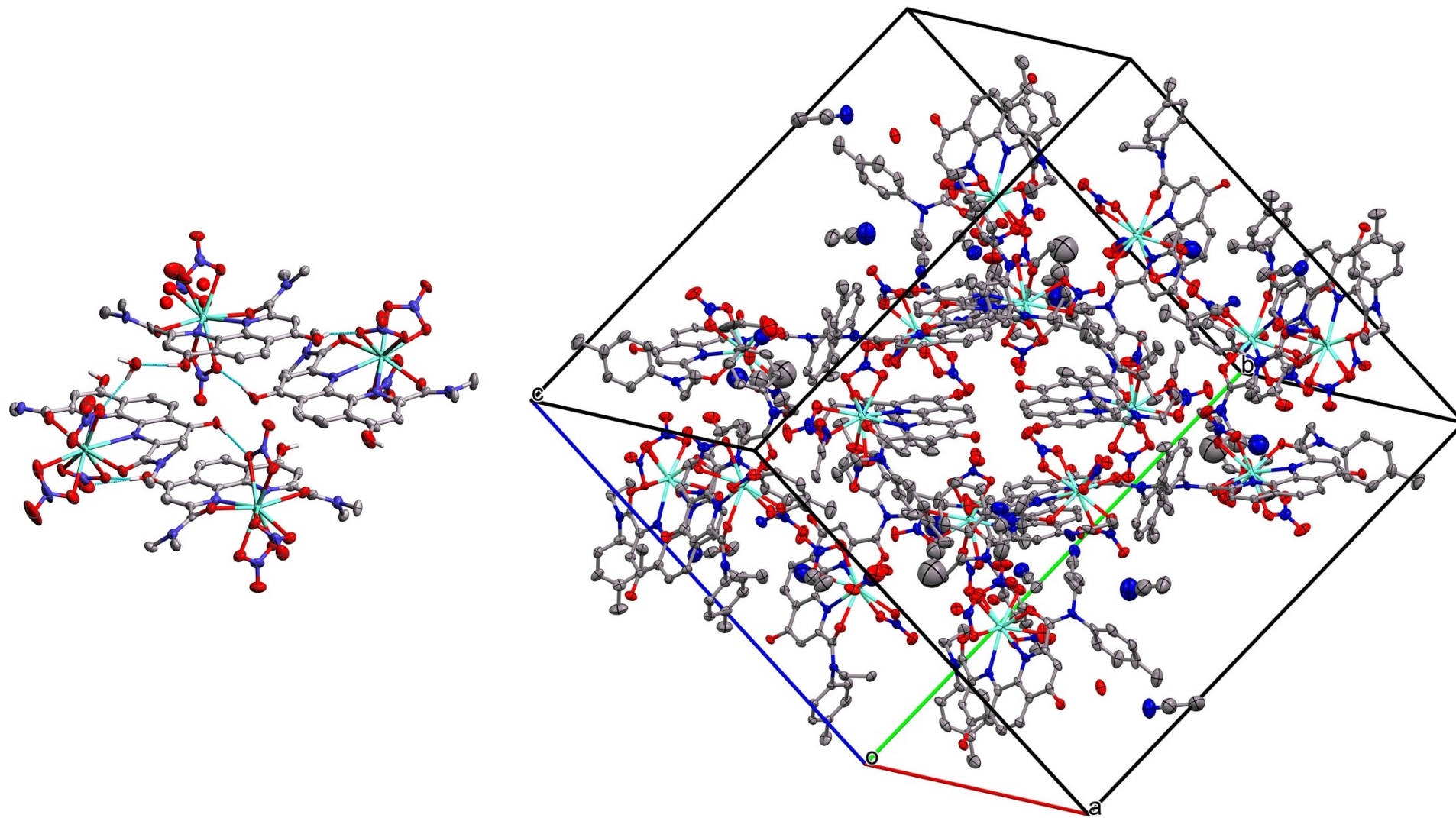


Figure S4. General view of a fragment of the $\text{LOH}\cdot\text{Eu}(\text{NO}_3)_3$ crystal and the crystal packing. Hydrogen atoms are omitted for clarity and the non-hydrogen atoms are shown as thermal ellipsoids at 50% probability level.

2. NMR and IR spectra of synthesized compounds

*N*²,*N*⁹-diethyl-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide europium trinitrate LH•Eu(NO₃)₃

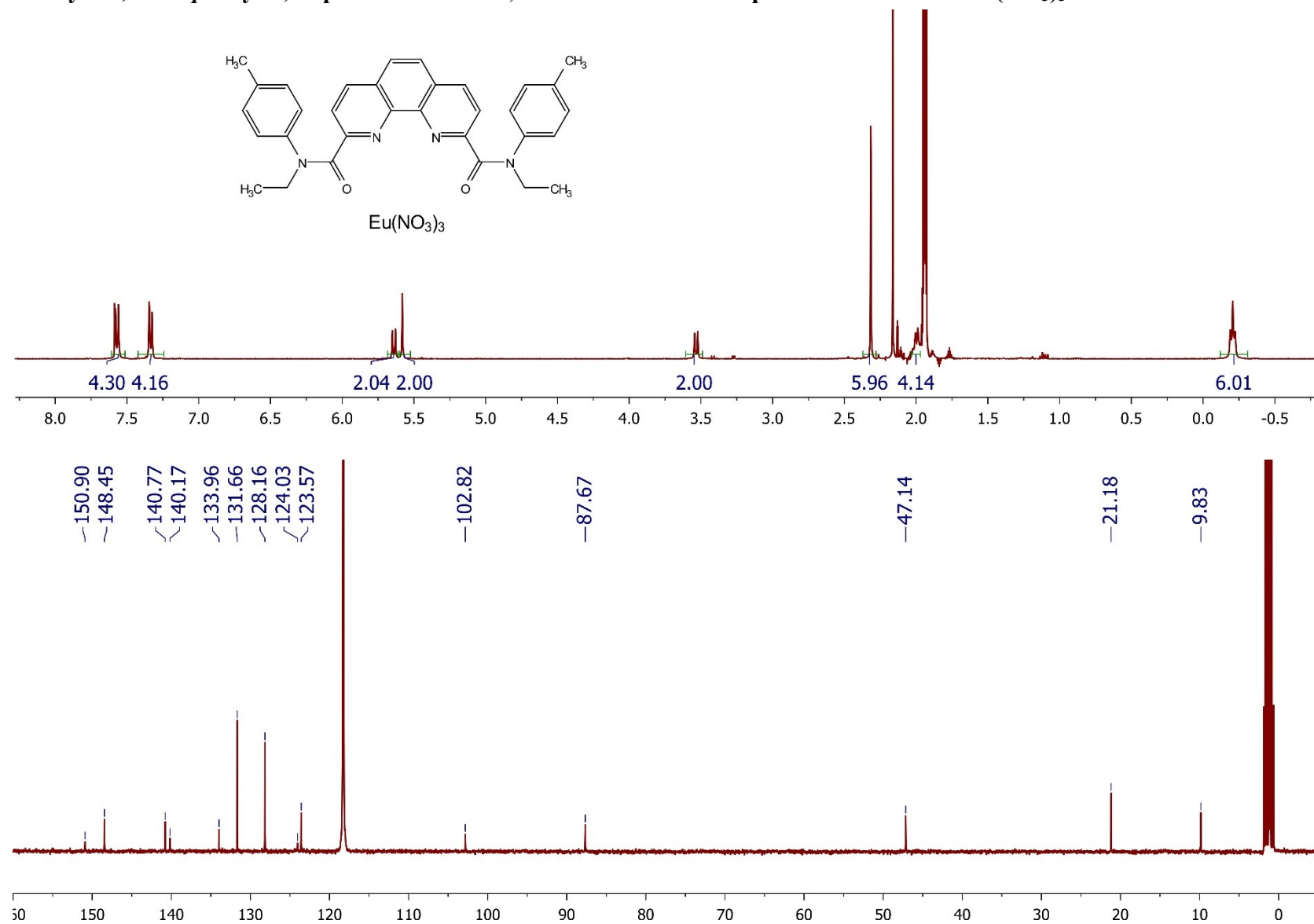


Figure S5. ^1H and ^{13}C NMR spectra in CD_3CN at 25°C

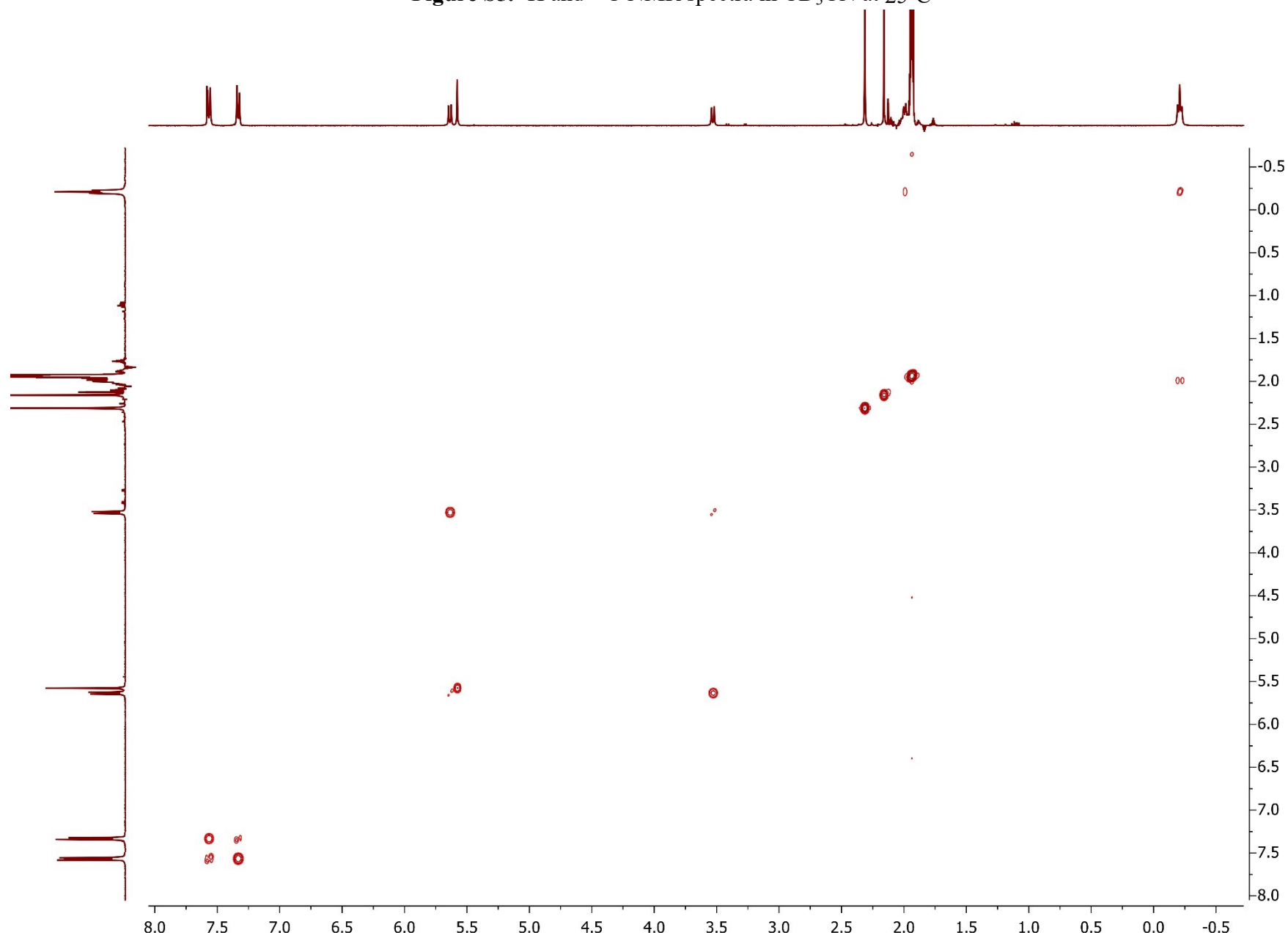


Figure S6. $^1\text{H}/^1\text{H}$ COSY NMR spectrum in CD_3CN at 25°C

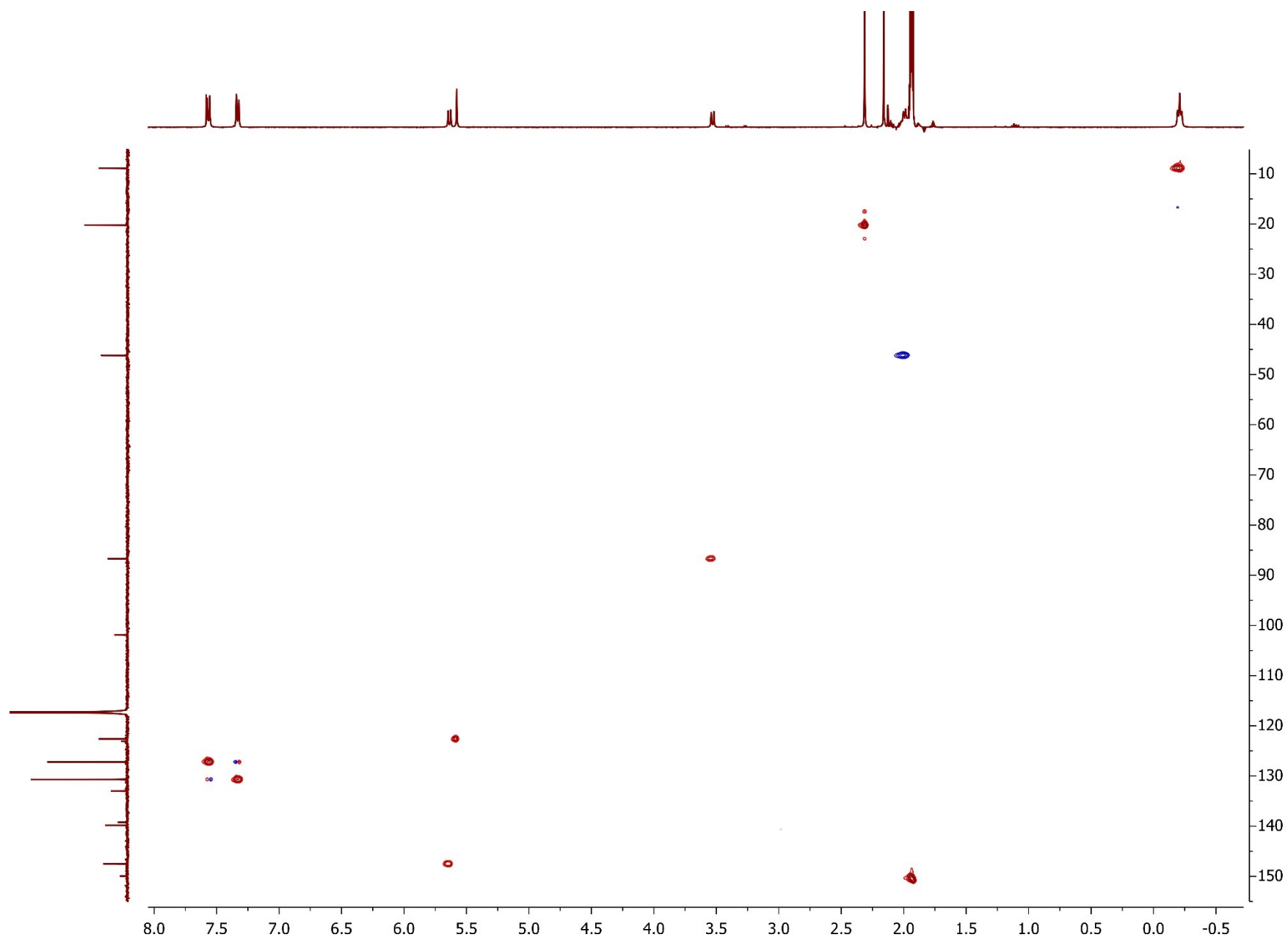


Figure S7. $^1\text{H}/^{13}\text{C}$ HSQC NMR spectrum in CD_3CN at 25°C

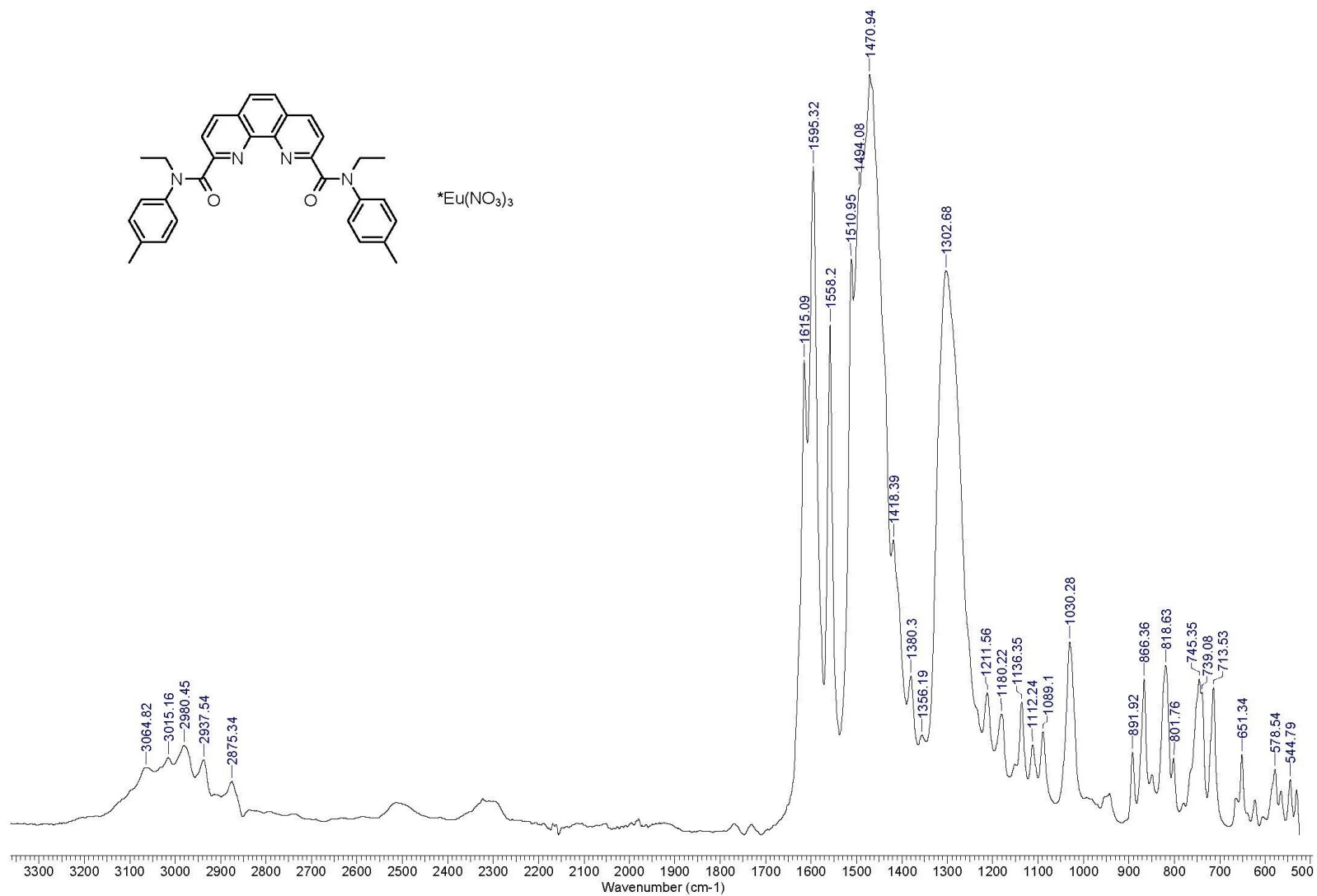


Figure S8. Solid-state IR spectrum at 25°C

*N*²,*N*⁹-diethyl-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide gadolinium trinitrate LH•Gd(NO₃)₃

