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Piperidine- and 2-(*p*-tolyl)piperidine-derived DAPhen ligands: the aryl substituent unexpectedly suppresses the extraction efficiency

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Experimental part

Materials

Deuterated solvents for NMR spectra were purchased from commercial sources and used without further purification. 3-Nitrobenzotrifluoride ("F-3") analytical grade was purchased from Rhodia (France) and was used as a solvent in the extraction experiments without further purification.

2-(*p*-Tolyl)piperidine was obtained according to ref. [S1]

Methods

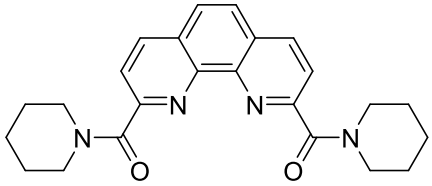
NMR spectra were recorded using standard 5 mm sample tubes on Agilent 400-MR spectrometer with operating frequencies of 400.1 MHz (^{1}H) and 100.6 MHz (^{13}C). IR spectra were recorded on FTIR spectrometer Nicolet iS5 (Thermo Scientific) using an internal reflectance attachment with diamond optical element – attenuated total reflection (ATR) with 45° angle of incidence. Resolution 4 cm^{-1}, the number of scans is 32. HRMS ESI mass spectra were recorded on an LCMS-IT-TOF (Shimadzu, Japan).

For solvent extraction experiments, 0.5 mL of organic solution of the ligand in "F-3" and 0.5 mL of aqueous phase containing nitric acid and both of Am^{III} and Eu^{III} nitrates were treated with a vortex shaker for 30 minutes in 1.5 mL polypropylene vial at temperature 25±1 °C. Then samples were centrifuged (5 minutes, 6000 rpm) and aliquots of each phase were taken for determination of Am^{III} or Eu^{III} concentration. Content of ^{241}Am ($E\gamma$= 59.5 keV) and ^{152}Eu ($E\gamma$=121.8 keV) was determined by gamma-spectrometry using a high-pure germanium detector GR 3818 (Canberra Ind.). The distribution coefficients were calculated as the ratio of count rates for the corresponding organic and aqueous phases, and separation factors were calculated as the ratio of distribution coefficients for the two elements. All extraction experiments were repeated three times. Errors for $0.01<D<100$ are within 10%.

General method for the synthesis of L1 and L2

A solution of the corresponding amine (10 mmol) and 1.4 mL of triethylamine (10 mmol) in 10 mL of dichloromethane was added at -10ºC under vigorous stirring to a suspension of 1.22 g (4 mmol) of the 1,10-phenanthroline-2,9-dicarbonyl dichloride in 50 mL of dichloromethane. The reaction mixture was allowed to reach room temperature and was stirred overnight. Next, the reaction mixture was diluted with 50 mL of dichloromethane, washed with water (2 × 50 mL), dried over sodium sulfate, and the solvent was distilled off. The residue was purified by flash chromatography (hexane : ethyl acetate 1:1).

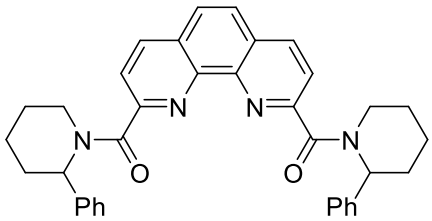
(1,10-Phenanthroline-2,9-diyl)bis(piperidin-1-ylmethanone) **L1**



Yield 68% (1.09 g), white solid, m.p. 256-258°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ, ppm: 8.32 (d, *J* = 8.3 Hz, 2H), 7.98 (d, *J* = 8.3 Hz, 2H), 7.82 (s, 2H), 3.84 – 3.78 (m, 4H), 3.77 – 3.71 (m, 4H), 1.79 – 1.67 (m, 8H), 1.67 – 1.58 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ, ppm: 166.9 (C=O), 153.8 (Phen), 144.0 (Phen), 136.7 (Phen), 128.6 (Phen), 126.8 (Phen), 123.0 (Phen), 48.2 (CH_2), 43.2 (CH_2), 26.2 (CH_2), 25.2

(CH_2), 24.3 (CH_2); IR (cm^{-1}) 2938, 2918, 2852 (C-H), 1622 (C=O), 1469, 1444 (C=C, C=N); HRMS (ESI-TOF) (*m*/*z*) $[M+H]^+$ calculated for $C_{24}H_{27}O_2N_4^+$ 403.2129, found 403.2107.

(1,10-Phenanthroline-2,9-diyl)bis(2-(p-tolyl)piperidin-1-yl)methanone **L2**



Yield 79% (1.84 g), white solid, m.p.. 175-185°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ, ppm: 8.51 – 7.61 (m, 6H, Phen), 7.53 – 6.97 (m, 8H, Tol), 6.35 – 5.49 (m, 2H, CH_2), 4.65 – 4.85 (m, 1H, CH), 4.53 – 3.06 (m, 2H, CH_2), 3.03 – 2.76 (m, 1H, CH), 2.70 – 1.42 (m, 18H, CH_2 + CH_3); ^{13}C NMR (101 MHz, $CDCl_3$) δ, ppm: 169.2 – 168.2 (C=O), 154.6 – 153.3 (Phen), 144.8 – 144.6 (Tol), 137.0 – 135.9 (Phen), 129.4 (Phen), 129.0 – 128.9 (Tol), 127.2 – 127.0 (Phen), 126.8 (Tol), 126.5 – 126.2 (Tol), 123.4 – 122.6 (Phen), 56.7 – 56.3 (CH), 51.5-51.4 (CH), 44.1-43.7 (CH_2), 38.8-38.6 (CH_2), 28.6 – 25.3 (CH_2), 21.1 – 20.7 (CH_3), 20.0 – 19.5 (CH_2); IR (cm^{-1}) 2935, 2860 (C-H), 1618 (C=O), 1546, 1513, 1446, 1423 (C=C, C=N); HRMS (ESI-TOF) (*m*/*z*) $[M+Na]^+$ calculated for $C_{38}H_{38}N_4NaO_2^+$ 605.2887, found 605.2887; $[2M+Na]^+$ calculated for $C_{76}H_{76}N_8NaO_4^+$ 1187.5882, found 1187.5881.