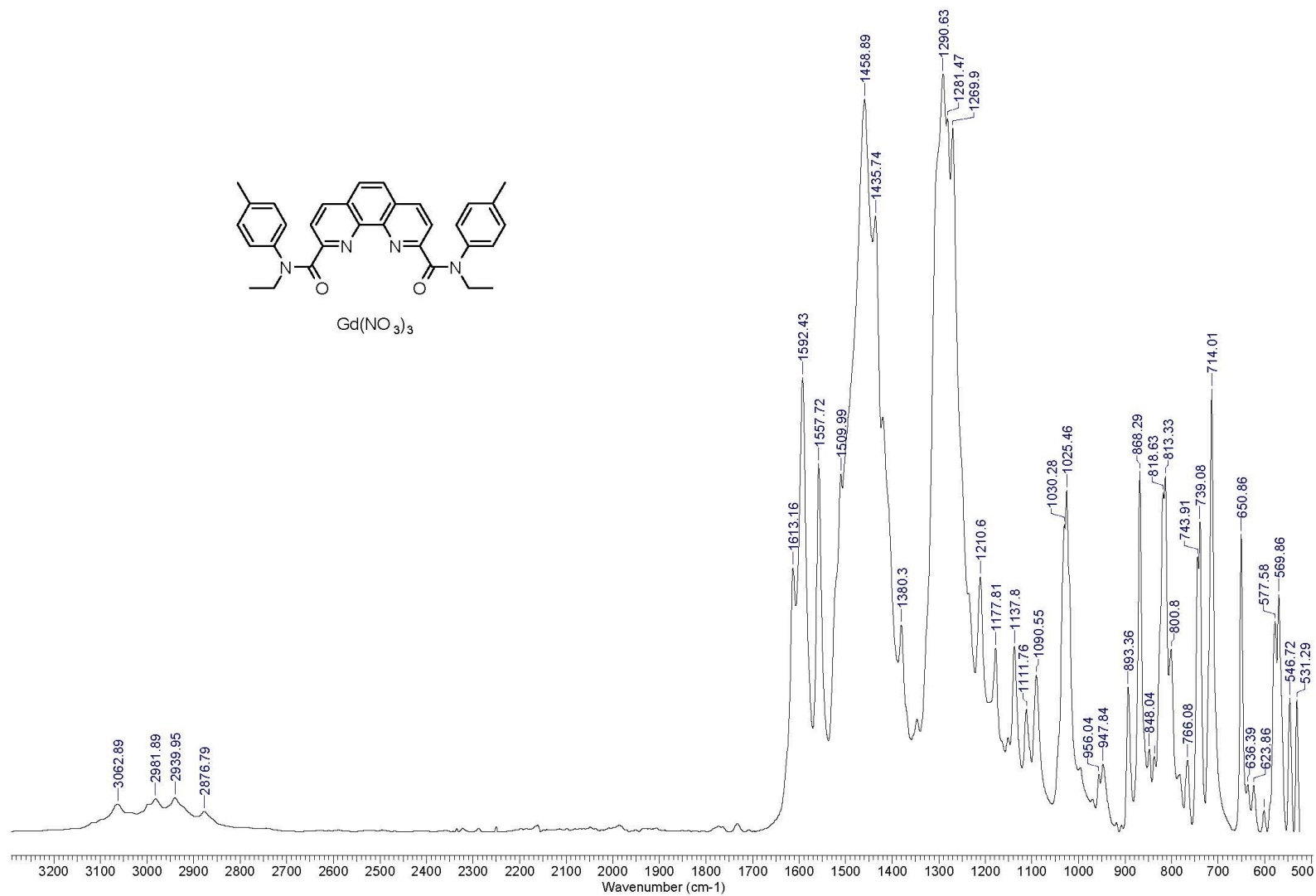


Figure S9. Solid-state IR spectrum at 25°C

*N*²,*N*⁹-diethyl-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide terbium trinitrate LH•Tb(NO₃)₃

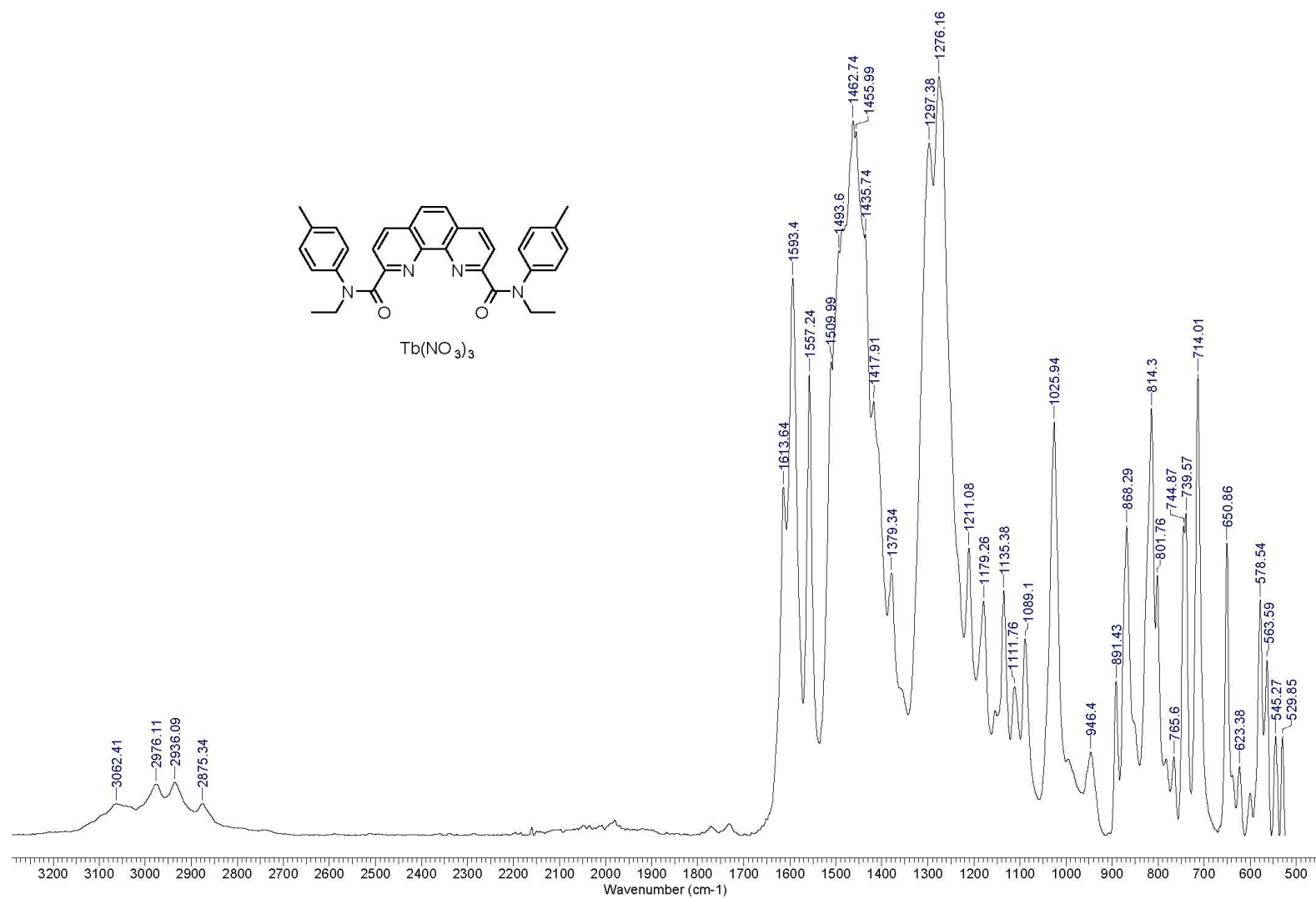


Figure S10. Solid-state IR spectrum at 25°C

4,7-dichloro-*N*²,*N*⁹-diethyl-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide europium trinitrate $\text{LCl} \cdot \text{Eu}(\text{NO}_3)_3$