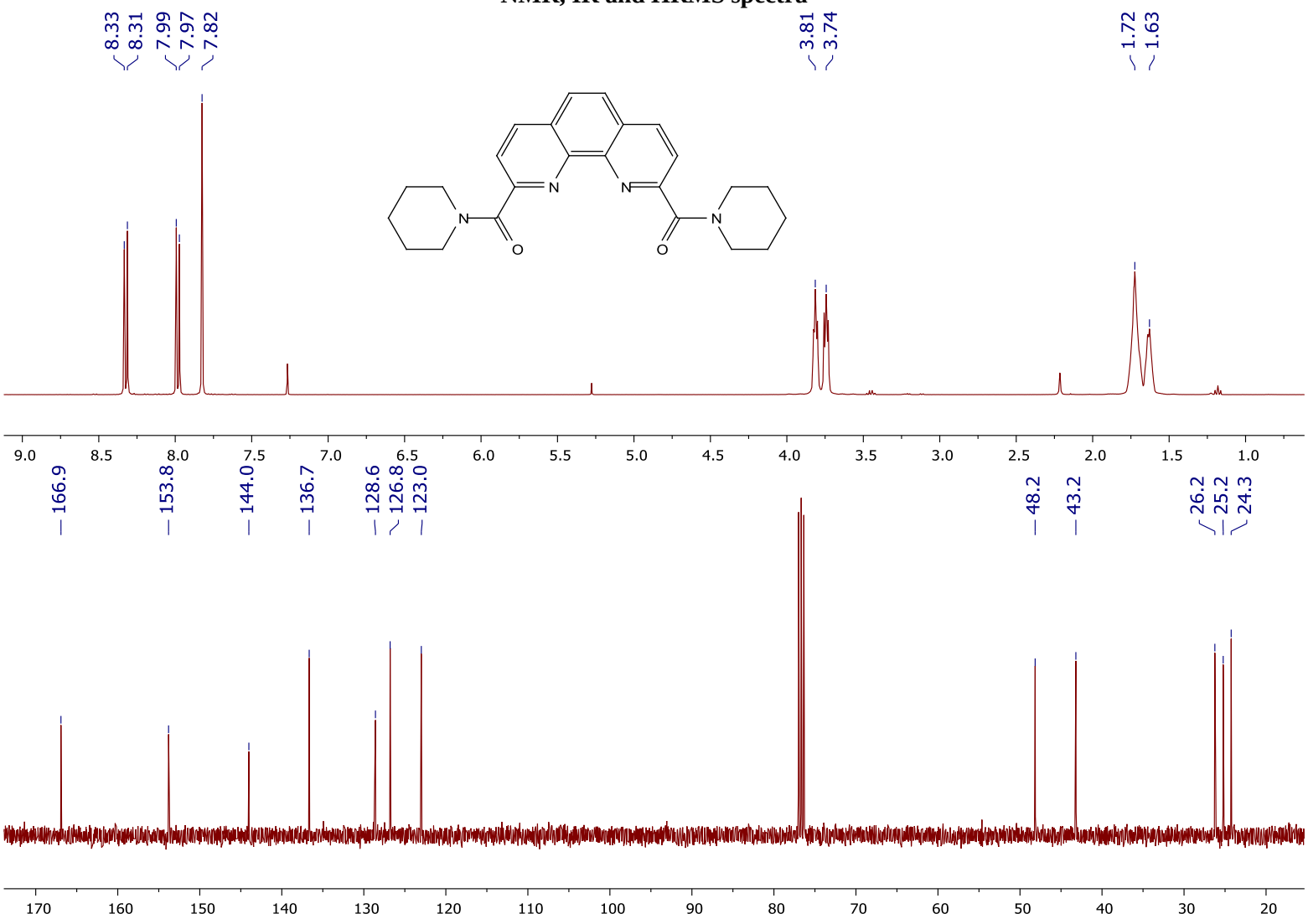


Figure S1. ^{1}H and ^{13}C NMR spectra of **L1** ($CDCl_3$, 25ºC)

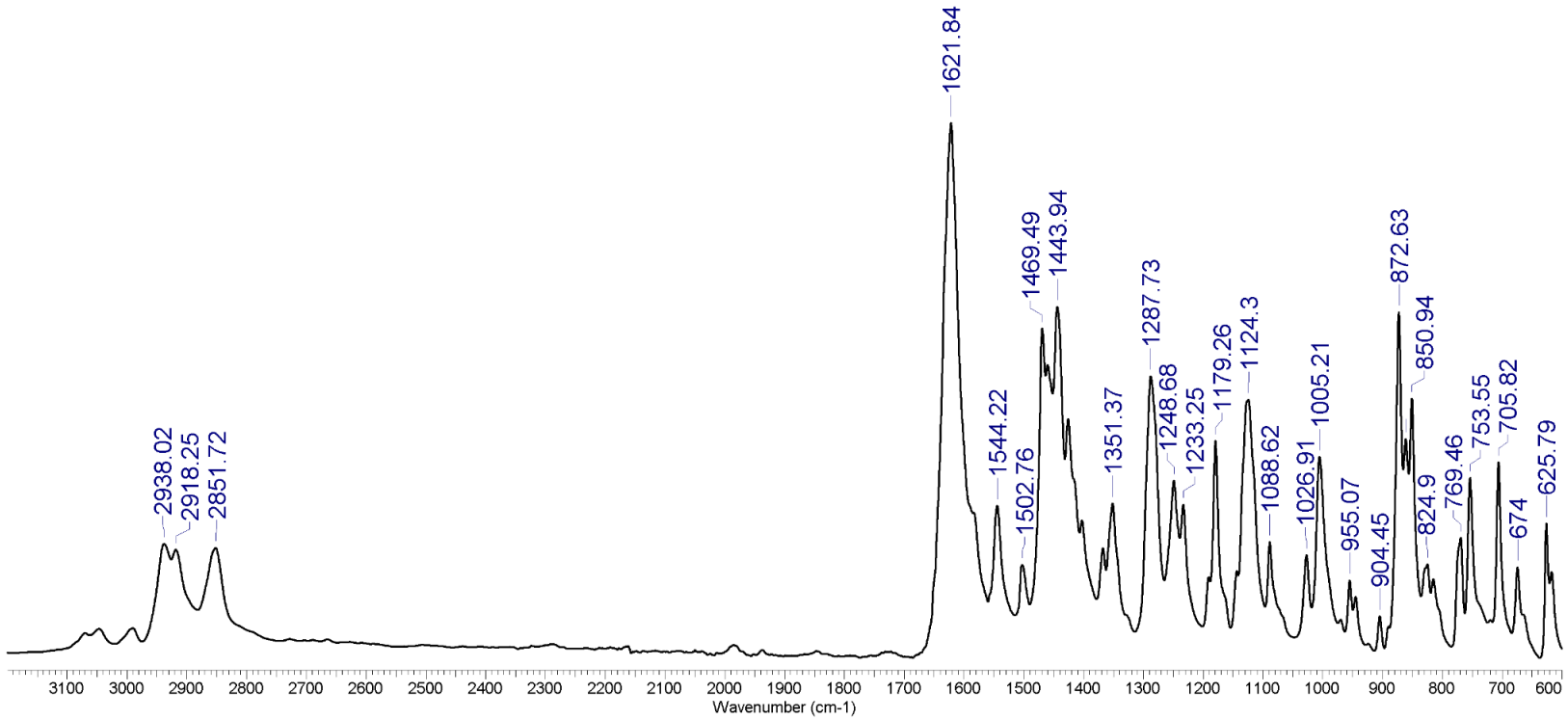


Figure S2. IR spectrum of **L1**

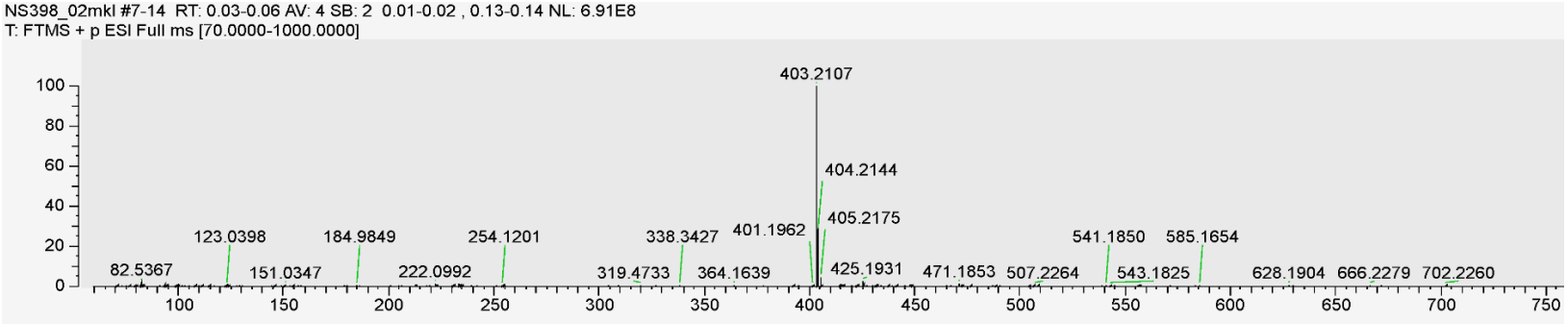


Figure S3. HRMS spectrum of **L1**

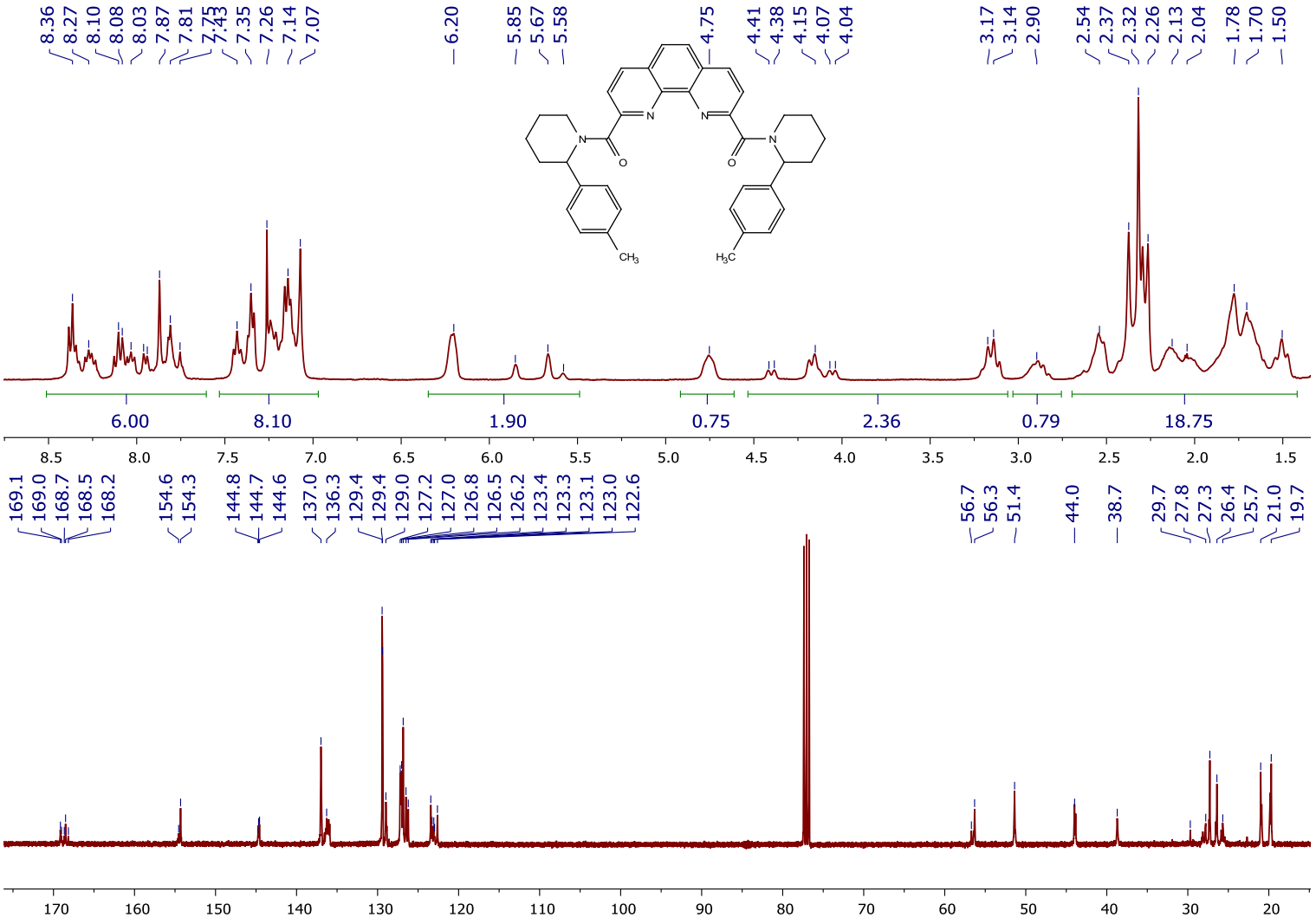


Figure S4. ^{1}H and ^{13}C NMR spectra of **L1** ($CDCl_3$, 25°C)

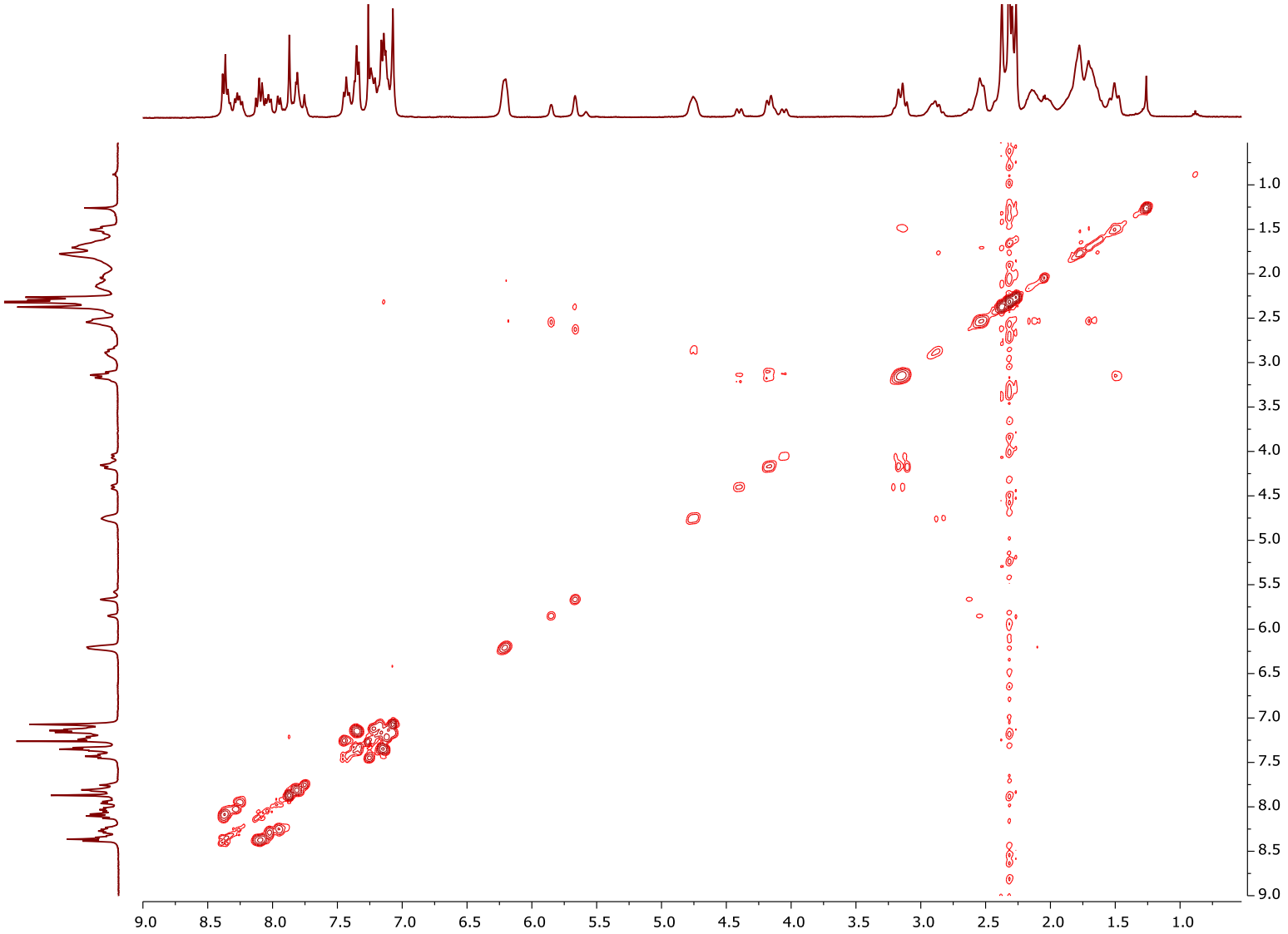


Figure S5. COSY spectrum of **L1** ($CDCl_3$, 25°C)

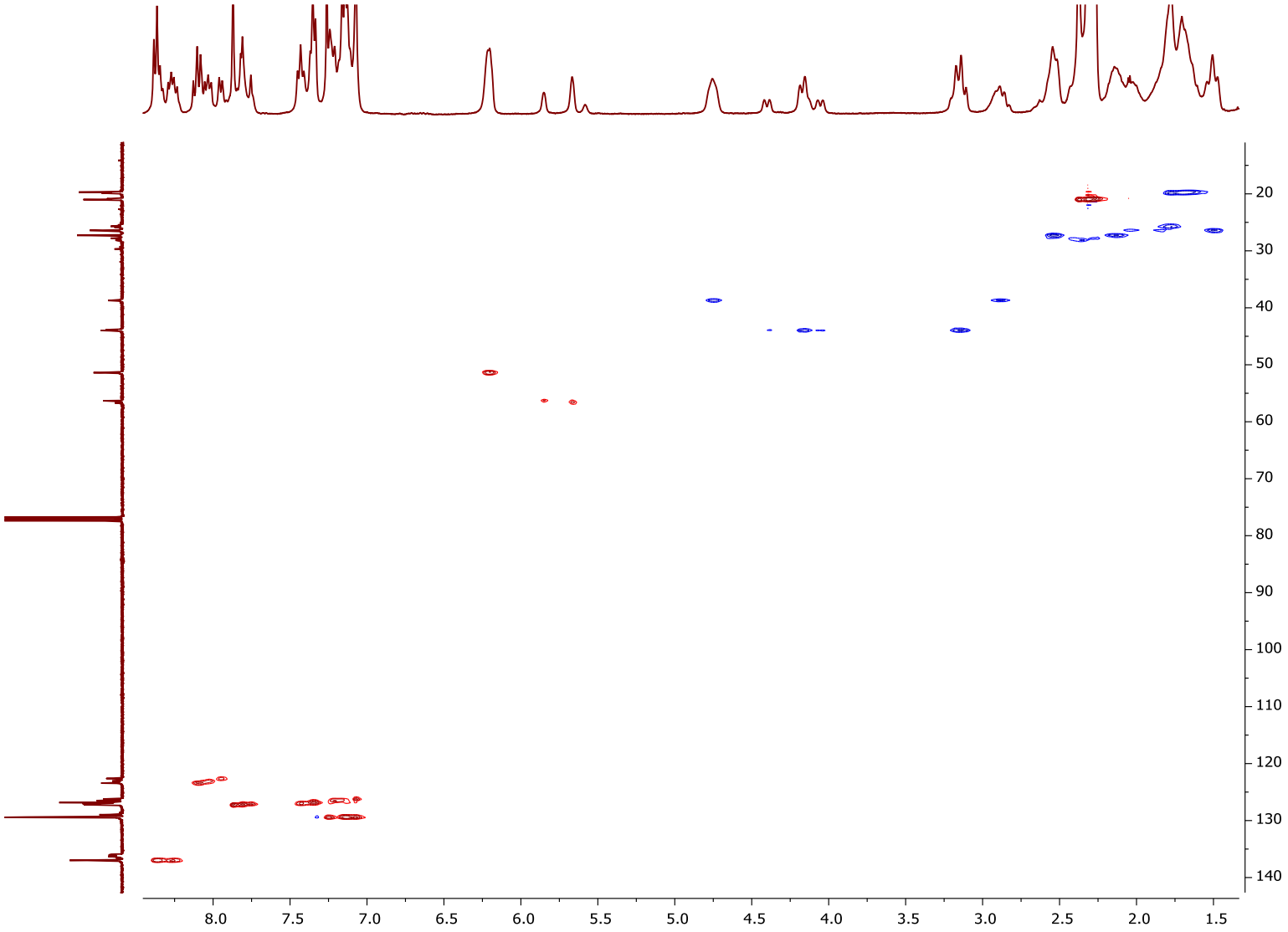


Figure S6. HSQC spectrum of **L1** ($CDCl_3$, 25°C)