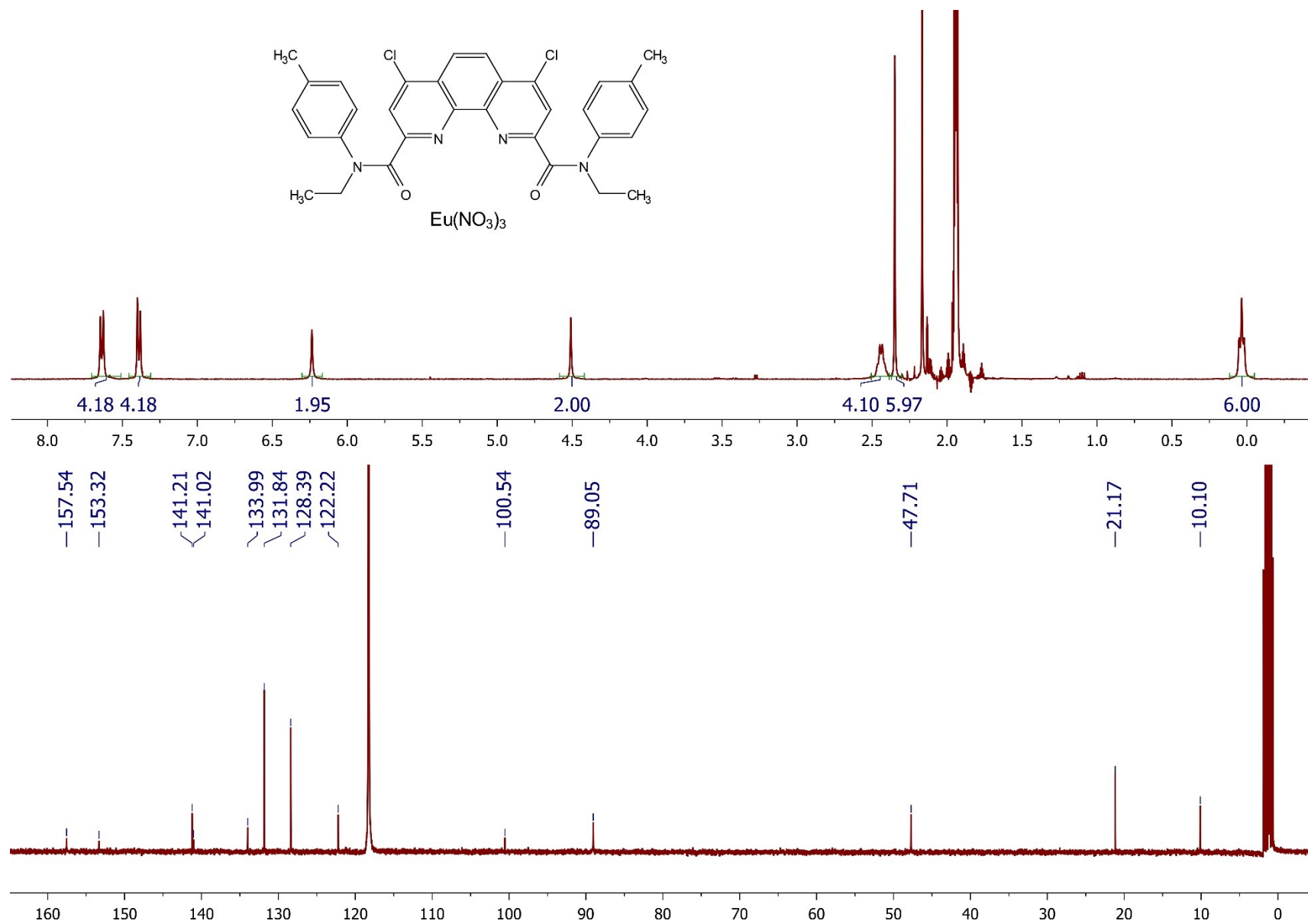


Figure S11. ¹H and ¹³C NMR spectra in CD₃CN at 25°C

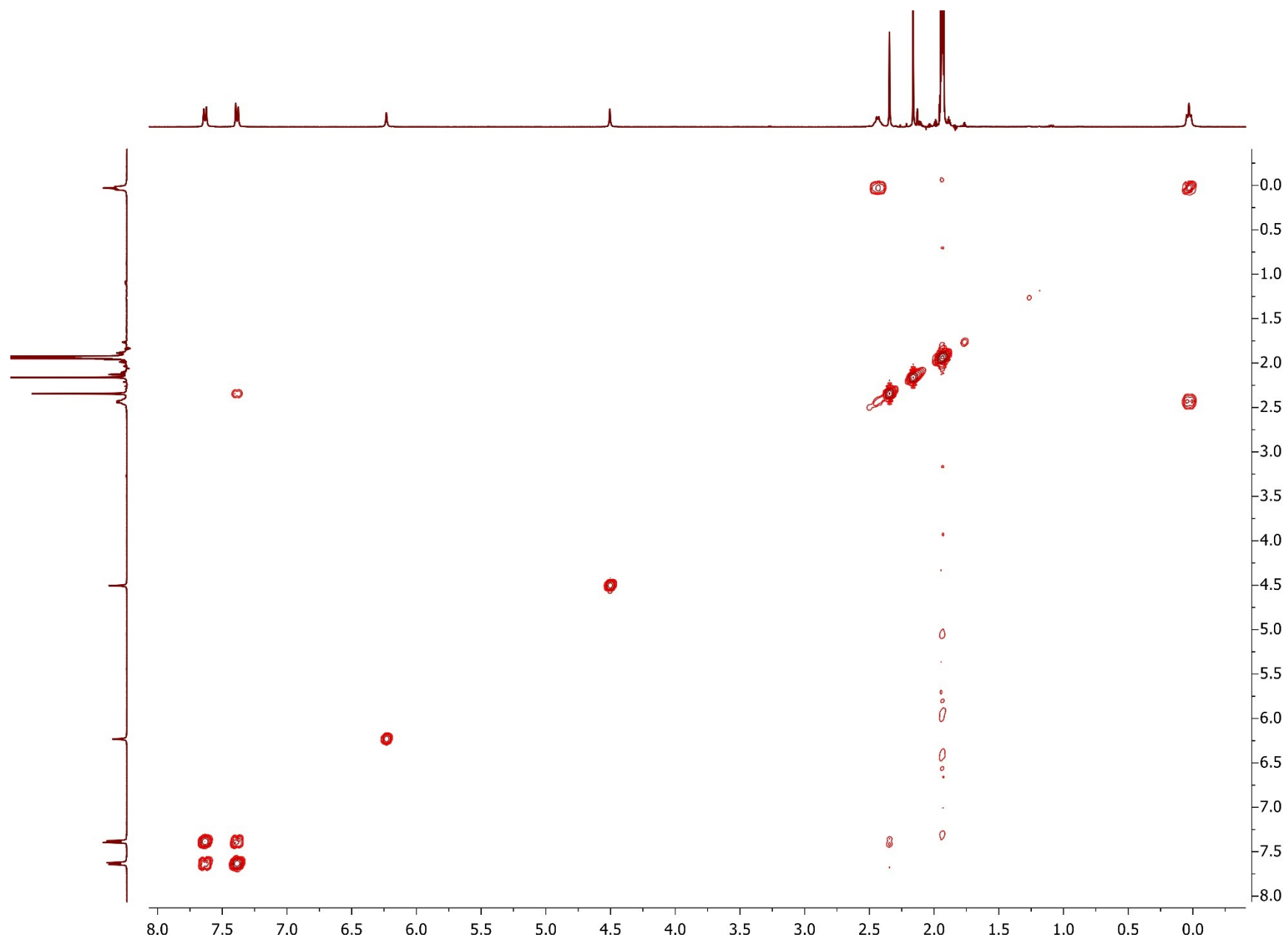


Figure S12. $^1\text{H}/^1\text{H}$ COSY NMR spectra in CD_3CN at 25°C

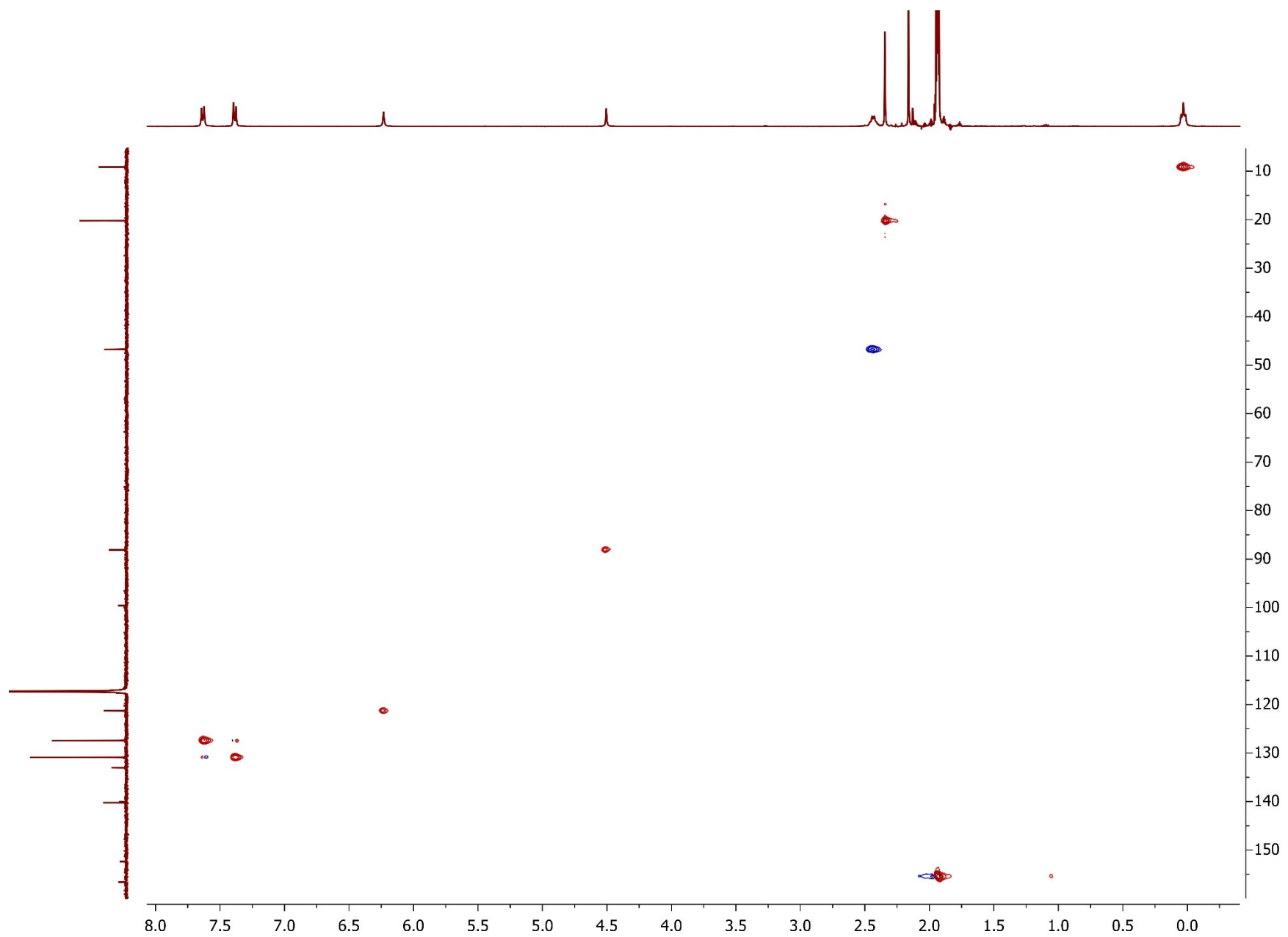


Figure S13. $^1\text{H}/^{13}\text{C}$ HSQC NMR spectra in CD_3CN at 25°C

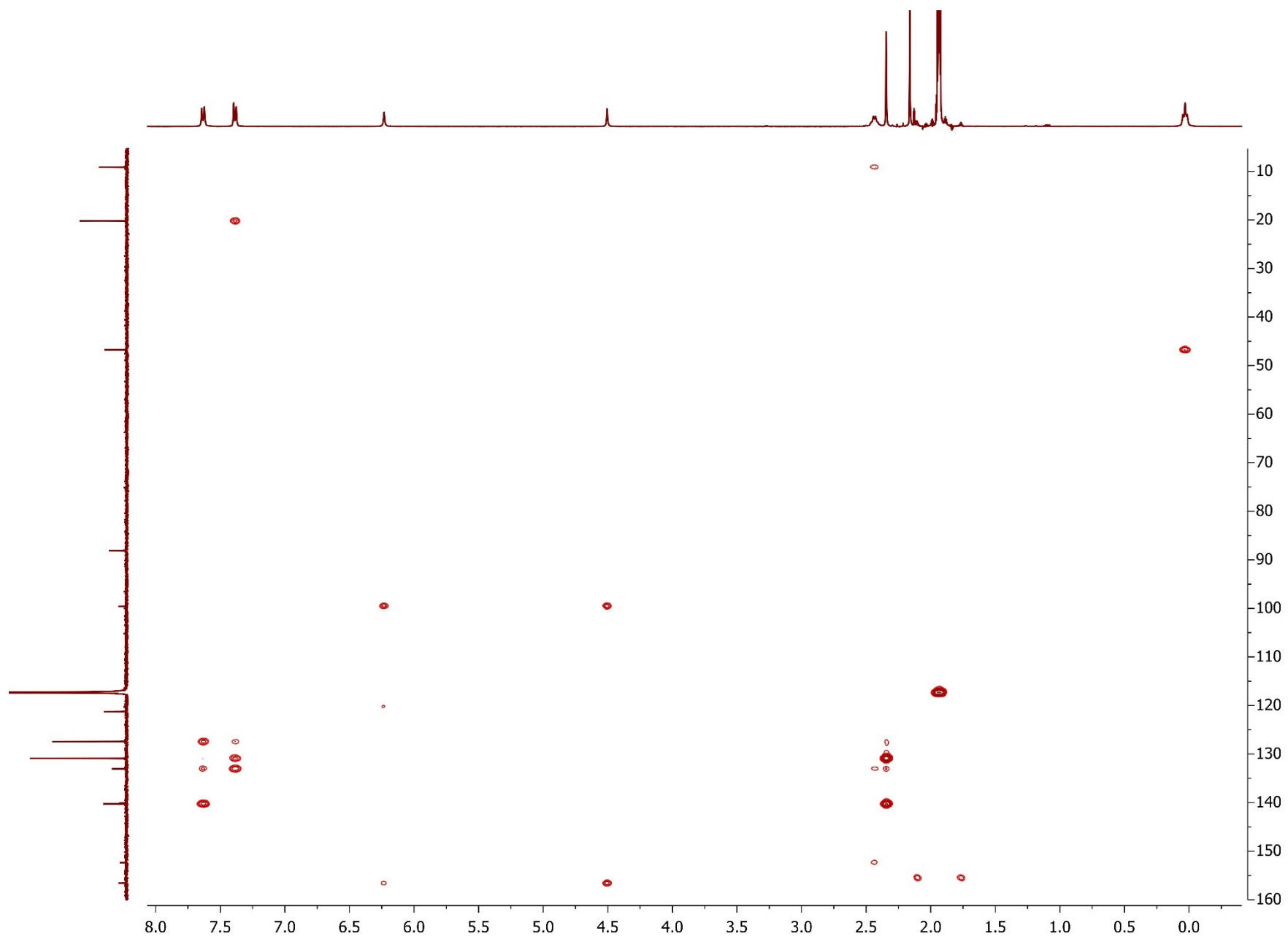


Figure S14. $^1\text{H}/^{13}\text{C}$ HMBC NMR spectra in CD_3CN at 25°C

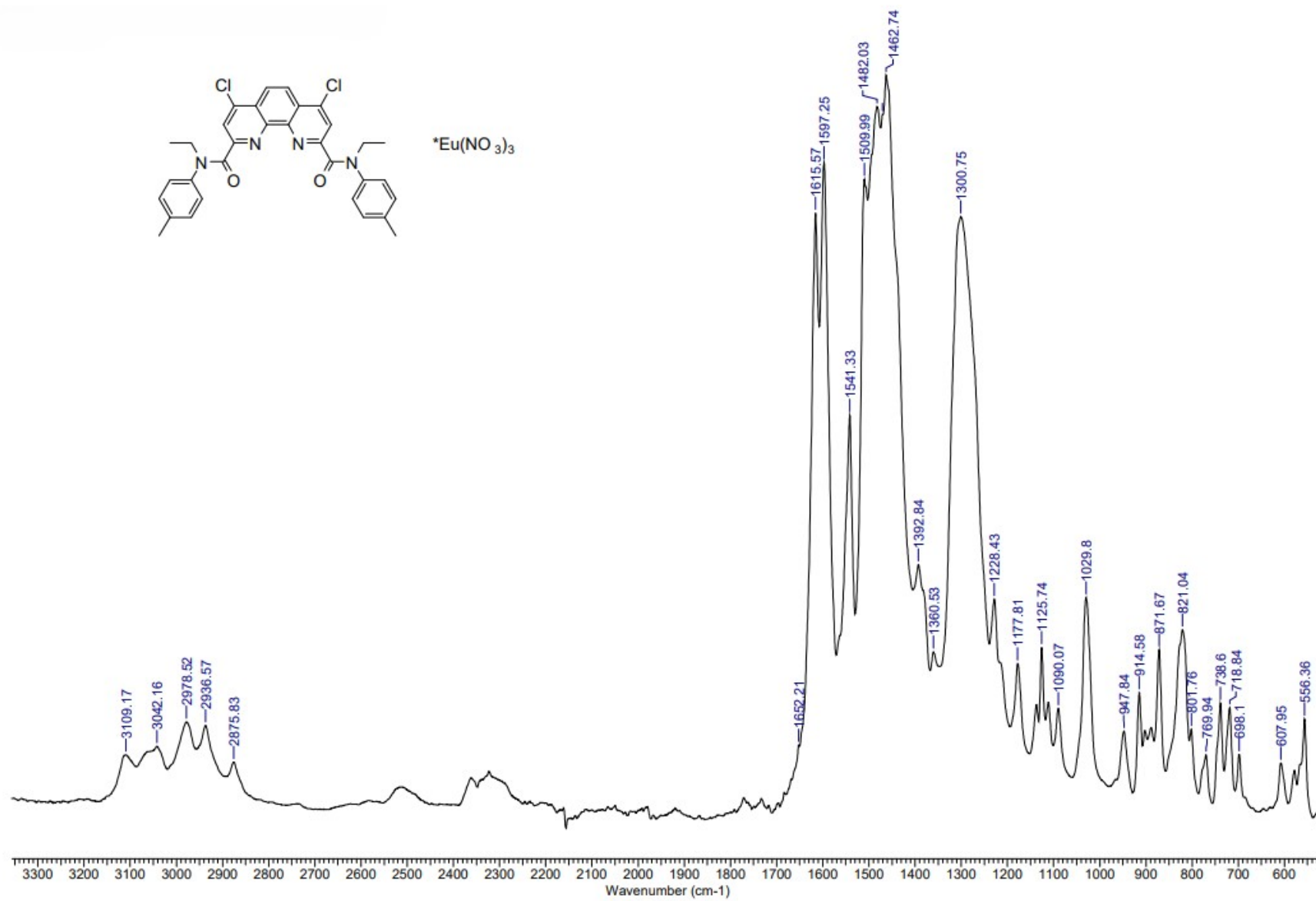


Figure S15. Solid-state IR spectrum at 25°C

4,7-dichloro-*N*²,*N*⁹-diethyl-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide gadolinium trinitrate $\text{LiCl} \cdot \text{Gd}(\text{NO}_3)_3$

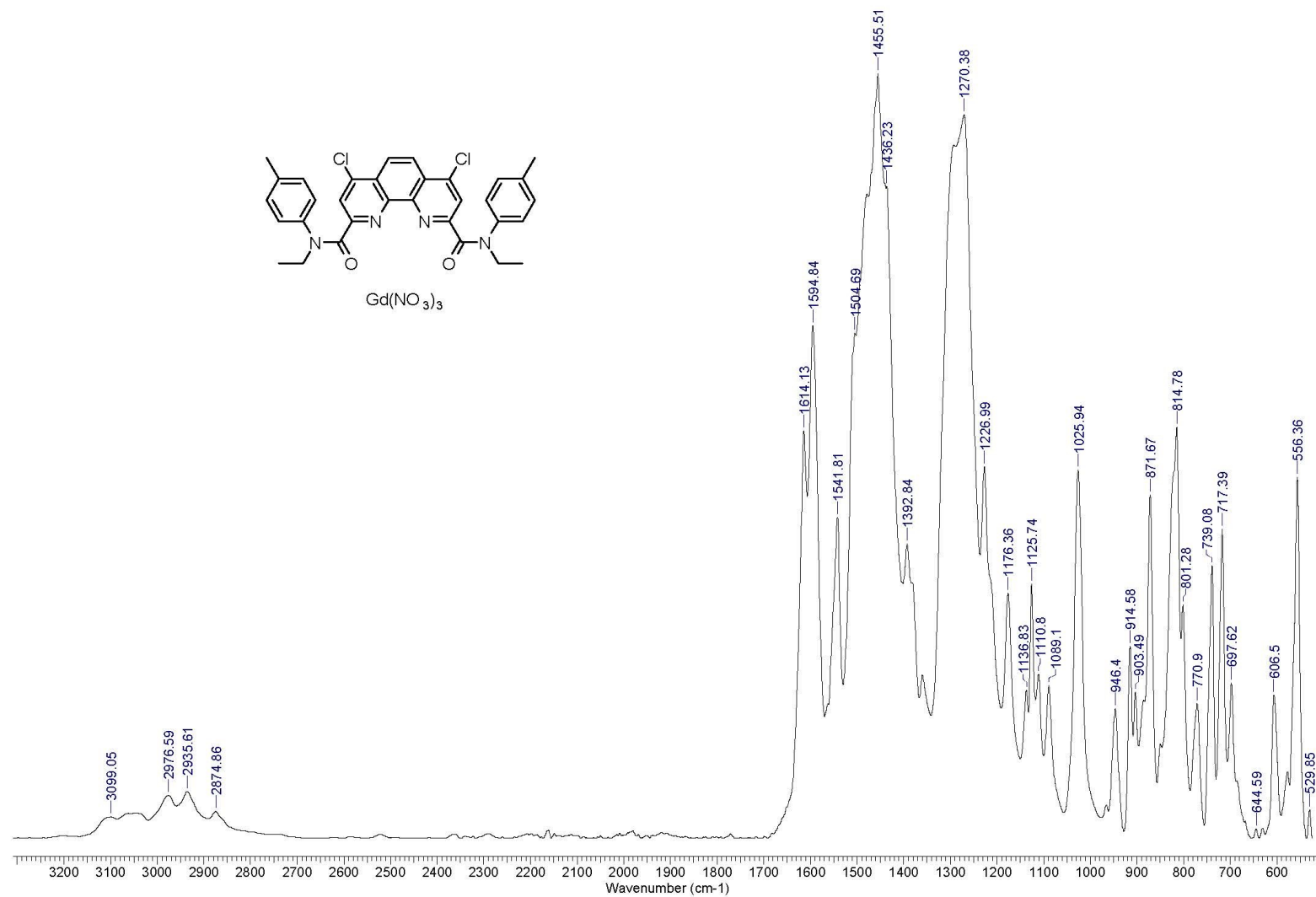


Figure S16. Solid-state IR spectrum at 25°C

4,7-dichloro- N^2,N^9 -diethyl- N^2,N^9 -di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide terbium trinitrate $\text{LCI}\cdot\text{Tb}(\text{NO}_3)_3$

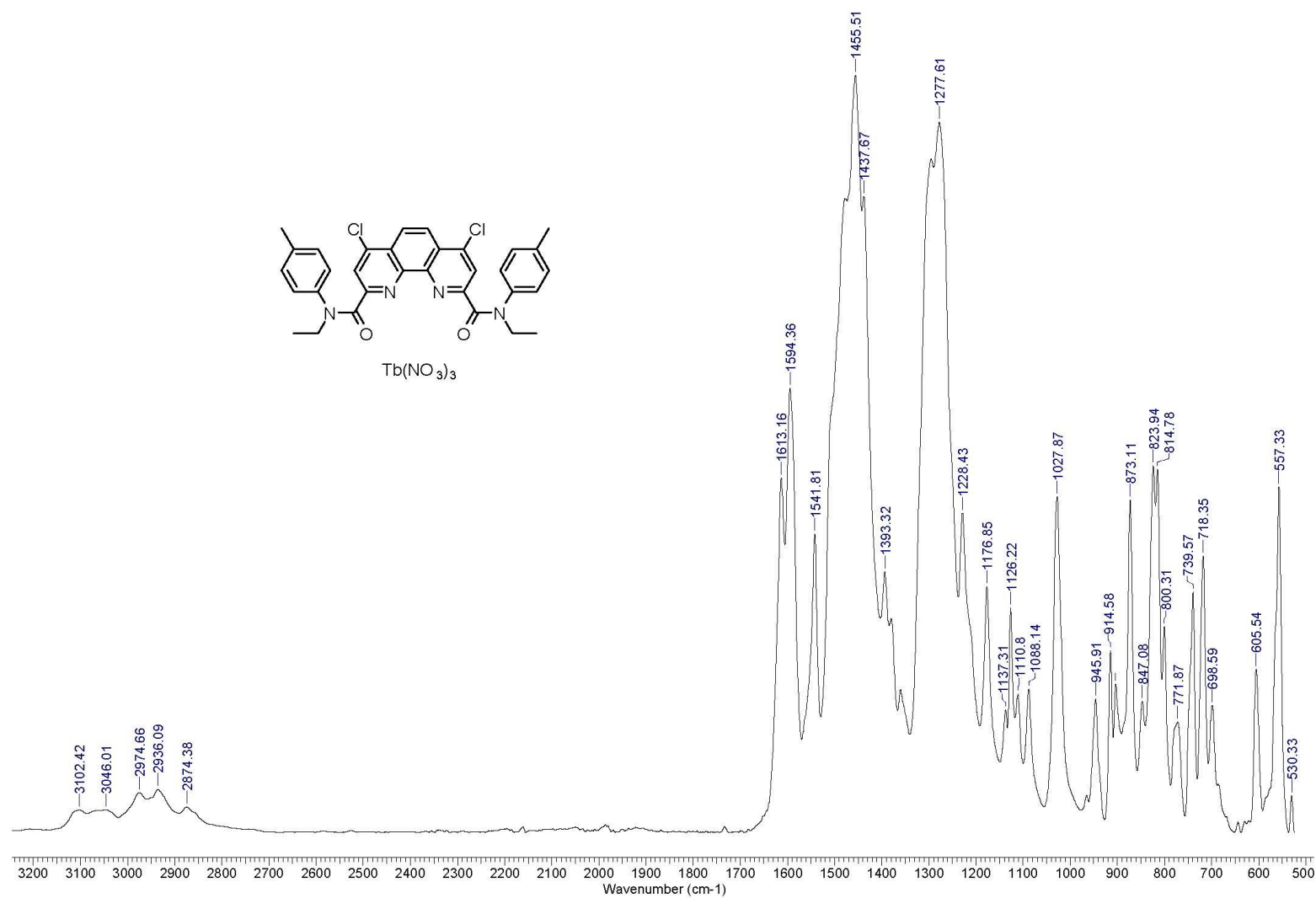


Figure S17. Solid-state IR spectrum at 25°C

*N*²,*N*⁹-diethyl-4,7-difluoro-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide europium trinitrate LF•Eu(NO₃)₃