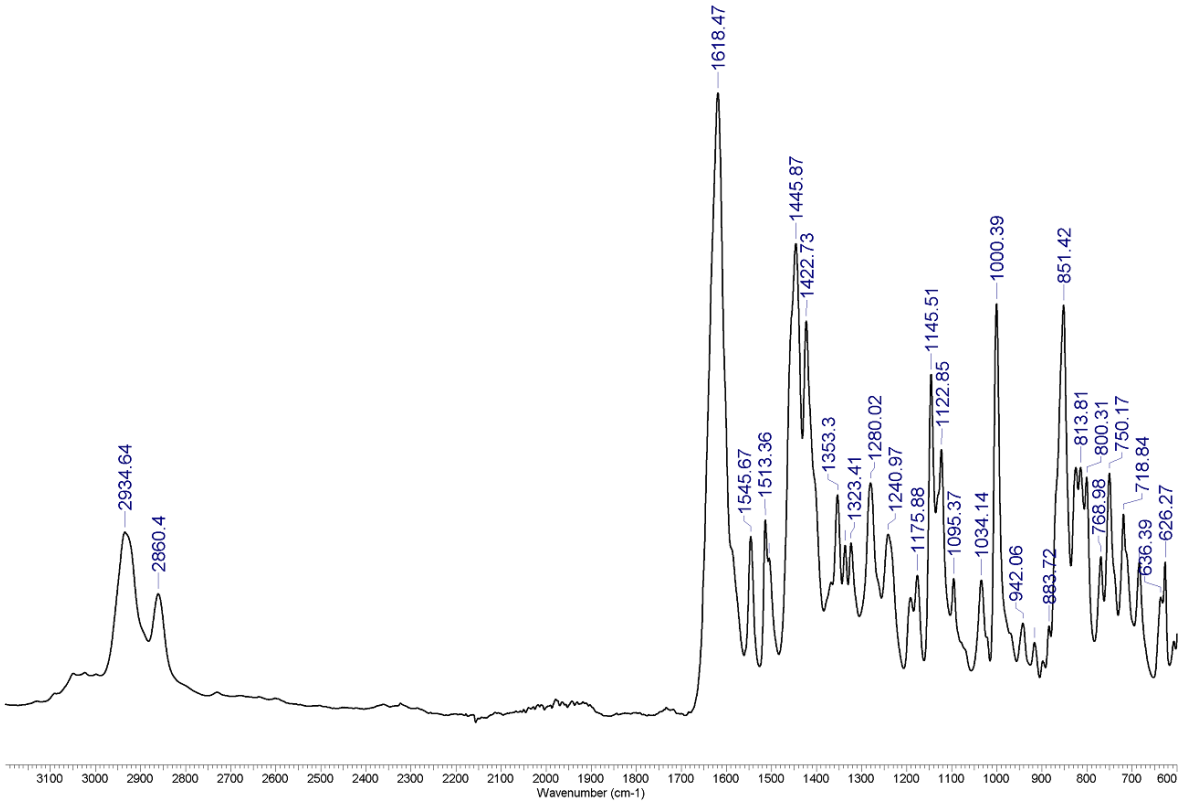


Figure S7. IR spectrum of **L2**

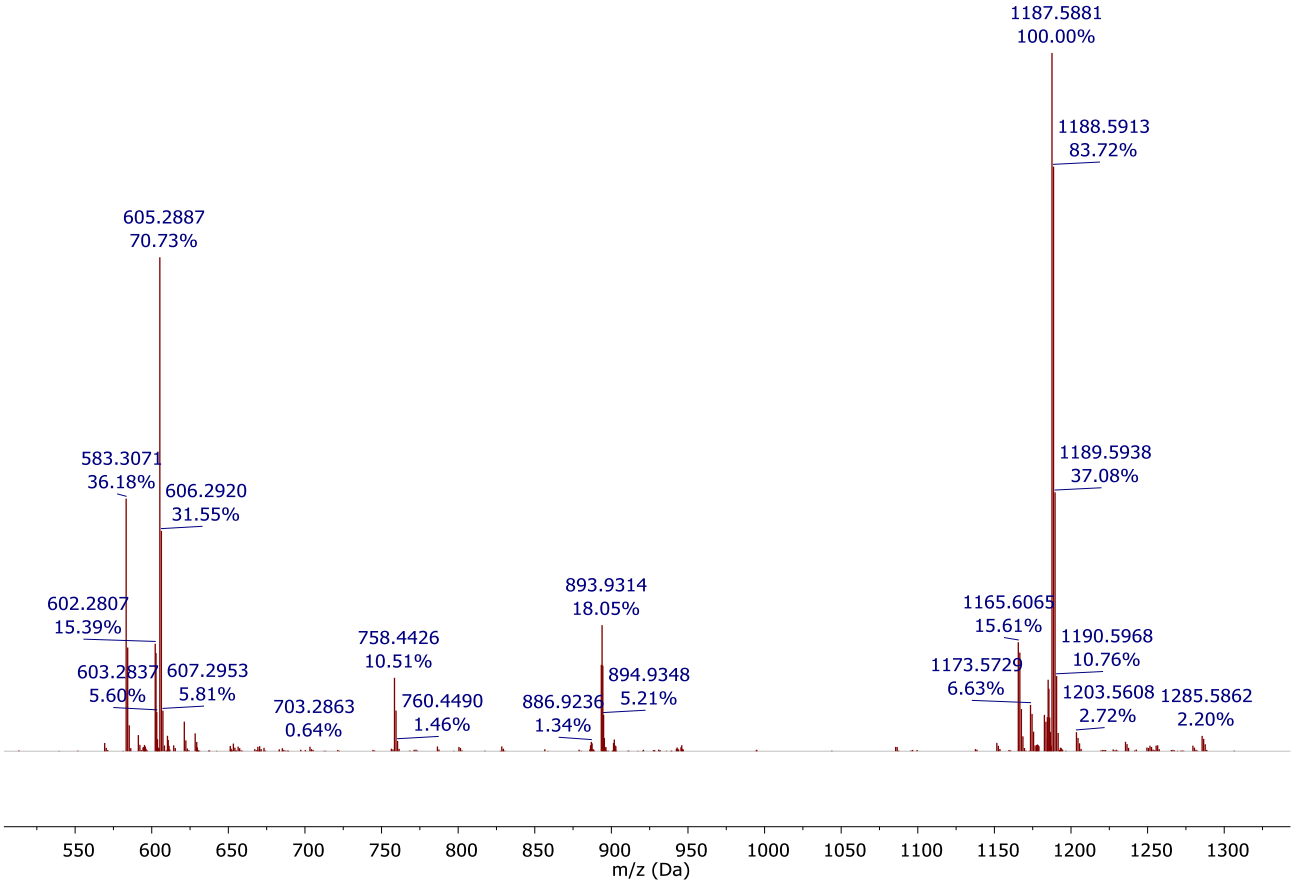


Figure S8. HRMS spectrum of **L2**

Theoretical computations

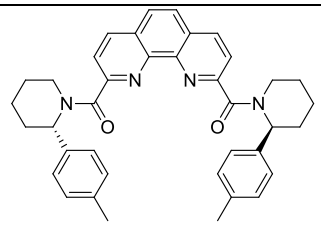
All structures were optimized at the DFT level in the gas phase (tolerance on gradient: 10^{-7} au). We used quantum chemical software PRIRODA-19 developed by Laikov [S2] to evaluate quantum chemical calculations. The generalized gradient approximation (GGA) functional PBE was used for the geometry optimization 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 [S3] of TZ quality including one polarization function was used for all the atoms to provide the most reliable result. For complexes of Eu^{III} and Am^{III} the highest spin 7 were chosen according (2S+1) rule. The data for **L4** complexes can be found in ref. [S4].

$$M(NO_3)_3(H_2O)_6 + \mathbf{L} = \mathbf{L}\bullet M(NO_3)_3 + (H_2O)_6 \qquad (1)$$