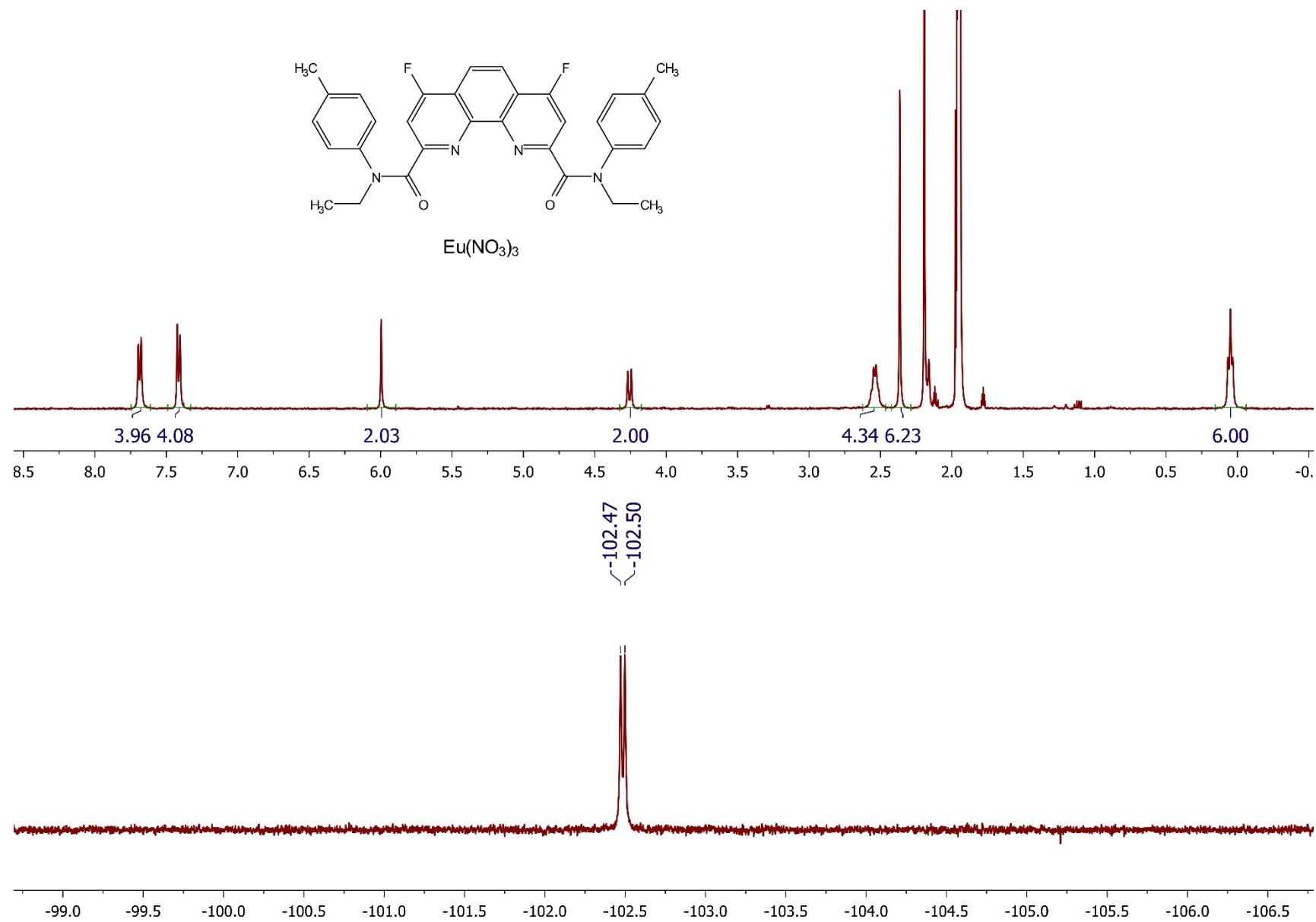


Figure S18. ¹H and ¹⁹F NMR spectra in CD₃CN at 25°C

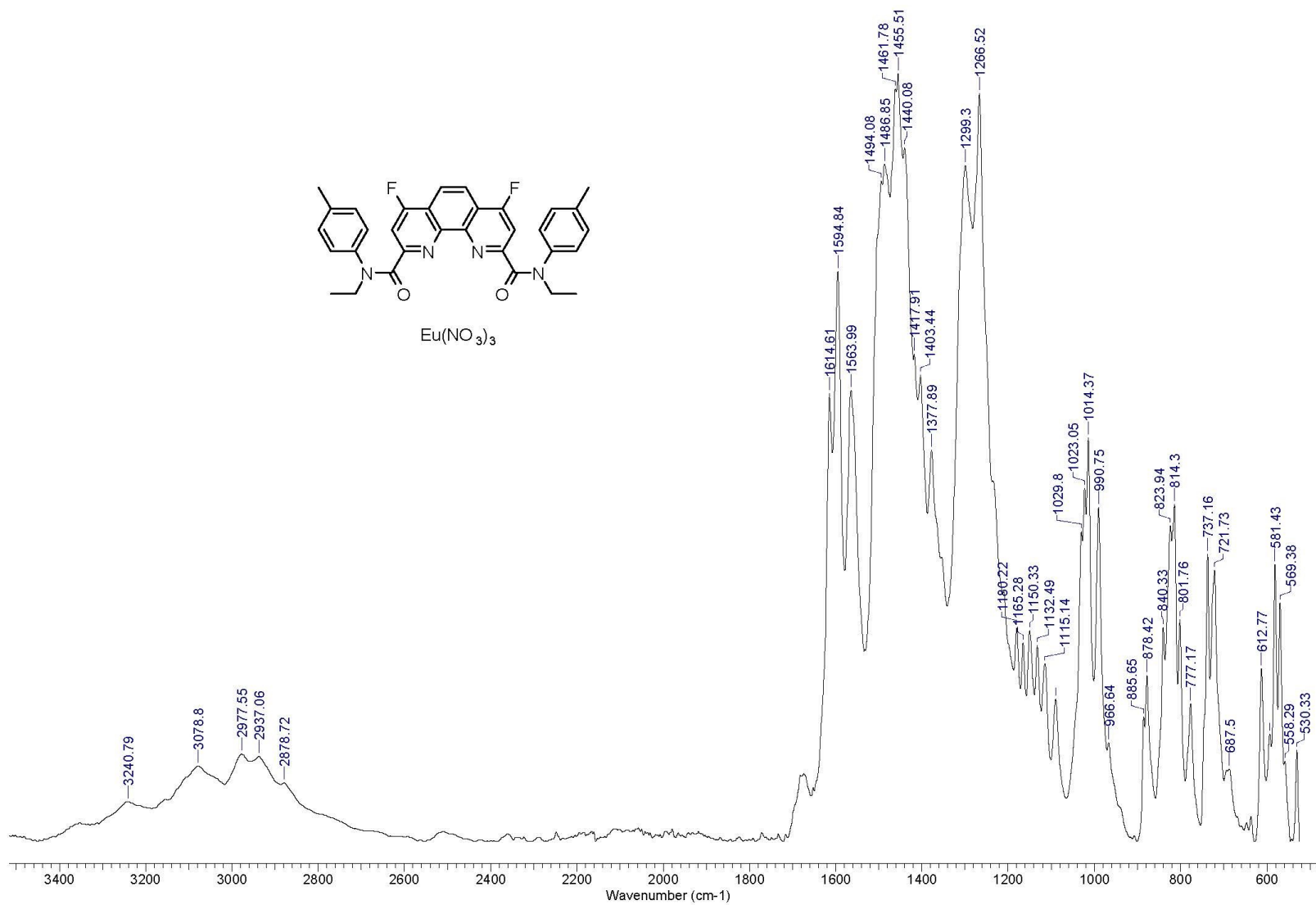


Figure S19. Solid-state IR spectrum at 25°C

*N*²,*N*⁹-diethyl-4,7-difluoro-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide gadolinium trinitrate LF•Gd(NO₃)₃

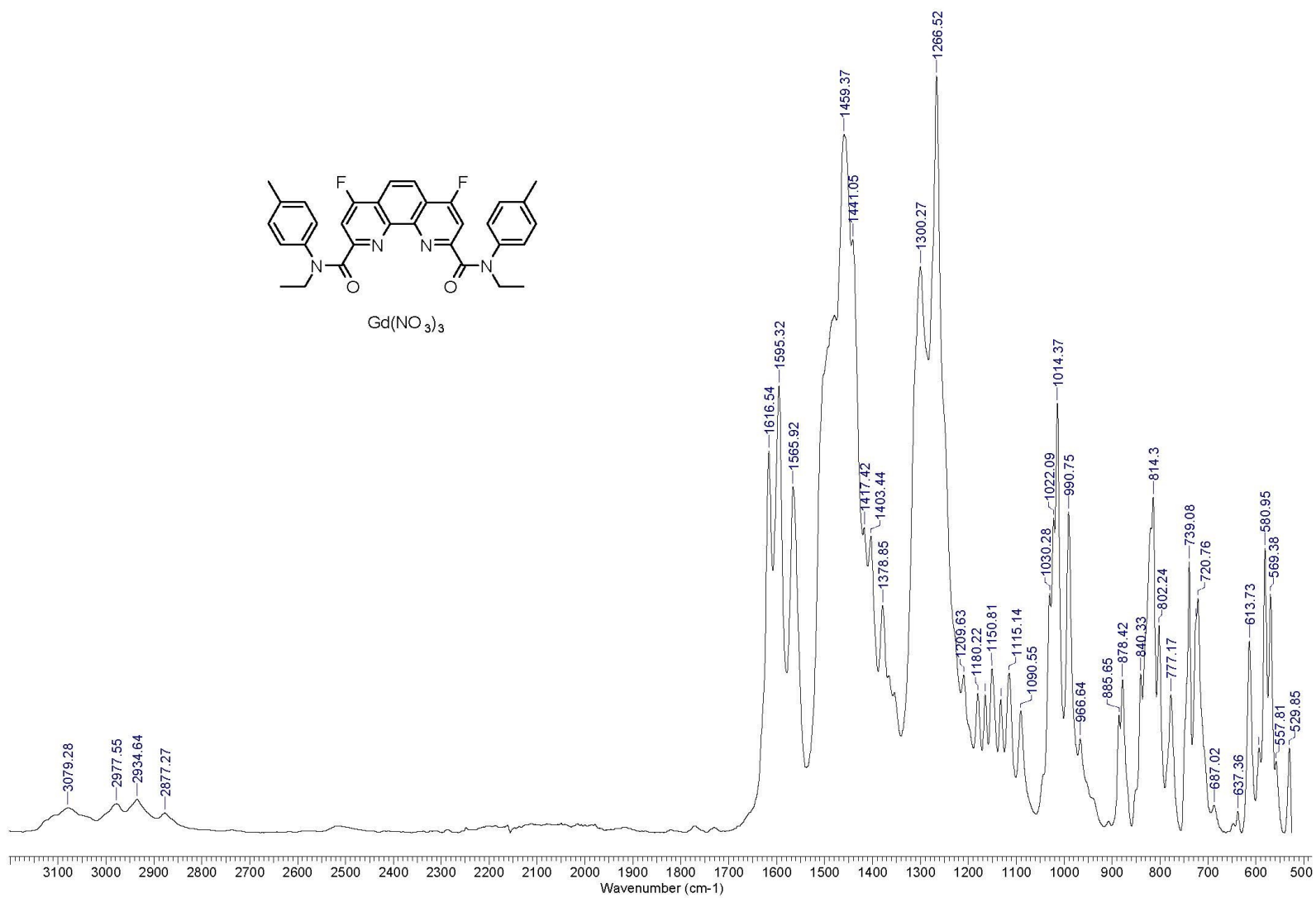


Figure S20. Solid-state IR spectrum at 25°C

*N*²,*N*⁹-diethyl-4,7-difluoro-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide terbium trinitrate LF•Tb(NO₃)₃

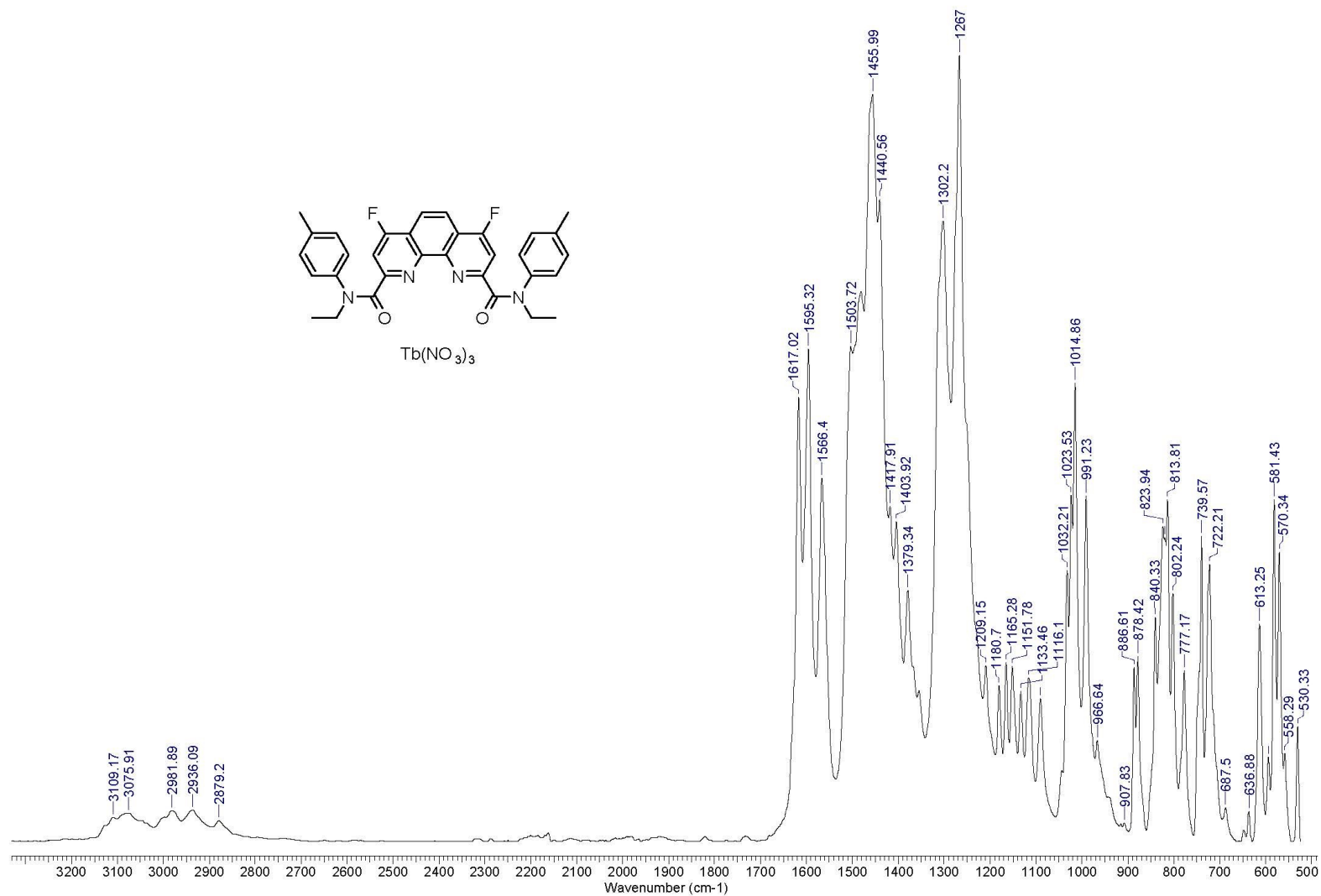


Figure S21. Solid-state IR spectrum at 25°C

***N*²,*N*⁹-diethyl-4-fluoro-7-hydroxy-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide europium trinitrate LFOH•Eu(NO₃)₃**