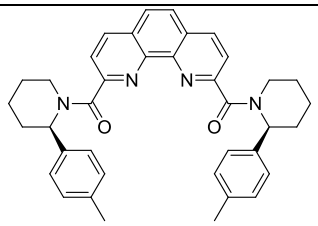
$$[\mathbf{L}\bullet H_3O]^+ + M(NO_3)_3(H_2O)_6 = \mathbf{L}\bullet M(NO_3)_3 + [(H_3O)(H_2O)_6]^+ \qquad (2)$$

Table S1 Δ*G* values during reaction (*2*) for **L1** and **L2**, kcal mol^{-1}

Ligand	$Eu(NO_3)_3$	$Am(NO_3)_3$
L1	8.2	6.7
$\mathbf{L2_{rac}}$	10.2	8.4
$\mathbf{L2_{meso}}$	10.2	8.6



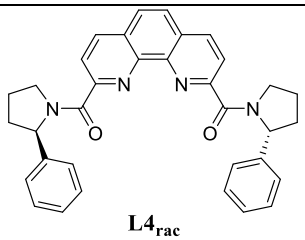
$\mathbf{L2_{rac}}$



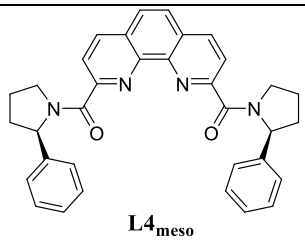
$\mathbf{L2_{meso}}$

Table S2 Δ*G* values during reaction (*2*) for **L3** and **L4**, kcal mol^{-1}

Ligand	$Eu(NO_3)_3$	$Am(NO_3)_3$
L3	10.6	7.0
$\mathbf{L4_{rac}}$	10.3	6.9
$\mathbf{L4_{meso}}$	10.0	6.4



$\mathbf{L4_{rac}}$



$\mathbf{L4_{meso}}$

References

[S1] S. Hussain, F. Leipold, H. Man, E. Wells, S.P. France, K. R. Mulholland, G. Grogan and N. J. Turner, *ChemCatChem*, 2015, **7**, 579; https://doi.org/10.1002/cctc.201402797.

[S2] D. N. Laikov and Y. A. Ustynyuk, *Russ. Chem. Bull.*, 2005, **54**, 820; https://doi.org/10.1007/s11172-005-0329-x.

[S3] D. N. Laikov, *J. Chem. Phys.*, 2020, **153**, 114121; htps://doi/org/10.1063/5.0014639.

[S4] V. S. Petrov, P. S. Lemport, M. V. Evsiunina, P. I. Matveev, P. Kalle, Y. V. Nelyubina, S. A. Aksenova, A. D. Averin, A. A. Yakushev, V. A. Roznyatovsky, R. V. Zonov, V. G. Petrov, I. P. Gloriozov, Y. A. Ustynyuk and V. G. Nenajdenko, *Chem. Eur. J.*, 2024, e202403056; https://doi.org/10.1002/chem.202403056.

Optimized structures of ligands and complexes

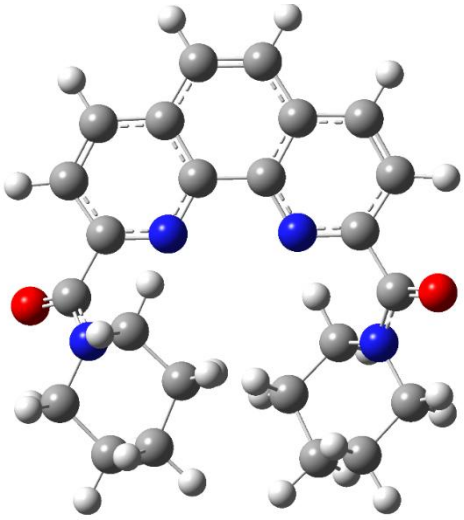


Figure S9. Optimized structure of **L1**

C	-0.53485060	-2.62501341	1.54971460
O	-2.05810025	-3.93192885	0.31339042
N	-0.11774921	-1.36498103	1.50487151
N	0.56927639	1.30391849	1.44946083
C	-0.68837597	-3.35495072	2.75263696
H	-1.08872500	-4.36917897	2.70892423
O	2.07374090	3.94208799	-0.15951335
C	-0.32430615	-2.75461290	3.93745686
H	-0.39150960	-3.29280192	4.88764168
C	0.13777489	-1.41704127	3.92905811
C	0.54443793	-0.73994312	5.12115888
C	0.98726672	0.55162005	5.07793412
C	1.03135273	1.27163783	3.84319080
C	1.48024403	2.61123981	3.76265462
H	1.82394615	3.11704831	4.66986786
C	1.48414072	3.25446536	2.54480294
H	1.85671011	4.27268754	2.42141307
C	0.98476027	2.56482277	1.41419525
C	0.61066825	0.64633777	2.63106796
C	0.19087409	-0.74867446	2.66907926
C	-1.00188905	-3.30017079	0.27205787
C	1.05775550	3.28936597	0.08120627
H	0.49946934	-1.28188463	6.07059706
H	1.30996571	1.06068199	5.99109022
C	1.11236687	-2.62462269	-0.94990602
C	-0.76692565	-3.70494323	-2.11856614
C	1.20833370	-1.54270297	-2.03174273
H	1.79636920	-3.46136961	-1.20129398
H	1.40097365	-2.21158461	0.02210522
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H	-0.14506881	-4.57187594	-2.41954710
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H	2.26151045	-1.22729955	-2.12679407
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H	-1.08110116	-3.09172205	-4.16527690
H	-1.45066123	-1.83710238	-2.95817222
H	0.67167520	-1.23815464	-4.12234158

H	1.35032778	-2.83797550	-3.76423443
C	-1.31974079	2.63520789	-0.49622025
C	0.13778152	3.77626632	-2.12095303
C	-1.75182128	1.61086358	-1.55137747
H	-2.03476181	3.48334213	-0.48771809
H	-1.30782453	2.17137543	0.49571369
C	-0.23572829	2.76713714	-3.21271590
H	-0.53522033	4.65554829	-2.17761796
H	1.17446306	4.13035457	-2.21140454
C	-1.63707619	2.18841350	-2.96901434
H	-2.78948930	1.29979870	-1.34154316
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H	0.51187493	1.95408426	-3.21652800
H	-1.86946795	1.41305149	-3.71873165
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N	-0.24974141	-3.15662137	-0.86349938

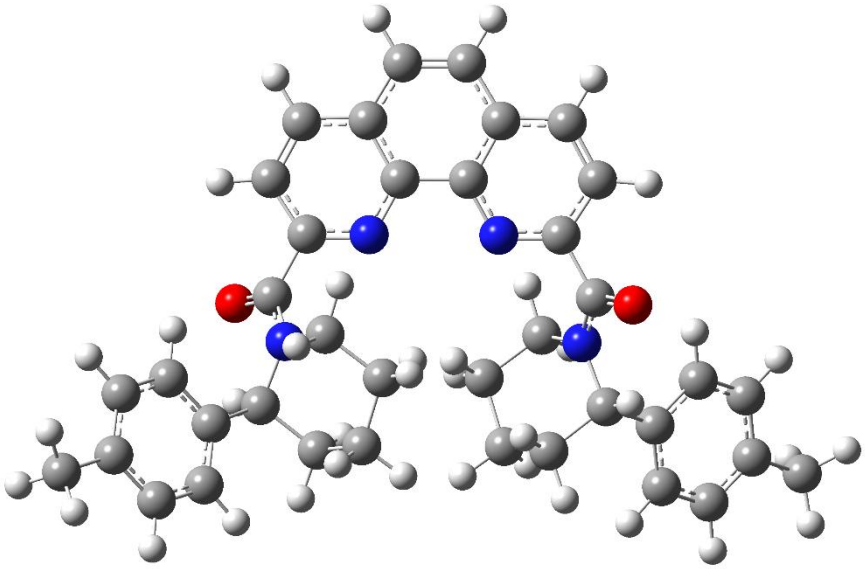

Figure S10. Optimized structure of **L2$_{rac}$**

O	0.84982387	4.19006935	1.34080634
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N	0.91858342	-3.12662726	-0.05973388
N	-0.16724715	1.18118897	2.53738858
C	-0.20815615	-1.80011864	4.74033146
N	-0.92373027	3.10491737	0.37113418
C	-0.04092640	-3.51304502	0.83651502
C	-0.08607662	3.18166122	3.89303444
H	-0.01653530	4.27087748	3.90361036
N	-0.01456762	-1.56559631	2.32127603
C	-0.21036926	0.19349587	6.13340122
H	-0.22747885	0.67280956	7.11680203
C	-0.44888159	2.61403453	-1.96943200
H	-0.27159656	3.04765724	-2.96724656
H	0.48025209	2.09054256	-1.68408335
C	-0.15794683	1.02376129	4.97037943
C	-2.26839594	5.58784562	-0.27189887