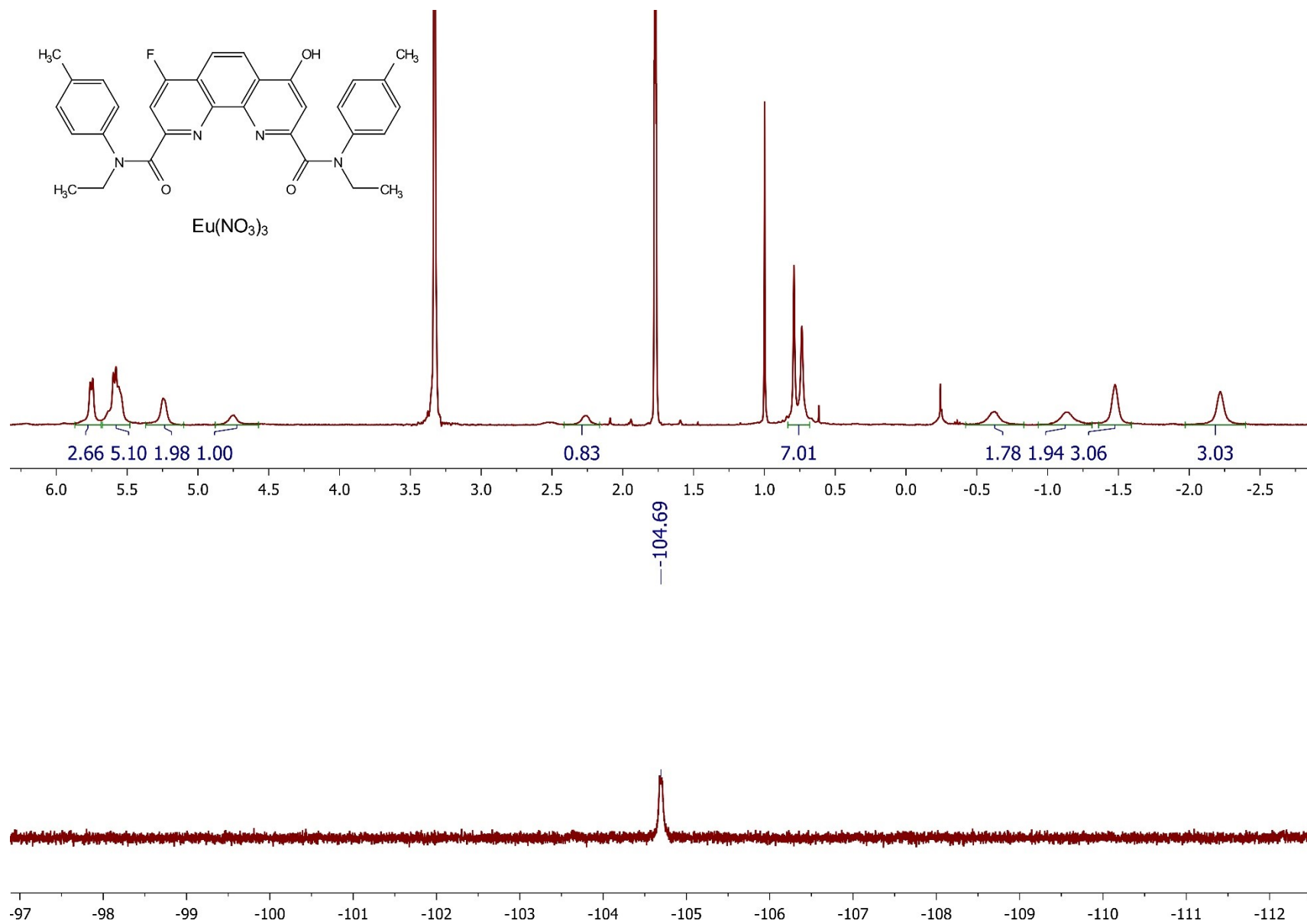


Figure S22. ¹H and ¹⁹F NMR spectra in CD₃OD at 25°C

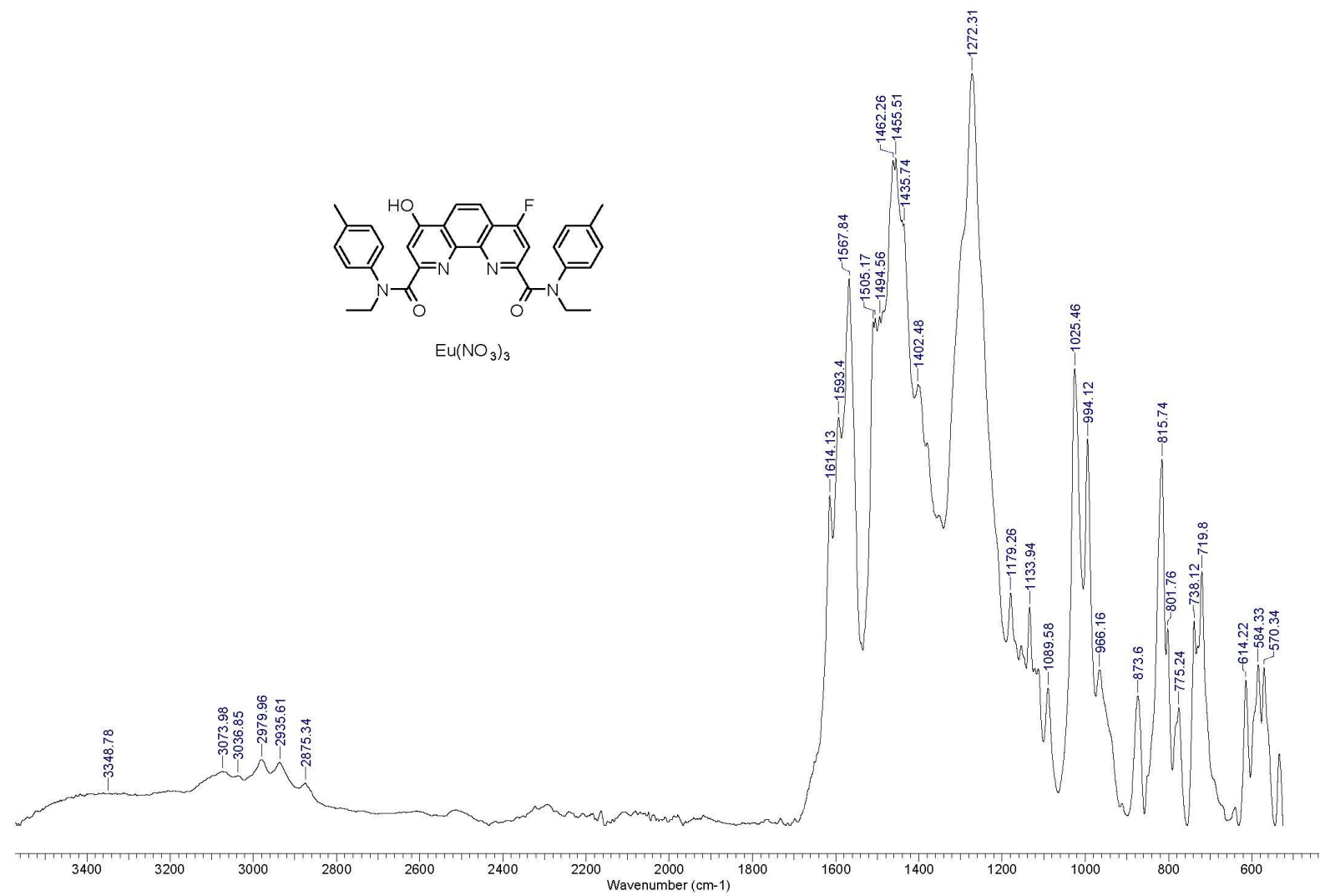


Figure S23. Solid-state IR spectrum at 25°C

*N*²,*N*⁹-diethyl-4-fluoro-7-hydroxy-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide gadolinium trinitrate LFOH•Gd(NO₃)₃

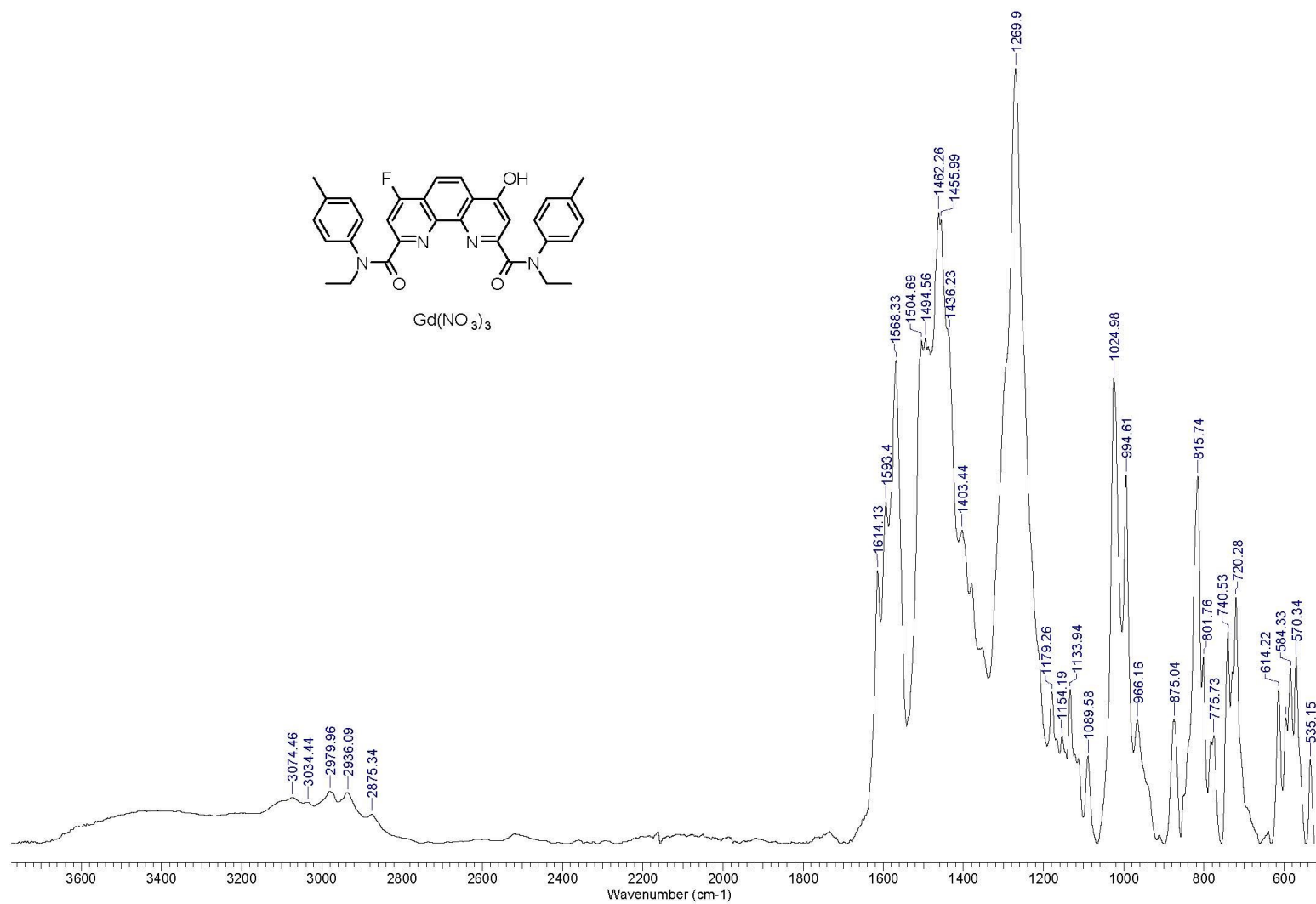


Figure S24. Solid-state IR spectrum at 25°C

*N*²,*N*⁹-diethyl-4-fluoro-7-hydroxy-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide terbium trinitrate LFOH•Tb(NO₃)₃

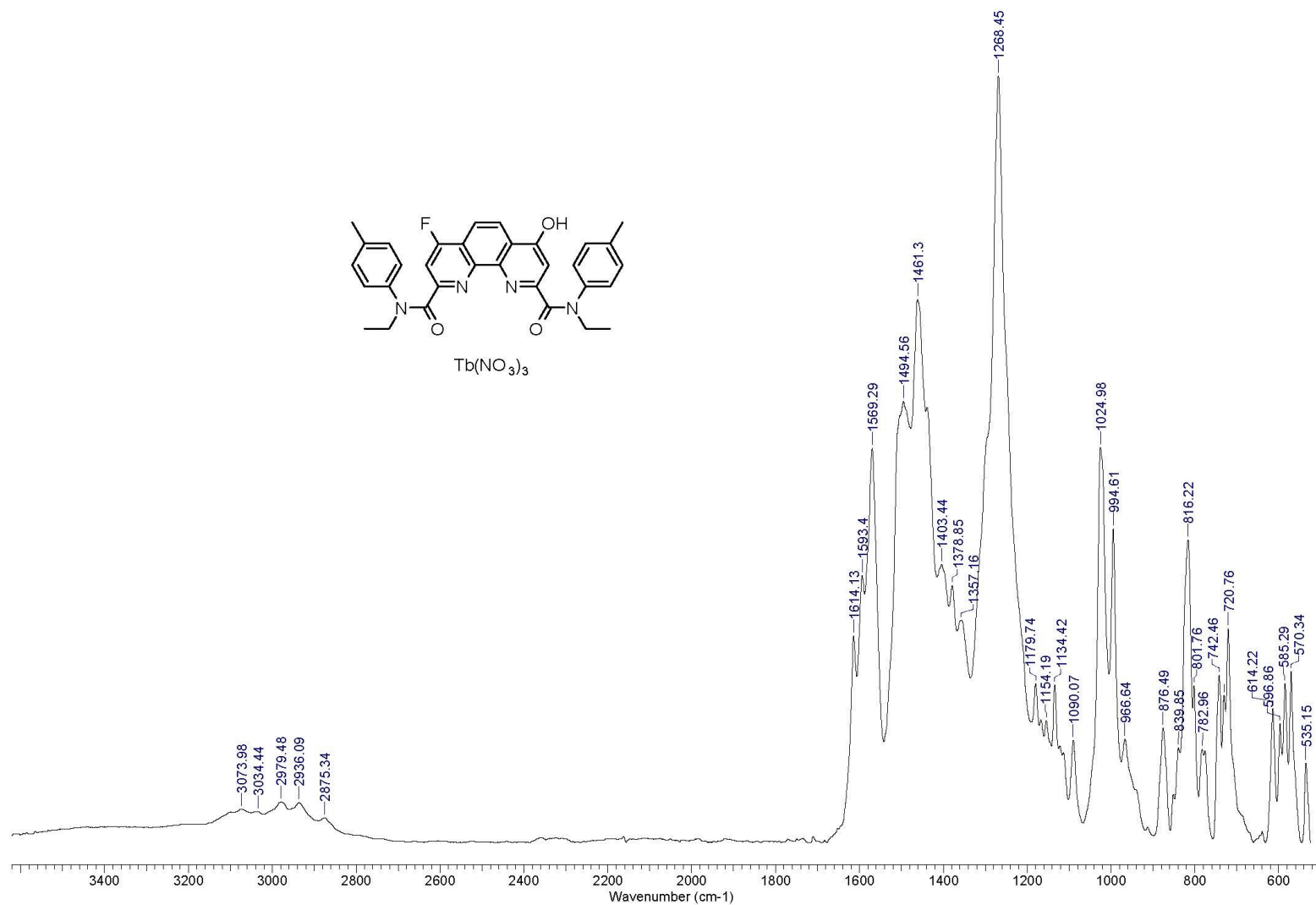


Figure S25. Solid-state IR spectrum at 25°C

*N*²,*N*⁹-diethyl-4,7-dihydroxy-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide gadolinium trinitrate LOH•Gd(NO₃)₃

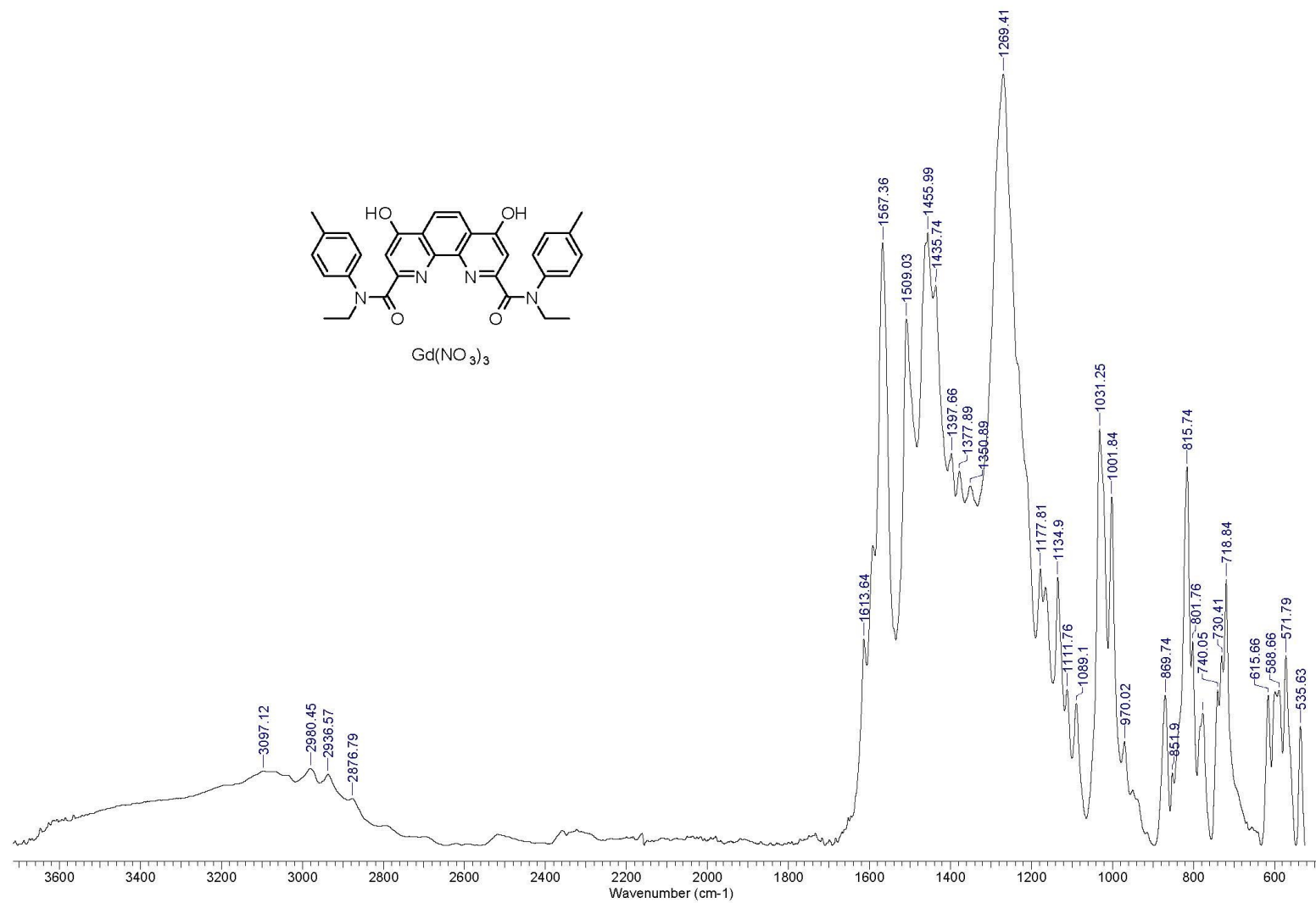


Figure S26. Solid-state IR spectrum at 25°C

*N*²,*N*⁹-diethyl-4,7-dihydroxy-*N*²,*N*⁹-di-*p*-tolyl-1,10-phenanthroline-2,9-dicarboxamide terbium trinitrate LOH•Tb(NO₃)₃

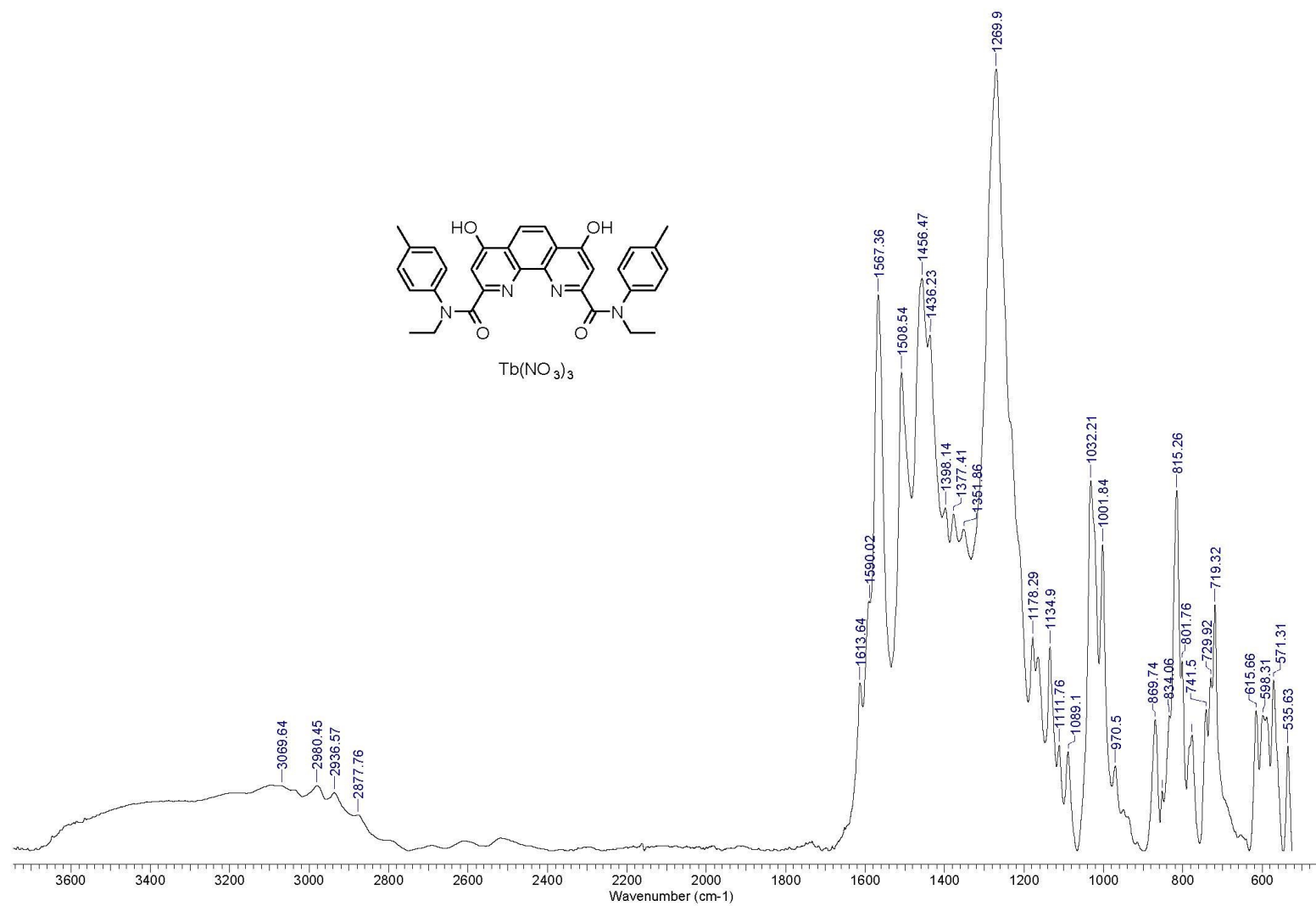


Figure S27. Solid-state IR spectrum at 25°C

3. Photoluminescence

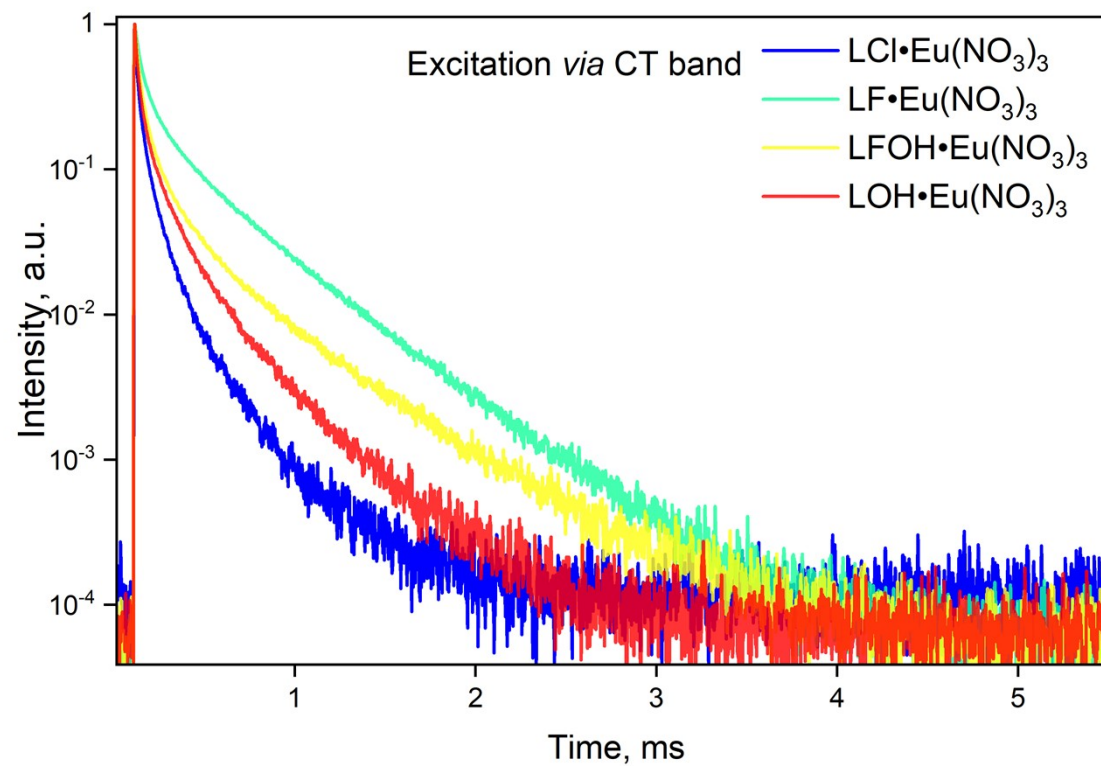
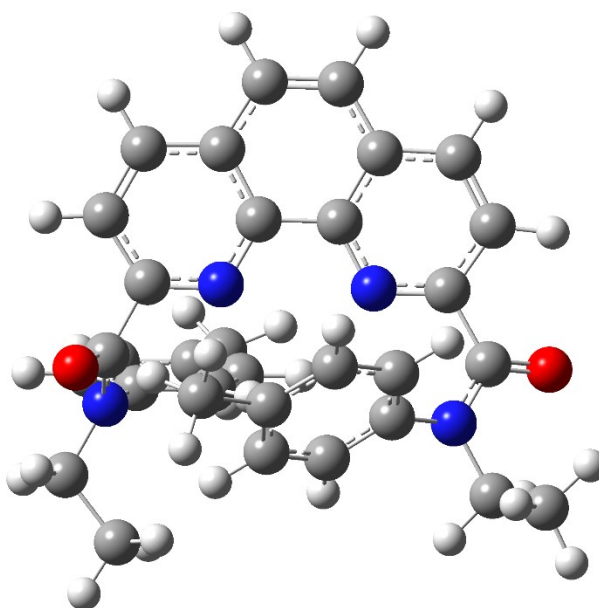


Figure S28. PL decays upon excitation via CT excitation band.

4. DFT calculations

All structures were optimized at the DFT level in the gas phase (tolerance on gradient: 10^{-7} au). We used quantum chemical software PRIODA-19 developed by Laikov [1] to evaluate quantum chemical calculations. The generalized gradient approximation (GGA) functional PBE was used for the geometry optimization and frequency calculations of all structures. All stationary points on the potential energy surface (PES) were checked by vibrational analysis and none of them had imaginary frequencies. Full electron relativistic L1 basis set [2] of TZ quality including one polarization function was used for all the atoms to provide the most reliable result. To make ESP maps for complexes we used Gaussian 16 [3] at B3LYP/6-31G(d,p)/RECP theoretical level. For light atoms, the 6-31G(d,p) basis sets were applied. For the europium, the relativistic effects were taken into account by using the scalar relativistic effective core potentials (RECPs), which replace 28 core electrons for Eu. The corresponding ECP28MWB-SEG valence basis sets were adopted for describing Eu atoms [4].

LH



E= -1606.160553

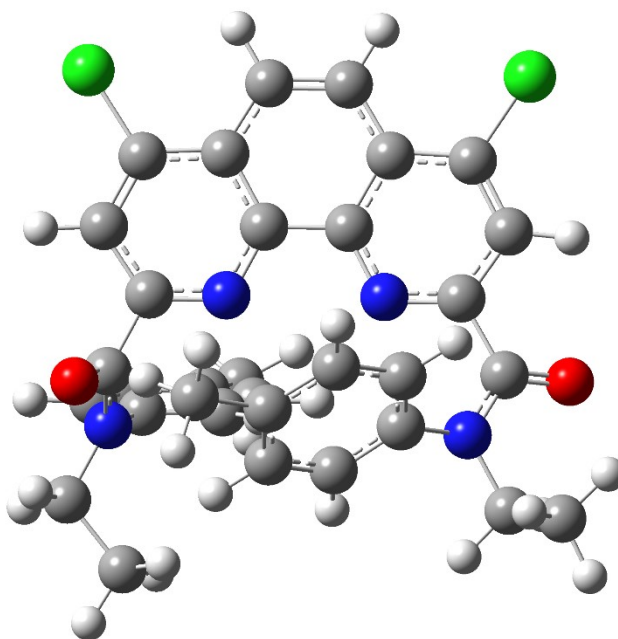
G= 291.8428 kcal/mol, H= 359.4870 kcal/mol, U= 358.8945 kcal/mol, S= 226.8798 cal/mol at T= 298.150 K

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N	-2.61227418	-1.82922185	0.70805077
N	-0.63266897	0.46946711	1.34097883

N	2.99591405	-0.03894810	-1.95552469
N	1.36922643	1.58561108	-0.17755243
C	2.80648608	-0.79062941	-0.75120050
C	-1.89979757	-1.54254084	1.85048895
C	-5.01122023	0.34001833	-1.15070152
H	-6.08687538	0.54132638	-1.15778350
C	0.82106298	2.32326473	0.81138479
C	-1.54772197	-0.09130386	2.11876508
C	1.82058823	-1.78378026	-0.69610258
H	1.18072624	-1.95386824	-1.56609995
C	-0.22052472	1.72166359	1.63510603
C	-4.49227868	-0.57782596	-0.23890411
H	-5.15646898	-1.09079938	0.46225157
C	-2.96973380	-3.23560477	0.44491400
H	-4.06470969	-3.30413743	0.32859973
H	-2.67809197	-3.78478483	1.35297399
C	2.34398947	2.12221752	-0.89795955
C	-0.30854977	3.80657609	2.96990728
H	-0.74825472	4.36007441	3.80516334
C	-1.73008259	1.83702045	3.53283344
C	0.65358566	4.37856662	2.18700959
H	0.99632773	5.39917843	2.38228804
C	2.80913677	3.44735473	-0.72073379
H	3.58181257	3.82505803	-1.39220442
C	-3.11666506	-0.83832732	-0.20313525
C	-2.11287364	0.54336266	3.24935076
H	-2.83670824	0.00987117	3.86899034
C	3.50760674	-0.76511079	-3.13434580
H	3.25256091	-0.15639585	-4.01393817
H	2.96843368	-1.72368776	-3.19179992
C	1.24483658	3.65573087	1.10367852
C	-4.17533717	1.01969286	-2.04885773
C	-0.75951574	2.47160566	2.72276914
C	1.62206046	-2.50871175	0.47296100
H	0.82606640	-3.25794539	0.51498683
C	2.96819254	1.33794259	-2.03919514
C	-2.79976502	0.75462271	-1.99488935
H	-2.12310049	1.28449814	-2.67208228
C	-2.26995355	-0.16798726	-1.09269769
H	-1.19269758	-0.33383124	-1.03200929
C	3.39873334	-1.29918926	1.54145716
H	4.02438265	-1.10136766	2.41717899
C	3.62048451	-0.57976258	0.36545187
H	4.41279344	0.17187278	0.31813384
C	2.26041358	4.20783156	0.28854955
C	2.38950834	-2.26612850	1.62350912
C	-4.74249217	1.99162290	-3.05328958
H	-4.00201082	2.75725971	-3.33028002

H	-5.63599618	2.49972376	-2.65869156
C	5.01831691	-0.99892126	-3.07412774
H	5.55138823	-0.03653246	-3.07157932
H	5.34463649	-1.57342541	-3.95615354
H	5.29464880	-1.56596242	-2.17164471
C	2.10083498	-3.01136965	2.90175817
H	2.26143467	-4.09555108	2.77712582
H	1.04799690	-2.86604138	3.19705145
C	-2.27043178	-3.80274178	-0.79036781
H	-2.51358115	-3.21860018	-1.69143940
H	-2.59542696	-4.84244419	-0.95627027
H	-1.17782245	-3.79997325	-0.65757349
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H	2.74744960	-2.66423154	3.72160930
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H	2.59997664	5.23138935	0.47358569

LCI



E= -2527.967506

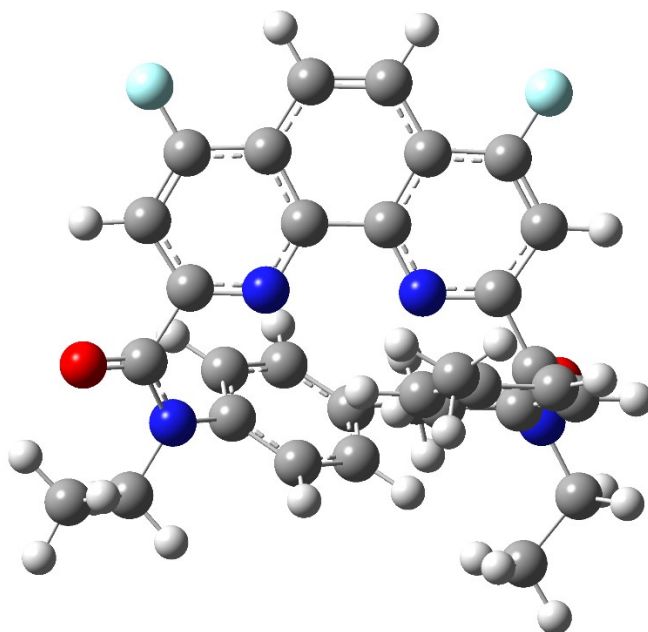
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N	-2.60429031	-1.84218593	0.67719175
N	-0.61164291	0.46577988	1.31547556
N	3.00938402	-0.07106938	-1.94857188
N	1.38131513	1.56618309	-0.17315545
C	2.82199639	-0.81872461	-0.74111600

C	-1.87368903	-1.55641727	1.80571158
C	-5.03840543	0.33604468	-1.12491556
H	-6.11426155	0.53530378	-1.11375011
C	0.83559543	2.31858516	0.80341110
C	-1.53809097	-0.09939771	2.07457311
C	1.83528444	-1.81060176	-0.68032552
H	1.19340197	-1.98401218	-1.54817967
C	-0.21685656	1.71903820	1.61973441
C	-4.50385917	-0.58918980	-0.22935711
H	-5.15601771	-1.10972872	0.47744759
C	-2.95183667	-3.25047981	0.40827255
H	-4.04748694	-3.32635144	0.30480083
H	-2.64495112	-3.80401580	1.30851788
C	2.36016203	2.09118164	-0.89396598
C	-0.32216706	3.81004200	2.93952026
H	-0.77056953	4.36786666	3.76341228
C	-1.75738405	1.82125481	3.47919816
C	0.65038363	4.37797340	2.16620777
H	0.98813086	5.39736652	2.36050401
C	2.83385558	3.41298723	-0.73240614
H	3.60599649	3.78852344	-1.40372845
C	-3.12773440	-0.84658587	-0.21835841
C	-2.13297250	0.52700599	3.19138751
H	-2.86669963	0.00073328	3.80274034
C	3.51501600	-0.80094892	-3.12871285
H	3.25180656	-0.19780012	-4.00969692
H	2.97778851	-1.76097082	-3.17639359
C	1.25464266	3.65556420	1.09520694
C	-4.21806645	1.02608865	-2.02915409
C	-0.77162703	2.47799508	2.69697179
C	1.63943784	-2.53103212	0.49200229
H	0.84379188	-3.28030662	0.53885818
C	2.98597256	1.30358168	-2.03492597
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H	-1.21794567	-0.33491408	-1.07548210
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H	4.04662750	-1.11643082	2.42548178
C	3.63754786	-0.60189694	0.37311320
H	4.43006543	0.14925828	0.32124765
C	2.28103750	4.18071045	0.26713818
C	2.41080962	-2.28509316	1.63937720
C	-4.80088016	2.00722869	-3.01511823
H	-4.09743632	2.82688958	-3.22703122
H	-5.73905377	2.44330078	-2.63930221
C	5.02657665	-1.03045678	-3.07708630
H	5.55747493	-0.06695642	-3.07998727

H	5.34820769	-1.60614932	-3.95992521
H	5.30964301	-1.59521191	-2.17524385
C	2.12811734	-3.02857465	2.91977299
H	2.28767170	-4.11284643	2.79524884
H	1.07672279	-2.88198218	3.21906056
C	-2.26216751	-3.80175360	-0.83939077
H	-2.52397328	-3.21494390	-1.73337389
H	-2.57787751	-4.84390201	-1.00726723
H	-1.16800863	-3.78757741	-0.72049455
H	-5.02799978	1.51123900	-3.97474257
H	2.77893642	-2.68069961	3.73588669
Cl	-2.50578775	2.64667993	4.83122987
Cl	2.86173408	5.81623838	0.51201275

LF



E= -1804.717679

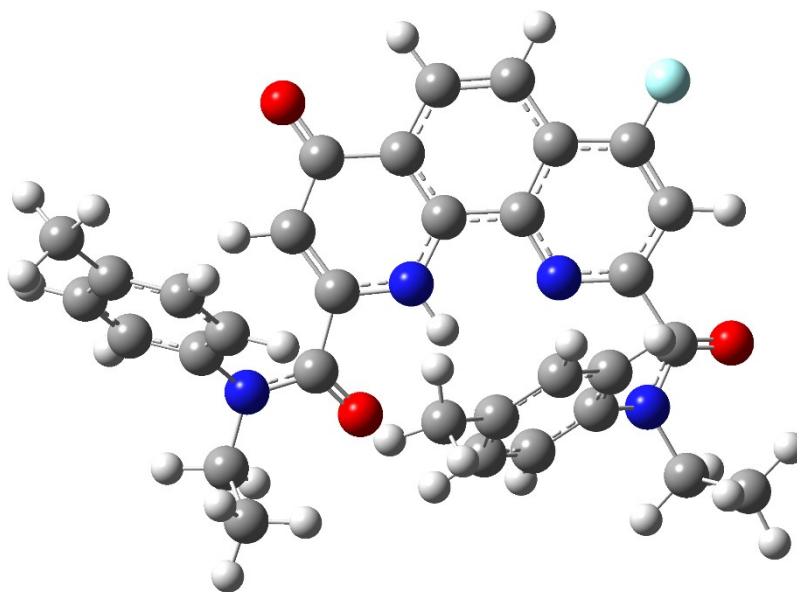
G= 281.4096 kcal/mol, H= 350.8702 kcal/mol, U= 350.2777 kcal/mol, S= 232.9721 cal/mol at T= 298.150 K

O	-1.51174787	-2.37377074	2.65215710
O	3.47934781	1.95966562	-2.98259565
N	-2.62174292	-1.83021178	0.71519925
N	-0.61134430	0.47269680	1.32630966
N	3.04858485	-0.03709407	-1.95025223
N	1.40788840	1.58037043	-0.17327550
C	2.84125726	-0.80010632	-0.75565384
C	-1.88874547	-1.53263353	1.83966817
C	-5.06062447	0.31605686	-1.11850489
H	-6.13804771	0.50721315	-1.11545305
C	0.84926040	2.32270093	0.80476007
C	-1.54643331	-0.07393613	2.09038909

C	1.84487126	-1.78337367	-0.71984832
H	1.20979897	-1.93714933	-1.59633573
C	-0.20749645	1.72778282	1.61491490
C	-4.52434275	-0.59598848	-0.21056187
H	-5.17703465	-1.11391496	0.49764653
C	-2.97618372	-3.24061035	0.46704283
H	-4.07330505	-3.31644416	0.37983742
H	-2.65793358	-3.78407764	1.36948248
C	2.39356114	2.11572246	-0.87887217
C	-0.31702052	3.83233538	2.93848555
H	-0.77330559	4.38720011	3.76031495
C	-1.74881367	1.85931981	3.46199197
C	0.66321555	4.39582394	2.17128096
H	1.00842396	5.41356469	2.36212080
C	2.86600924	3.43688571	-0.70220153
H	3.64534931	3.82929619	-1.35633046
C	-3.14674369	-0.84525792	-0.19090090
C	-2.14324806	0.56970585	3.19734653
H	-2.88511808	0.06680980	3.81968967
C	3.56670204	-0.75455588	-3.13243825
H	3.31732414	-0.13983097	-4.00945907
H	3.02640505	-1.71177531	-3.19849864
C	1.26263128	3.65671271	1.10732709
C	-4.24067048	1.00185311	-2.02623476
C	-0.75936145	2.49925933	2.68176494
C	1.63048391	-2.51928863	0.43951001
H	0.82757289	-3.26179769	0.46632999
C	3.03339864	1.33879606	-2.01948420
C	-2.86212730	0.74751322	-1.98826386
H	-2.19759503	1.28019417	-2.67520915
C	-2.31536426	-0.16991103	-1.09144685
H	-1.23673518	-0.33238097	-1.04605499
C	3.41069560	-1.33919341	1.53541976
H	4.03169176	-1.15792038	2.41793659
C	3.64758333	-0.60783997	0.36973399
H	4.44726231	0.13678286	0.33679198
C	2.29362404	4.18408546	0.29684827
C	2.39248203	-2.29824989	1.59807773
C	-4.82674338	1.96463432	-3.02843899
H	-4.12664977	2.78316907	-3.25406569
H	-5.76787321	2.40186992	-2.66126698
C	5.07661622	-0.99077824	-3.06460398
H	5.61100968	-0.02934299	-3.04851603
H	5.40738043	-1.55640574	-3.95059749
H	5.34607340	-1.56809685	-2.16654977
C	2.08974905	-3.05749410	2.86470218
H	2.23583451	-4.14177090	2.72481393
H	1.03840403	-2.90041632	3.15903251