H	-1.93375277	5.44234389	0.75853533
C	2.05725545	-2.24252037	0.21113512
H	2.97974969	-2.78998961	-0.05866036
H	2.08923554	-2.01776467	1.28310795
C	-2.17733297	4.99960037	-2.59442537
H	-1.78595384	4.39872909	-3.41851114
C	-3.20016308	6.58258311	-0.55809525
H	-3.58716102	7.20574570	0.25460273
C	0.62130545	-2.26205260	-2.32011724
H	-0.32940602	-1.78431514	-2.02569906
C	-0.12663456	-1.01393368	3.55171092
C	2.40111061	-4.53081415	-3.18948000
H	2.07379237	-3.79892474	-3.93144186
C	-0.03593744	-2.88965867	2.22077620
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C	-0.24830706	-1.16735592	6.02201679
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C	3.35961600	-5.47656796	-3.56043008
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C	-3.11199789	5.99845795	-2.87955692
H	-3.43158756	6.15239203	-3.91511438
C	-1.74006935	4.77074350	-1.28397446
C	-0.66682317	3.73873259	-0.93655574
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C	-3.64718521	6.80506596	-1.86923882
C	-0.14702095	2.50408603	2.65227948
C	-1.89839600	1.05464872	-0.59912851
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C	3.81808713	-6.44226975	-2.65660396
C	3.28437241	-6.42020809	-1.36005412
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C	-0.04174173	3.34171853	1.39047374
C	1.95421388	-0.95405706	-0.61047160
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C	-0.12024875	2.43611991	5.05063875
C	-0.24366065	-3.20680974	4.59007853
C	-0.18637647	-3.75695051	3.32867254
H	-0.25022465	-4.83334465	3.15938301
C	-2.07334854	2.19470624	0.40855159
H	-2.97656320	2.78309808	0.16053062
H	-2.18522047	1.80048715	1.42477219
H	-0.11274999	2.91730703	6.03316730
H	-0.32239227	-3.83919574	5.47937535
H	-1.07050025	0.41396506	-0.25131095
C	-1.61381611	1.61263416	-2.00124978
H	-2.52098186	2.11285289	-2.38500818
H	-1.38061139	0.79081548	-2.69980583

H	0.52262813	-2.52816535	-3.38526008
C	1.78047432	-1.27746481	-2.10162963
H	2.71674462	-1.71660432	-2.49026327
H	1.59767863	-0.35237959	-2.67481788
C	4.82974708	-7.48298744	-3.06779143
H	5.46032199	-7.78730459	-2.21803622
H	4.32849210	-8.39077276	-3.44670650
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C	-4.67856016	7.86368763	-2.17100748
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H	-5.69342369	7.51031470	-1.91862035
H	-4.49687990	8.77815328	-1.58425556

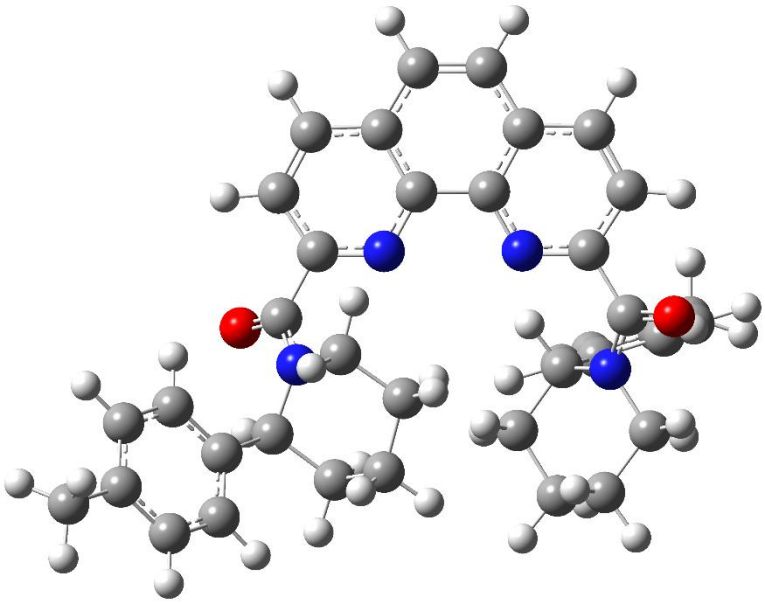

Figure S11. Optimized structure of **L2$_{meso}$**

O	0.60275362	3.81942955	1.09617706
O	-1.16743899	-4.80169393	-0.09998395
N	0.42877144	-3.35045907	-0.87651378
N	-0.38425890	0.73160249	2.12097348
C	-0.36830263	-2.39616619	4.10912034
N	-1.19628823	2.78551709	0.11737067
C	-0.38128390	-3.87496899	0.10071360
C	-0.21961602	2.63139373	3.60706610
H	-0.13610547	3.71648352	3.68988166
N	-0.28761151	-1.99552037	1.70632636
C	-0.28263414	-0.50571566	5.63707797
H	-0.24861872	-0.09689740	6.65135819
C	-0.77480340	2.40790609	-2.25417281
H	-0.63350270	2.88972027	-3.23569804
H	0.16975623	1.88622387	-2.02145460
C	-0.27157055	0.40378508	4.53379122
C	-2.50310126	5.33879048	-0.37928004
H	-2.09285662	5.18400495	0.62217407
C	1.52615634	-2.39153736	-0.64873249
H	1.29190106	-1.87826987	0.29666464
C	-2.58743018	4.76653537	-2.70668160

H	-2.26212925	4.16852016	-3.56099743
C	-3.44451980	6.34289962	-0.58967484
H	-3.76514748	6.96387771	0.25302094
C	0.26029046	-2.85585327	-3.29831703
H	-0.68938354	-2.30071634	-3.19453840
C	-0.33197235	-1.52919601	2.97639472
C	-0.32661349	-3.30855588	1.51117677
C	-0.32374900	-0.08853280	3.19483225
C	-0.34217774	-1.85484908	5.43235052
H	-0.36313725	-2.54677694	6.27957088
C	0.33507252	-3.93943250	-2.22181499
H	-0.55462486	-4.58443991	-2.21192212
C	-3.53246911	5.77486995	-2.91559057
H	-3.92665276	5.93851925	-3.92357127
C	-2.05752224	4.52521000	-1.43362643
C	-0.97344235	3.48183614	-1.16491202
H	-0.02337840	4.02535611	-1.01505320
C	-3.98375906	6.57914610	-1.86359467
C	-0.34283399	2.04310228	2.32631563
C	-2.17712236	0.77252615	-0.91602230
H	-3.08707351	0.14842266	-0.93319473
C	-0.28323188	2.96379911	1.12069407
C	1.48148534	-1.30835486	-1.75052902
H	0.57248927	-0.70788347	-1.57614882
H	2.33921674	-0.62914035	-1.62920336
C	-0.21183384	1.80656557	4.71025925
C	-0.42575454	-3.78798635	3.86220600
C	-0.43156569	-4.24845820	2.56463312
H	-0.51348452	-5.30825390	2.31962028
C	-2.34350811	1.87209844	0.13634017
H	-3.24976344	2.46912791	-0.07735953
H	-2.44272471	1.44052179	1.13855737
H	-0.15446345	2.21740670	5.72259771
H	-0.46920646	-4.48117796	4.70743425
H	-1.33846036	0.12753089	-0.60323290
C	-1.92483546	1.38877765	-2.30016541
H	-2.84753654	1.88637887	-2.64819409
H	-1.69140399	0.59823489	-3.03410923
H	0.25416710	-3.34169435	-4.28900147
C	1.44531858	-1.89360842	-3.16534792
H	2.38680709	-2.43574962	-3.36898727
H	1.37199640	-1.07970241	-3.90643907
C	2.88518217	-3.08272073	-0.49363125
C	4.07084871	-2.33257977	-0.48180572
C	2.99401672	-4.46347831	-0.27704928
C	5.30965696	-2.93985483	-0.27584610
C	4.23457582	-5.06969006	-0.07494959
C	5.41855937	-4.32137461	-0.07006449
H	4.03562511	-1.24965203	-0.62601607
H	2.09257415	-5.08086682	-0.26424777
H	6.21436667	-2.32373883	-0.27382324
H	4.28136437	-6.15203414	0.08271563
H	1.22112862	-4.57646546	-2.40466142

C	-5.02392339	7.64964104	-2.08188678
H	-5.10485429	7.91704822	-3.14646869
H	-6.01890290	7.30931992	-1.74655980
H	-4.78257711	8.56271812	-1.51476308
C	6.75563907	-4.97521677	0.17672944
H	6.92293072	-5.13792901	1.25550394
H	6.81759547	-5.95779173	-0.31708032
H	7.58091633	-4.34986315	-0.19672932