C	-2.30475261	-3.80749810	-0.78348260
H	-2.57662491	-3.22998207	-1.68049564
H	-2.62518642	-4.85064228	-0.93537745
H	-1.20907784	-3.79474966	-0.67942413
H	-5.04393147	1.44888247	-3.97962055
H	2.73924135	-2.73078192	3.69062646
F	-2.30010289	2.53655294	4.48515555
F	2.71229424	5.44181618	0.52760627

LFOH



E= -1780.694250

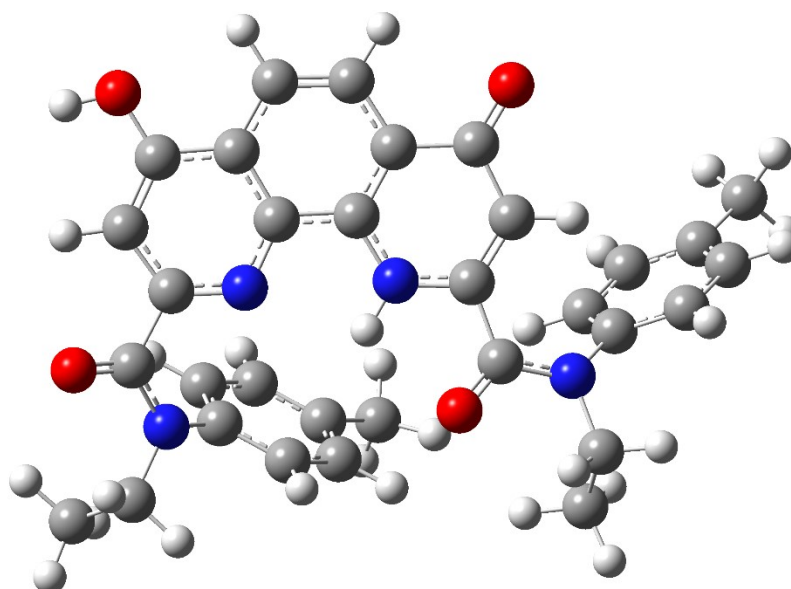
G= 288.7924 kcal/mol, H= 359.0517 kcal/mol, U= 358.4592 kcal/mol, S= 235.6509 cal/mol at T= 298.150 K

F	4.78962431	4.67607113	0.61069299
O	6.10201491	0.19265565	-1.20627706
O	-0.69866648	-0.93731906	-2.20576893
O	-2.23048302	4.49223450	-0.38862276
N	2.82174940	1.23754299	-0.58089733
N	0.12095656	1.20169823	-0.92938592
N	4.38033663	-1.20864025	-0.64468005
N	-2.90056205	-0.68366497	-1.65356201
C	4.96665771	0.03479469	-0.76544670
C	4.13698799	1.25599340	-0.41415765
C	4.85805603	2.40996103	-0.02554754
H	5.94556679	2.37210887	0.04600922
C	4.14938761	3.56009154	0.22248260
C	2.74326958	3.60705859	0.06913368
C	1.95033938	4.76774998	0.28993578
H	2.43927825	5.69021065	0.60791776

C	0.59186732	4.71081952	0.09093938
H	-0.05566998	5.57935210	0.23944156
C	-0.05042782	3.51765045	-0.32583537
C	-1.51988798	3.49782418	-0.54920654
C	-2.03677822	2.19766210	-0.97565300
H	-3.10869091	2.13079623	-1.15431515
C	-1.22829814	1.10556982	-1.14427578
C	0.71379144	2.36502354	-0.53829858
C	2.14079564	2.38162232	-0.35014377
C	-1.58965916	-0.26281740	-1.68763837
C	3.26539136	-1.49851384	0.20256572
C	3.30026932	-1.17871103	1.56581040
H	4.18049517	-0.67795023	1.97700482
C	2.21736204	-1.48487316	2.38820846
H	2.25690111	-1.21376425	3.44771768
C	1.08681338	-2.14542275	1.88608257
C	1.07493982	-2.47837955	0.52383482
H	0.20093775	-2.98066944	0.09908007
C	2.14409432	-2.15986832	-0.31149231
H	2.09359534	-2.39480330	-1.37731333
C	-0.06661543	-2.50696627	2.78901528
C	5.14946934	-2.35715617	-1.16723331
H	5.71247660	-1.98895102	-2.03704389
H	4.42269544	-3.11164349	-1.50623735
C	6.10553657	-2.95278964	-0.13242667
H	6.63158448	-3.81915107	-0.56474466
H	5.56027691	-3.29241934	0.76204439
C	-3.88682029	-0.21184497	-0.72947266
C	-3.64455570	-0.22897992	0.64843456
H	-2.68188692	-0.58782626	1.02137945
C	-4.61626047	0.23196782	1.53599150
H	-4.40500676	0.22876950	2.60928959
C	-5.85792677	0.69532465	1.08103283
C	-6.09476883	0.68678097	-0.30254146
H	-7.05133291	1.05358116	-0.68667499
C	-5.12658513	0.24171938	-1.19931141
H	-5.31829460	0.27167249	-2.27516041
C	-6.91606837	1.17027057	2.04414207
H	-6.48112199	1.42128561	3.02300690
C	-3.21420772	-1.92872948	-2.38897086
H	-2.54277742	-1.96073070	-3.25873234
H	-4.25272477	-1.84314846	-2.74420270
C	-3.03992643	-3.18595616	-1.53627348
H	-3.32136383	-4.07565253	-2.12196805
H	-3.67754790	-3.14868410	-0.63937327
H	-1.98944398	-3.29354838	-1.22832901
H	-7.43397182	2.06200342	1.65804086
H	-7.67971240	0.39020934	2.20633062

H	-0.27286105	-1.70551851	3.51572581
H	-0.98377816	-2.69509728	2.20980237
H	0.15338487	-3.42244341	3.36493686
H	6.85578244	-2.20544357	0.16492206
H	0.71199757	0.39000187	-1.1537379

LOH



E= -1756.650935

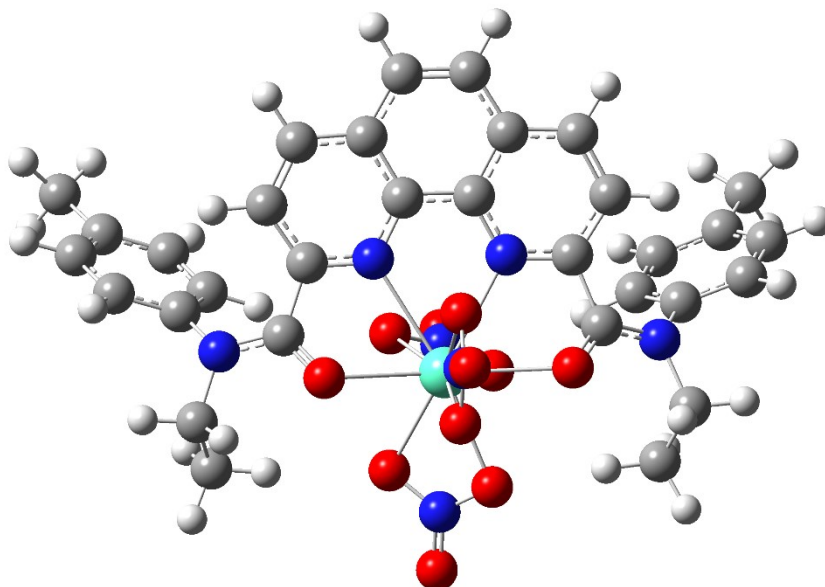
G= 297.2662 kcal/mol, H= 366.3025 kcal/mol, U= 365.7100 kcal/mol, S= 231.5489 cal/mol at T= 298.150 K

O	1.11451059	0.51528834	6.02293215
O	0.56628392	-2.48942337	-0.26572147
O	3.62602549	1.80546675	-2.96531523
N	1.41577137	0.85562939	2.54450448
N	1.47971910	-0.03194344	-0.01996977
N	-0.37734041	-0.31008453	4.49632585
N	0.29961766	-2.37804513	-2.53197755
C	0.68600814	0.48728627	4.87146049
C	1.39433369	1.29101181	3.79703145
C	2.09560716	2.43286204	4.23961079
H	2.05974615	2.67982897	5.30432242
C	2.82970472	3.17224903	3.32913219
C	2.87817527	2.74944131	1.96802763
C	3.61733903	3.42859386	0.95948313
H	4.17027693	4.32977441	1.22934834
C	3.63339403	2.94093673	-0.32556690
H	4.19560862	3.42729575	-1.12732129
C	2.92203587	1.76835863	-0.68237659
C	2.97602903	1.25247964	-2.07512285
C	2.19394000	0.03511420	-2.28612190

H	2.20285709	-0.38687602	-3.28981422
C	1.47600594	-0.55991521	-1.28293982
C	2.18208339	1.09426833	0.29516062
C	2.14462086	1.56774535	1.65424670
C	0.72309345	-1.87389852	-1.32068288
C	-1.17855626	-0.09641169	3.33151741
C	-1.78770198	1.14371189	3.10082206
H	-1.61898955	1.96245310	3.80493065
C	-2.58886159	1.33635691	1.97685229
H	-3.04369917	2.31691300	1.80565223
C	-2.83323486	0.29412287	1.07089464
C	-2.23379663	-0.94769986	1.32560557
H	-2.39165097	-1.77583937	0.62868766
C	-1.41538045	-1.14574720	2.43618154
H	-0.92708027	-2.11098117	2.58939098
C	-3.73144889	0.49817262	-0.12415664
C	-0.91128509	-1.22800793	5.52316528
H	-0.05816244	-1.53282987	6.14639575
H	-1.30383505	-2.11375182	4.99979685
C	-1.99599561	-0.58703329	6.39052679
H	-2.37728405	-1.32246711	7.11720609
H	-2.84146713	-0.24010537	5.77618191
C	0.03334433	-1.58973018	-3.69629500
C	-0.81488950	-0.47872807	-3.63205571
H	-1.26232610	-0.19800116	-2.67519942
C	-1.06620802	0.27790447	-4.77601306
H	-1.71694421	1.15435042	-4.70517607
C	-0.50496051	-0.06342701	-6.01372930
C	0.32663810	-1.19292062	-6.06764323
H	0.78796124	-1.47610841	-7.01850234
C	0.59642160	-1.94750396	-4.92865848
H	1.27236423	-2.80483532	-4.98486383
C	-0.79667642	0.74237624	-7.25410433
H	-1.17377044	1.74408655	-6.99967141
C	-0.22814054	-3.75982523	-2.52393272
H	0.32326457	-4.30474766	-1.74461516
H	0.00832169	-4.20485643	-3.50280094
C	-1.73186135	-3.82439786	-2.25424343
H	-2.07406764	-4.87082596	-2.29650539
H	-2.29497505	-3.24768527	-3.00432705
H	-1.95561301	-3.42865543	-1.25262208
H	0.10658512	0.86152005	-7.87258328
H	-1.55938890	0.24502870	-7.87773349
H	-3.57161770	1.48743408	-0.58124051
H	-3.55609010	-0.27119694	-0.89192484
H	-4.79502598	0.43907065	0.16488483
H	-1.58090949	0.26639915	6.94662901
H	1.00816098	-0.54755933	0.73487412

O	3.52730393	4.28970748	3.65568149
H	3.42608203	4.44882672	4.61406477

LH•Eu(NO₃)₃



E= -13294.937077

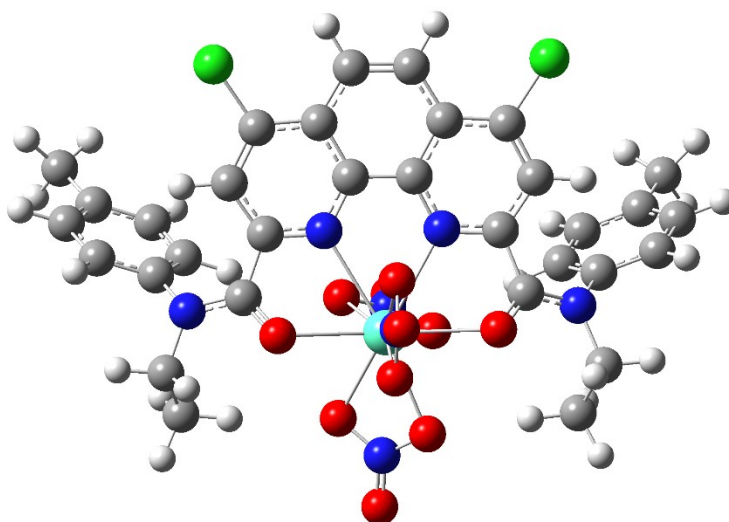
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O	-2.48619629	-2.27688954	0.93086684
O	2.50280956	-2.21042518	1.05665831
O	-0.01832720	-4.96965481	-2.34687485
O	0.01540212	-1.92638578	3.04076198
O	-0.03996094	-3.90237686	2.10920368
N	-4.42216313	-1.30923212	0.21057468
O	0.95039310	-3.99312912	-0.62951112
N	-1.37748336	0.06729783	1.47066391
N	4.42657948	-1.25782135	0.28713894
O	1.31924111	-1.06046422	-1.40103130
N	-0.00313716	-4.10810014	-1.48612474
N	1.31477310	0.13955412	1.38967102
O	-0.11682353	-3.72631175	4.30101414
N	-0.05024347	-3.20943915	3.19993325
O	0.56024054	0.50210052	-2.75522917
O	-0.95464435	-3.23224906	-1.36961598
N	0.39052083	-0.26507107	-1.81839046
O	-0.72429327	-0.31800143	-1.16725250
C	5.02753704	-0.13092742	-0.36441128
C	-3.20539144	-1.26888471	0.81854135
C	-6.98063851	1.27197707	-0.62781064
H	-8.02668926	1.49314276	-0.39510612
C	0.67822218	1.17151784	1.97512757
C	-2.70568022	0.02363883	1.42925802
C	6.33881070	0.24712293	-0.04805274

H	6.89307564	-0.30291079	0.71760192
C	-0.76541271	1.13416764	2.01490972
C	-6.37988472	0.14740038	-0.06624060
H	-6.94558379	-0.50207081	0.60729420
C	-4.91955431	-2.63311491	-0.24755279
H	-6.01818913	-2.59721832	-0.17413520
H	-4.54119700	-3.37528717	0.46981839
C	2.64624196	0.12630211	1.35351763
C	-0.75351660	3.29141424	3.20080695
H	-1.31539662	4.10402651	3.66960488
C	-2.89012167	2.10615776	2.62010423
C	0.61395453	3.32153280	3.17409136
H	1.15707427	4.15788867	3.62292317
C	3.42076944	1.16812379	1.90966447
H	4.50937223	1.12533468	1.86672671
C	-5.03894526	-0.14190874	-0.34836870
C	-3.50786213	1.03023388	2.01111421
H	-4.59508805	0.95404955	1.98156675
C	4.96714863	-2.60599758	-0.02721528
H	4.64475226	-3.27353815	0.78512628
H	6.06459108	-2.51536451	0.00047620
C	1.36639992	2.26702109	2.56355008
C	-6.26624739	2.13055903	-1.47868682
C	-1.48036664	2.20177721	2.62216681
C	6.92192677	1.33385545	-0.69601965
H	7.94370556	1.62767877	-0.43703113
C	3.19102833	-1.19746588	0.85308732
C	-4.92639326	1.82151347	-1.75216337
H	-4.34814545	2.46954743	-2.41768509
C	-4.31390069	0.69265277	-1.20856576
H	-3.27208129	0.45440168	-1.45072898
C	4.91103515	1.66469754	-1.97541054
H	4.34431564	2.20942763	-2.73659050
C	4.31662925	0.57118679	-1.34536307
H	3.30663182	0.24186789	-1.61650861
C	2.77749239	2.23237452	2.51326706
C	6.21903312	2.06428744	-1.66818514
C	-6.93251213	3.32793476	-2.10753482
H	-6.20363934	4.12301928	-2.32562588
H	-7.71464966	3.74192332	-1.45274151
C	4.49073158	-3.13720888	-1.37750591
H	3.39904235	-3.27657777	-1.37607961
H	4.96136164	-4.11499389	-1.56718531
H	4.76776283	-2.45427630	-2.19540253
C	6.86845890	3.22018459	-2.38639547
H	7.41777929	2.86747000	-3.27640458
H	7.59072172	3.74072461	-1.73880176
C	-4.47320953	-2.97768959	-1.66669113

H	-4.82038191	-2.22173907	-2.38810281
H	-4.90452718	-3.95001592	-1.95335668
H	-3.37654971	-3.05912755	-1.72479644
H	-7.41375173	3.04999597	-3.06115299
H	6.11919512	3.94956184	-2.72939341
H	-3.48504518	2.89047637	3.09572509
H	3.35374907	3.04594917	2.96221360

LCI•Eu(NO₃)₃



E= -14216.741643

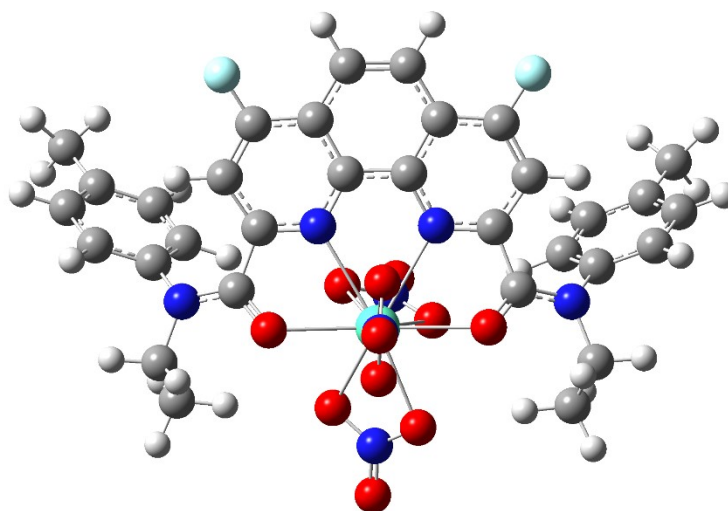
G= 296.9106 kcal/mol, H= 388.0832 kcal/mol, U= 387.4907 kcal/mol, S= 305.7945 cal/mol at T= 298.150 K

Eu	0.00021507	-2.05338357	0.55570563
O	-2.49016350	-2.30336816	0.94478190
O	2.49728326	-2.22399670	1.05516453
O	-0.01240844	-5.00597963	-2.33068155
O	0.02374176	-1.95254677	3.04596089
O	-0.03445713	-3.93019095	2.11832201
N	-4.41266651	-1.32412818	0.19865490
O	0.95551712	-4.02064163	-0.61778598
N	-1.37492918	0.04453710	1.48386613
N	4.41084022	-1.26333282	0.26787769
O	1.29846207	-1.08090929	-1.39774433
N	0.00120341	-4.14234042	-1.47263622
N	1.29967032	0.12407534	1.39355990
O	-0.08117600	-3.75131338	4.31062817
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N	0.36007685	-0.29615948	-1.81392019
O	-0.75214345	-0.35992359	-1.15846766