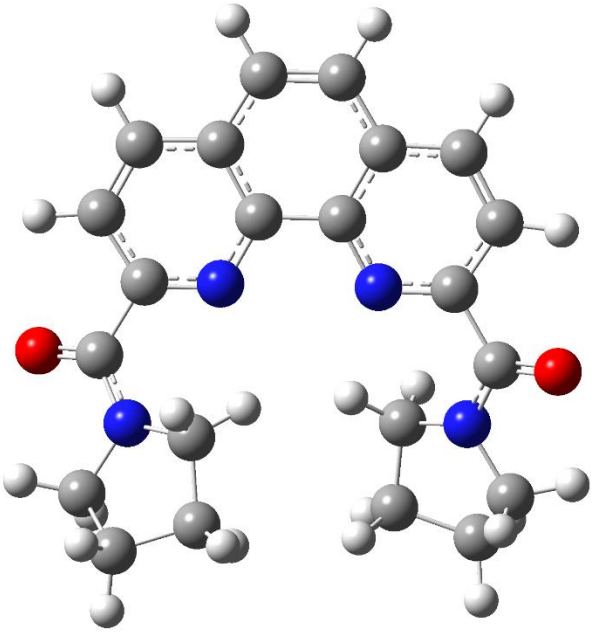

Figure S12. Optimized structure of **L3**

C	1.61228857	-2.48267690	0.17315241
O	0.57818318	-4.48594036	0.91357696
N	1.41032275	-1.17573152	0.06484509
N	0.99005356	1.54259239	-0.07022742
C	2.89849621	-3.06305063	0.28833082
H	2.96911894	-4.14345245	0.42277119
O	-0.80280795	4.44343712	-0.92569542
N	-0.74161062	-3.10676687	-0.32290672
C	4.00081369	-2.23918623	0.24059219
C	3.82270907	-0.84117446	0.11409935
N	-1.64347205	2.73711093	0.32139425
C	4.92325296	0.07033445	0.05675534
H	5.93879015	-0.33378305	0.10710512
C	4.71534357	1.41536726	-0.06056568
H	5.56146490	2.10727839	-0.11057374
C	3.39096023	1.95204254	-0.11838835
C	3.13877318	3.33860363	-0.24476206
C	1.83917340	3.79121345	-0.29304034
H	1.58062227	4.84257541	-0.42769879
C	0.78818863	2.84961105	-0.17829734
C	2.26093893	1.08301855	-0.05231952
C	2.48308095	-0.35389059	0.04737834
C	0.43595151	-3.43846550	0.27869241
C	-1.86260927	-4.06160278	-0.23595623
H	-2.35403464	-3.97646687	0.75034698

H	-1.48291608	-5.09108396	-0.32571819
C	-2.79791609	-3.63593697	-1.37411317
H	-3.84840522	-3.88425603	-1.16192646
H	-2.50790613	-4.14050302	-2.31092167
C	-2.54004173	-2.12511415	-1.48970027
H	-3.07106494	-1.58731952	-0.68586374
H	-2.85353351	-1.70008092	-2.45496205
C	-1.02559324	-2.01324680	-1.27854047
H	-0.48659160	-2.18584351	-2.22948737
H	-0.69656646	-1.04986765	-0.87118036
C	-0.62177488	3.40543806	-0.28523397
C	-3.00033991	3.30913710	0.23452766
H	-2.94831618	4.40571148	0.31754159
C	-3.05909064	1.26633347	1.50118338
H	-3.40580876	0.58885927	0.70226318
C	-1.58194150	1.61499410	1.28403230
H	-1.11758491	1.94796751	2.23172121
H	-3.44592630	3.07387571	-0.74915633
C	-3.76081793	2.62835260	1.37895583
H	-4.83780810	2.54692623	1.16997035
H	-3.63419111	3.20273139	2.31188030
H	-3.22723034	0.77241089	2.46990874
H	-0.97902117	0.79311080	0.87985731
H	3.98200707	4.03324232	-0.30482522
H	5.01438756	-2.64683534	0.30117856

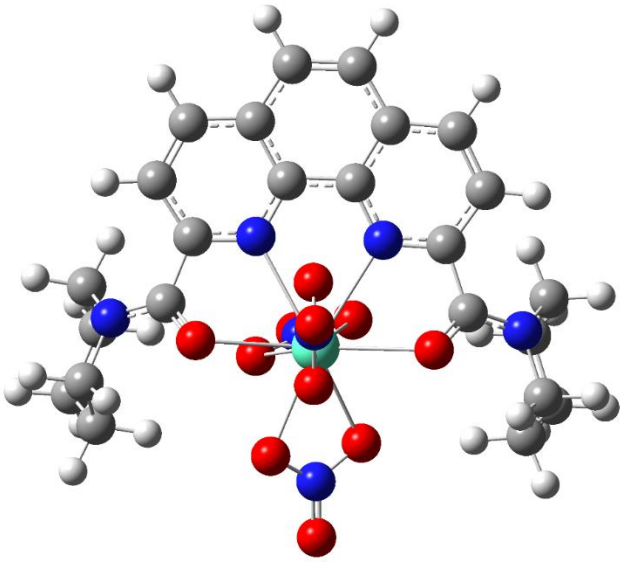

Figure S13. Optimized structure of **L1·Eu(NO$_3$)$_3$**

N	-1.39416599	1.27441701	-0.94977806
N	1.28651898	1.30734901	-0.82896117
O	-2.52385862	-1.07358244	-1.48134547
O	2.50039910	-0.98359781	-1.47491213
C	-2.72148677	1.21148216	-0.96065572
C	-3.52273775	2.35552307	-1.17078914
H	-4.60844666	2.26162055	-1.23540227
C	-2.90658325	3.58375054	-1.33496244
C	-1.49837069	3.67857051	-1.27066982

C	-0.76739051	4.90063136	-1.42811438
H	-1.32557110	5.82796939	-1.58394117
C	0.60029488	4.91434087	-1.39995972
H	1.14526385	5.85268877	-1.53563949
C	1.35084726	3.70963692	-1.20318599
C	2.76177866	3.64705631	-1.21228854
C	3.39731111	2.43104284	-1.03398281
H	4.48553534	2.35749895	-1.07906510
C	2.61731513	1.27099115	-0.83139984
C	0.65832453	2.48282022	-1.01652499
C	-0.78512311	2.46617105	-1.06818821
C	-3.21424544	-0.21942142	-0.89211446
C	3.15323550	-0.14780998	-0.82405039
Eu	-0.02495039	-1.02793554	-0.97914583
N	-0.00950995	-0.94146908	-3.88592903
O	-0.02428967	-2.03921938	-3.20576285
O	0.03412797	0.14476664	-3.18209055
O	-0.03329691	-0.92660905	-5.10353158
N	-0.08627260	-3.78314900	-0.03898215
O	-1.02318240	-2.92384299	0.23080163
O	0.87272626	-3.33299058	-0.76681447
O	-0.12282984	-4.92849286	0.37505257
N	0.31431187	-0.52818499	1.92087496
O	0.44544770	-0.32939158	3.11945394
O	1.25351134	-1.04365873	1.19907629
O	-0.77184184	-0.22441189	1.28879548
H	3.34229501	4.55812164	-1.38179008
H	-3.50058132	4.48225549	-1.52321334
C	-4.89758239	0.27832768	0.87712801
C	-4.83299674	-1.91428344	-0.25938480
C	-4.53450038	-0.38901319	2.21298209
H	-5.99500849	0.34644281	0.75949924
H	-4.48152738	1.29341280	0.83937268
C	-4.48143561	-2.62856956	1.04978169
H	-5.92857512	-1.88306953	-0.40570268
H	-4.36530600	-2.40757809	-1.12193290
C	-5.01250475	-1.84588659	2.25740229
H	-4.98459109	0.19954323	3.03096903
H	-3.43663210	-0.34708305	2.33329105
H	-4.90924199	-3.64502047	1.02145000
H	-3.38425982	-2.73904123	1.10582579
H	-4.67727002	-2.32104642	3.19438062
H	-6.11952103	-1.87068929	2.26179548
C	4.84147863	-1.80881112	-0.29782715
C	4.84173824	0.32786536	0.94992469
C	4.58004318	-2.59850636	0.98830991
H	5.92782878	-1.72601772	-0.48879821
H	4.35437436	-2.27952785	-1.16236530
C	4.58159679	-0.42613628	2.26375543
H	5.92696987	0.47746444	0.79509862
H	4.35821033	1.31348596	0.98268634
C	5.13909105	-1.85391455	2.20717065
H	5.03761101	-3.59719811	0.88897340