C	5.00259360	-0.13256808	-0.38651153
C	-3.20422543	-1.29356140	0.82033115
C	-6.93264857	1.28676483	-0.66611066
H	-7.97883910	1.51931307	-0.44584972
C	0.67278441	1.15558624	1.98893917
C	-2.70211738	-0.00287879	1.43641421
C	6.31280954	0.25301888	-0.07501351
H	6.87435706	-0.29395241	0.68746160
C	-0.77422371	1.11443427	2.03338282
C	-6.35371782	0.15143015	-0.10305069
H	-6.94027933	-0.49502613	0.55542492
C	-4.91943466	-2.64436740	-0.26048489
H	-6.01809307	-2.59710831	-0.19572245
H	-4.55444048	-3.38847478	0.46189839
C	2.63044495	0.11154318	1.34735213
C	-0.76257279	3.26742348	3.22533404
H	-1.32458981	4.07498635	3.69716681
C	-2.90158215	2.06649632	2.62986692
C	0.60477137	3.30043863	3.19565638
H	1.14649392	4.13421605	3.64507720
C	3.41413411	1.14510361	1.89736291
H	4.50193056	1.11234872	1.84776767
C	-5.01194164	-0.15024240	-0.36705008
C	-3.51546503	0.99218035	2.01422788
H	-4.60166008	0.92098269	1.98151832
C	4.95889819	-2.60892369	-0.04572027
H	4.64650550	-3.27628501	0.77072326
H	6.05570312	-2.51028375	-0.02453308
C	1.35702975	2.25452870	2.58041155
C	-6.19631316	2.14265579	-1.50070962
C	-1.48744750	2.18287492	2.64573781
C	6.88517158	1.34532824	-0.72306916
H	7.90541292	1.64651152	-0.46688972
C	3.18045338	-1.21000459	0.84234976
C	-4.85695646	1.81852589	-1.75893033
H	-4.26212820	2.46296600	-2.41317878
C	-4.26545150	0.67936074	-1.21387321
H	-3.22349744	0.42928078	-1.44423014
C	4.86663719	1.66468207	-1.99357087
H	4.29324838	2.20675105	-2.75158469
C	4.28235731	0.56601304	-1.36311588
H	3.27397023	0.22934598	-1.63125977
C	2.77282723	2.20533122	2.51007818
C	6.17290540	2.07311183	-1.69043273
C	-6.83846543	3.35381687	-2.12772974
H	-6.09693967	4.14261279	-2.32467294
H	-7.62627825	3.76966715	-1.48113994
C	4.47863669	-3.14740325	-1.39170406

H	3.38764357	-3.29171121	-1.38573522
H	4.95352261	-4.12353388	-1.57893552
H	4.74957211	-2.46675441	-2.21350645
C	6.81008433	3.23681637	-2.40662078
H	7.35788819	2.89192963	-3.30058803
H	7.53116324	3.75961125	-1.75968013
C	-4.46495508	-2.99636827	-1.67514669
H	-4.79827965	-2.23820214	-2.40068428
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H	-3.36889589	-3.08967238	-1.72445289
H	-7.30669554	3.09136320	-3.09211171
H	6.05359664	3.96192382	-2.74248907
Cl	-3.88959459	3.29229984	3.38094725
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LF•Eu(NO₃)₃



E= -13493.491865

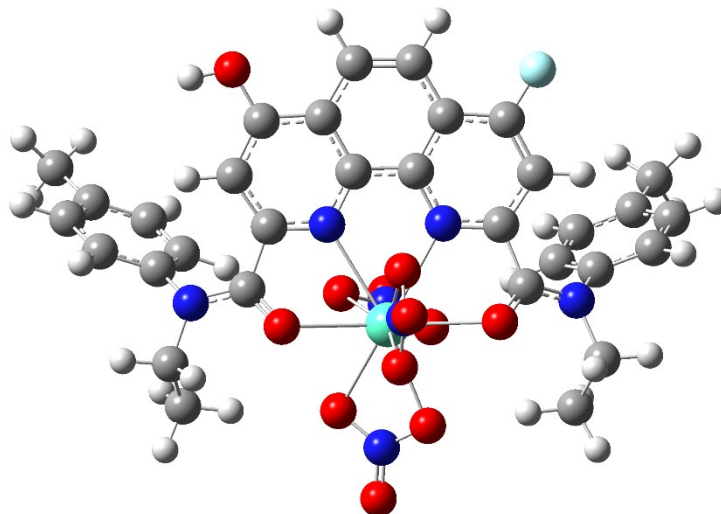
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O	-2.48914887	-2.27888512	0.91947982
O	2.50613813	-2.21482498	1.05277604
O	-0.01114270	-4.99026212	-2.34714276
O	0.01486333	-1.93479456	3.02712105
O	-0.04574269	-3.91236884	2.09939975
N	-4.42730637	-1.31242879	0.20183067
O	0.95528474	-4.00862949	-0.63127138
N	-1.37606612	0.06123280	1.45399725
N	4.43203150	-1.26314241	0.28509834
O	1.32762014	-1.07810384	-1.41022577
N	0.00336375	-4.12617896	-1.48952654
N	1.31332320	0.13237552	1.37461985
O	-0.11418090	-3.73255288	4.29113749

N	-0.05146558	-3.21764532	3.18934938
O	0.56991033	0.48112884	-2.76896134
O	-0.94819937	-3.24915590	-1.37729356
N	0.39900284	-0.28454454	-1.83141032
O	-0.71772926	-0.33833555	-1.18308885
C	5.03374782	-0.13524567	-0.36504224
C	-3.20967902	-1.27279469	0.80530230
C	-6.98508058	1.27869486	-0.60715528
H	-8.02653444	1.50567862	-0.36023997
C	0.67849610	1.16424677	1.96058438
C	-2.70409455	0.02094278	1.41376892
C	6.33990884	0.25027821	-0.03719195
H	6.89054554	-0.29522558	0.73430321
C	-0.76561518	1.12751989	1.99983305
C	-6.38342229	0.15024083	-0.05439588
H	-6.94409282	-0.49696969	0.62550731
C	-4.92731526	-2.63694324	-0.25268221
H	-6.02575789	-2.59818685	-0.17993049
H	-4.55080491	-3.37759189	0.46730986
C	2.64497951	0.12125672	1.34229642
C	-0.75382922	3.29263684	3.19267096
H	-1.31981306	4.10023144	3.66009658
C	-2.87741594	2.08951953	2.59373566
C	0.61444673	3.32199154	3.16706898
H	1.16217468	4.15283281	3.61520754
C	3.42297235	1.15911776	1.89414493
H	4.51254520	1.14138606	1.86095832
C	-5.04723189	-0.14424337	-0.35284687
C	-3.50996519	1.02453700	1.98979382
H	-4.59873615	0.97480771	1.96662873
C	4.97626577	-2.61123860	-0.02475250
H	4.65514938	-3.27731840	0.78934854
H	6.07331151	-2.51728433	0.00407695
C	1.35410521	2.26457738	2.55328530
C	-6.27659666	2.13518464	-1.46516140
C	-1.46783846	2.20118935	2.60955845
C	6.92193313	1.34020088	-0.68081709
H	7.93908276	1.64113881	-0.41227905
C	3.19576093	-1.20411378	0.84641749
C	-4.94195650	1.81942105	-1.75633576
H	-4.36902830	2.46505198	-2.42870998
C	-4.32854905	0.68692943	-1.22139777
H	-3.29094791	0.44341077	-1.47600675
C	4.92083536	1.65703486	-1.97939957
H	4.35826971	2.19701958	-2.74697362
C	4.32720668	0.56088179	-1.35326841
H	3.32159618	0.22518615	-1.63289729
C	2.76415934	2.21254842	2.49179416

C	6.22329227	2.06545146	-1.65994779
C	-6.94386480	3.33817722	-2.08129174
H	-6.21488559	4.13244137	-2.30165153
H	-7.71943431	3.75014822	-1.41762762
C	4.50230065	-3.14756751	-1.37383400
H	3.41077502	-3.28791703	-1.37394530
H	4.97429184	-4.12558841	-1.55852359
H	4.78063066	-2.46779752	-2.19388520
C	6.87128227	3.22602937	-2.37156370
H	7.43136700	2.87726533	-3.25636684
H	7.58361466	3.75095682	-1.71668651
C	-4.47965745	-2.98697028	-1.67008930
H	-4.82542002	-2.23368737	-2.39491391
H	-4.91234996	-3.95972398	-1.95304886
H	-3.38310941	-3.07026311	-1.72683700
H	-7.43434578	3.06692452	-3.03220469
H	6.12016672	3.95035130	-2.72093282
F	-3.60378887	3.05404962	3.17499730
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LFOH•Eu(NO₃)₃



E= -13469.450064

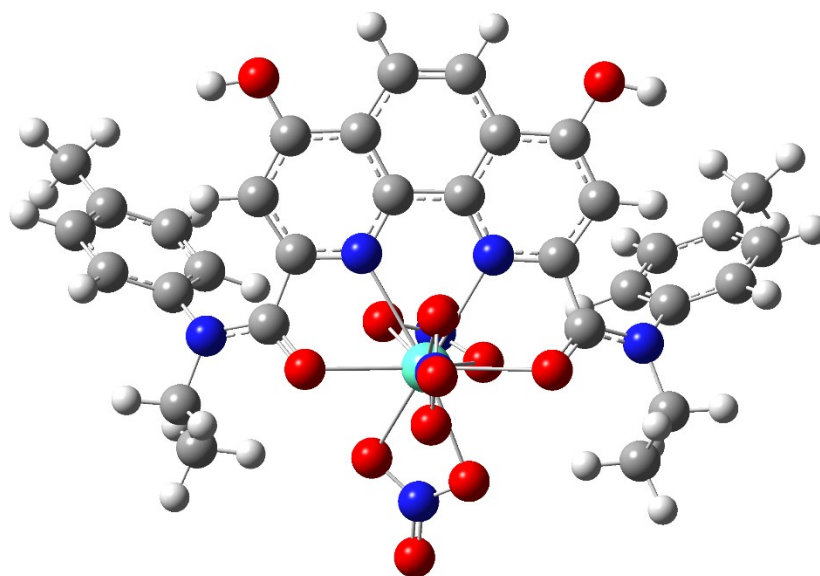
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O	-2.48914887	-2.27888512	0.91947982
O	2.50613813	-2.21482498	1.05277604
O	-0.01114270	-4.99026212	-2.34714276
O	0.01486333	-1.93479456	3.02712105
O	-0.04574269	-3.91236884	2.09939975

N	-4.42730637	-1.31242879	0.20183067
O	0.95528474	-4.00862949	-0.63127138
N	-1.37606612	0.06123280	1.45399725
N	4.43203150	-1.26314241	0.28509834
O	1.32762014	-1.07810384	-1.41022577
N	0.00336375	-4.12617896	-1.48952654
N	1.31332320	0.13237552	1.37461985
O	-0.11418090	-3.73255288	4.29113749
N	-0.05146558	-3.21764532	3.18934938
O	0.56991033	0.48112884	-2.76896134
O	-0.94819937	-3.24915590	-1.37729356
N	0.39900284	-0.28454454	-1.83141032
O	-0.71772926	-0.33833555	-1.18308885
C	5.03374782	-0.13524567	-0.36504224
C	-3.20967902	-1.27279469	0.80530230
C	-6.98508058	1.27869486	-0.60715528
H	-8.02653444	1.50567862	-0.36023997
C	0.67849610	1.16424677	1.96058438
C	-2.70409455	0.02094278	1.41376892
C	6.33990884	0.25027821	-0.03719195
H	6.89054554	-0.29522558	0.73430321
C	-0.76561518	1.12751989	1.99983305
C	-6.38342229	0.15024083	-0.05439588
H	-6.94409282	-0.49696969	0.62550731
C	-4.92731526	-2.63694324	-0.25268221
H	-6.02575789	-2.59818685	-0.17993049
H	-4.55080491	-3.37759189	0.46730986
C	2.64497951	0.12125672	1.34229642
C	-0.75382922	3.29263684	3.19267096
H	-1.31981306	4.10023144	3.66009658
C	-2.87741594	2.08951953	2.59373566
C	0.61444673	3.32199154	3.16706898
H	1.16217468	4.15283281	3.61520754
C	3.42297235	1.15911776	1.89414493
H	4.51254520	1.14138606	1.86095832
C	-5.04723189	-0.14424337	-0.35284687
C	-3.50996519	1.02453700	1.98979382
H	-4.59873615	0.97480771	1.96662873
C	4.97626577	-2.61123860	-0.02475250
H	4.65514938	-3.27731840	0.78934854
H	6.07331151	-2.51728433	0.00407695
C	1.35410521	2.26457738	2.55328530
C	-6.27659666	2.13518464	-1.46516140
C	-1.46783846	2.20118935	2.60955845
C	6.92193313	1.34020088	-0.68081709
H	7.93908276	1.64113881	-0.41227905
C	3.19576093	-1.20411378	0.84641749
C	-4.94195650	1.81942105	-1.75633576

H	-4.36902830	2.46505198	-2.42870998
C	-4.32854905	0.68692943	-1.22139777
H	-3.29094791	0.44341077	-1.47600675
C	4.92083536	1.65703486	-1.97939957
H	4.35826971	2.19701958	-2.74697362
C	4.32720668	0.56088179	-1.35326841
H	3.32159618	0.22518615	-1.63289729
C	2.76415934	2.21254842	2.49179416
C	6.22329227	2.06545146	-1.65994779
C	-6.94386480	3.33817722	-2.08129174
H	-6.21488559	4.13244137	-2.30165153
H	-7.71943431	3.75014822	-1.41762762
C	4.50230065	-3.14756751	-1.37383400
H	3.41077502	-3.28791703	-1.37394530
H	4.97429184	-4.12558841	-1.55852359
H	4.78063066	-2.46779752	-2.19388520
C	6.87128227	3.22602937	-2.37156370
H	7.43136700	2.87726533	-3.25636684
H	7.58361466	3.75095682	-1.71668651
C	-4.47965745	-2.98697028	-1.67008930
H	-4.82542002	-2.23368737	-2.39491391
H	-4.91234996	-3.95972398	-1.95304886
H	-3.38310941	-3.07026311	-1.72683700
H	-7.43434578	3.06692452	-3.03220469
H	6.12016672	3.95035130	-2.72093282
F	-3.60378887	3.05404962	3.17499730
F	3.46877447	3.21216215	3.04036409

LOH•Eu(NO₃)₃



E= -13445.408132

G= 314.5416 kcal/mol, H= 405.9504 kcal/mol, U= 405.3579 kcal/mol, S= 306.5863 cal/mol at T= 298.150 K

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O	-2.48914887	-2.27888512	0.91947982
O	2.50613813	-2.21482498	1.05277604
O	-0.01114270	-4.99026212	-2.34714276
O	0.01486333	-1.93479456	3.02712105
O	-0.04574269	-3.91236884	2.09939975
N	-4.42730637	-1.31242879	0.20183067
O	0.95528474	-4.00862949	-0.63127138
N	-1.37606612	0.06123280	1.45399725
N	4.43203150	-1.26314241	0.28509834
O	1.32762014	-1.07810384	-1.41022577
N	0.00336375	-4.12617896	-1.48952654
N	1.31332320	0.13237552	1.37461985
O	-0.11418090	-3.73255288	4.29113749
N	-0.05146558	-3.21764532	3.18934938
O	0.56991033	0.48112884	-2.76896134
O	-0.94819937	-3.24915590	-1.37729356
N	0.39900284	-0.28454454	-1.83141032
O	-0.71772926	-0.33833555	-1.18308885
C	5.03374782	-0.13524567	-0.36504224
C	-3.20967902	-1.27279469	0.80530230
C	-6.98508058	1.27869486	-0.60715528
H	-8.02653444	1.50567862	-0.36023997
C	0.67849610	1.16424677	1.96058438
C	-2.70409455	0.02094278	1.41376892
C	6.33990884	0.25027821	-0.03719195
H	6.89054554	-0.29522558	0.73430321
C	-0.76561518	1.12751989	1.99983305
C	-6.38342229	0.15024083	-0.05439588
H	-6.94409282	-0.49696969	0.62550731
C	-4.92731526	-2.63694324	-0.25268221
H	-6.02575789	-2.59818685	-0.17993049
H	-4.55080491	-3.37759189	0.46730986
C	2.64497951	0.12125672	1.34229642
C	-0.75382922	3.29263684	3.19267096
H	-1.31981306	4.10023144	3.66009658
C	-2.87741594	2.08951953	2.59373566
C	0.61444673	3.32199154	3.16706898
H	1.16217468	4.15283281	3.61520754
C	3.42297235	1.15911776	1.89414493
H	4.51254520	1.14138606	1.86095832
C	-5.04723189	-0.14424337	-0.35284687
C	-3.50996519	1.02453700	1.98979382
H	-4.59873615	0.97480771	1.96662873
C	4.97626577	-2.61123860	-0.02475250

H	4.65514938	-3.27731840	0.78934854
H	6.07331151	-2.51728433	0.00407695
C	1.35410521	2.26457738	2.55328530
C	-6.27659666	2.13518464	-1.46516140
C	-1.46783846	2.20118935	2.60955845
C	6.92193313	1.34020088	-0.68081709
H	7.93908276	1.64113881	-0.41227905
C	3.19576093	-1.20411378	0.84641749
C	-4.94195650	1.81942105	-1.75633576
H	-4.36902830	2.46505198	-2.42870998
C	-4.32854905	0.68692943	-1.22139777
H	-3.29094791	0.44341077	-1.47600675
C	4.92083536	1.65703486	-1.97939957
H	4.35826971	2.19701958	-2.74697362
C	4.32720668	0.56088179	-1.35326841
H	3.32159618	0.22518615	-1.63289729
C	2.76415934	2.21254842	2.49179416
C	6.22329227	2.06545146	-1.65994779
C	-6.94386480	3.33817722	-2.08129174
H	-6.21488559	4.13244137	-2.30165153
H	-7.71943431	3.75014822	-1.41762762
C	4.50230065	-3.14756751	-1.37383400
H	3.41077502	-3.28791703	-1.37394530
H	4.97429184	-4.12558841	-1.55852359
H	4.78063066	-2.46779752	-2.19388520
C	6.87128227	3.22602937	-2.37156370
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C	-4.47965745	-2.98697028	-1.67008930
H	-4.82542002	-2.23368737	-2.39491391
H	-4.91234996	-3.95972398	-1.95304886
H	-3.38310941	-3.07026311	-1.72683700
H	-7.43434578	3.06692452	-3.03220469
H	6.12016672	3.95035130	-2.72093282
F	-3.60378887	3.05404962	3.17499730
F	3.46877447	3.21216215	3.04036409

5. References

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