H	3.49097387	-2.74082988	1.09545848
H	5.04041283	0.14525549	3.08881434
H	3.49138539	-0.46119035	2.43466742
H	4.88008496	-2.39265230	3.13385364
H	6.24454172	-1.82196684	2.15029761
N	-4.36458468	-0.51402413	-0.24441010
N	4.31468689	-0.43467852	-0.19333103

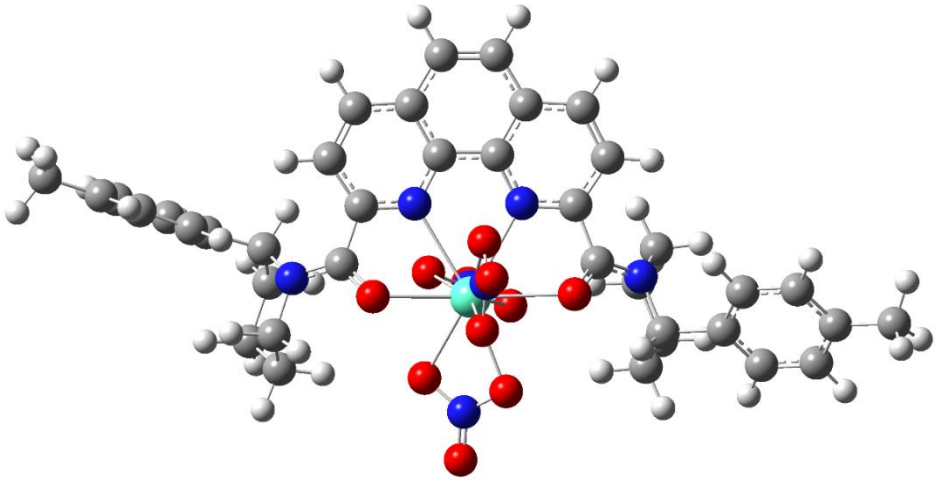

Figure S14. Optimized structure of **$L2_{rac}$•$Eu(NO_3)_3$**

N	-1.23708504	1.34397886	-0.76182451
N	1.43952122	1.14963261	-0.86035037
O	-2.57675950	-0.93336370	-1.15544145
O	2.42889630	-1.29651640	-1.12204665
C	-2.56775991	1.38158014	-0.77189451
C	-3.28114708	2.55208458	-1.11306435
H	-4.37167889	2.53496444	-1.15981342
C	-2.57778467	3.70375897	-1.41829231
C	-1.16572106	3.69012275	-1.39877894
C	-0.34878115	4.82477388	-1.71239132
H	-0.84047238	5.77112804	-1.95430163
C	1.01628767	4.73522230	-1.71719236
H	1.62609705	5.60989519	-1.95976847
C	1.67773939	3.49939327	-1.42121851
C	3.07959076	3.32592061	-1.44474800
C	3.62786019	2.09101292	-1.14521942
H	4.70989579	1.94170647	-1.16503806
C	2.76198868	1.01593745	-0.84289303
C	0.89738843	2.35411423	-1.10649464
C	-0.54324479	2.45489957	-1.07260254
C	-3.18312940	0.00469390	-0.60556171
C	3.17184362	-0.42797632	-0.62603770
Eu	-0.05560548	-1.06135385	-0.64651745
N	-0.07045237	-1.29308101	-3.54572476
O	-0.11227874	-2.30905506	-2.74964416
O	-0.05714893	-0.13553791	-2.96501408
O	-0.04659746	-1.41267898	-4.75761946
N	-0.14724470	-3.69613690	0.58987428

O	-1.08001160	-3.27508924	-0.18823462
O	0.83766809	-2.86777986	0.76791116
O	-0.17656770	-4.78906667	1.12784647
N	-0.36333168	-0.23135789	2.17903772
O	-0.48286190	0.10351443	3.34806205
O	0.73722204	-0.05737368	1.52330931
O	-1.32955544	-0.77103737	1.51240363
H	3.72451325	4.16970732	-1.70462193
H	-3.10577709	4.62092613	-1.69346166
C	-4.84846702	0.78700746	1.08018632
C	-4.96286327	-1.50336784	0.09249510
C	-4.60673346	0.20761114	2.48125973
H	-5.92604926	0.95448547	0.90446822
C	-4.74486641	-2.10152798	1.49358945
C	-5.24303699	-1.18059988	2.61536341
H	-5.02622498	0.90738917	3.22418361
H	-3.51805184	0.13707435	2.65082499
H	-5.21651132	-3.09633916	1.54364014
H	-3.65888524	-2.26137684	1.60706419
H	-4.98374205	-1.61762968	3.59419735
H	-6.34351702	-1.08816228	2.58082361
C	4.69193508	-2.14825053	0.17123084
C	4.90332691	0.18375146	1.05659601
C	4.35152614	-2.70185203	1.55640173
H	5.77888882	-2.20660047	-0.01063234
C	4.56404263	-0.36832679	2.46272901
H	4.37037211	1.14512970	0.96902984
C	4.98551381	-1.82979353	2.64569505
H	4.71892771	-3.74017158	1.61743584
H	3.25356919	-2.73595579	1.66850560
H	5.02270147	0.27858060	3.22727598
H	3.46917159	-0.28154239	2.58430185
H	4.67240310	-2.17811596	3.64409741
H	6.08726002	-1.91221790	2.60173311
N	-4.35729001	-0.14426037	0.04907940
N	4.30615374	-0.72441017	0.05088693
H	-4.36719503	-2.09419602	-0.62382529
H	-4.32479406	1.74624579	0.97623261
H	4.15916592	-2.69117125	-0.62071523
C	-6.40225044	-1.44342021	-0.41624786
C	-6.69397405	-0.70727038	-1.57567313
C	-7.45062950	-2.15072626	0.18432277
C	-7.98140793	-0.67400392	-2.10621869
H	-5.89216947	-0.15686195	-2.07652774
C	-8.74060157	-2.11756216	-0.35062977
H	-7.26891415	-2.74412562	1.08286607
C	-9.03300424	-1.38086589	-1.50423396
H	-8.17452720	-0.09264320	-3.01347384
H	-9.53891960	-2.67918811	0.14465282
C	-10.41896115	-1.37354765	-2.09907658
H	-10.51823085	-2.15547432	-2.87189651
H	-11.18488134	-1.56747965	-1.33257368
H	-10.64499576	-0.40810450	-2.57792997

C	6.38192738	0.44884902	0.77607114
C	7.22526039	0.97406754	1.76578509
C	6.92065731	0.26253478	-0.50525753
C	8.55440432	1.28918020	1.48461438
H	6.84474532	1.15105310	2.77455918
C	8.25148171	0.57705517	-0.78292294
H	6.28722202	-0.14264298	-1.29963248
C	9.09752766	1.09258096	0.20732405
H	9.18567972	1.69972050	2.27884682
H	8.64010212	0.41657210	-1.79347307
C	10.54522461	1.39938552	-0.08188241
H	11.18092661	0.52077351	0.12353945
H	10.69333820	1.67353715	-1.13765316
H	10.91272407	2.22563738	0.54593447

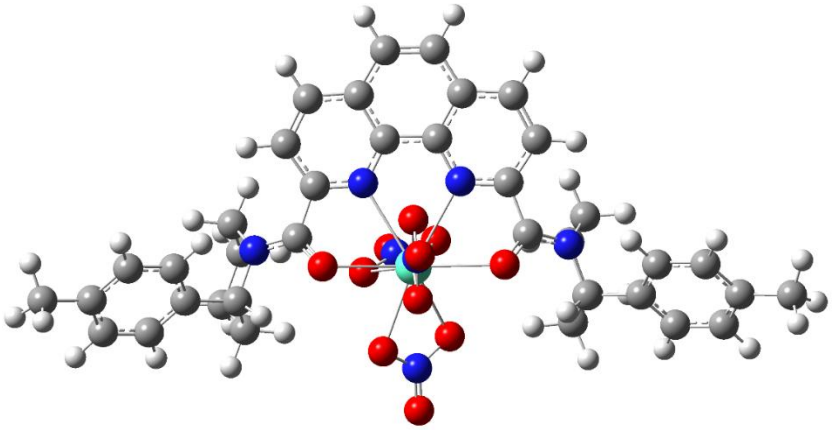

Figure S15. Optimized structure of **$L2_{meso}$•$Eu(NO_3)_3$**

N	-1.35458006	1.74415612	-0.70904432
N	1.32583890	1.75309047	-0.55946796
O	-2.51588918	-0.62945154	-0.99808370
O	2.51225526	-0.61116640	-0.93035762
C	-2.68246391	1.69937119	-0.72925103
C	-3.46367466	2.82278605	-1.07986850
H	-4.55013555	2.73842853	-1.14537624
C	-2.82658636	4.01501114	-1.37589557
C	-1.41790236	4.09684081	-1.30444827
C	-0.66682211	5.28237673	-1.59206529
H	-1.20914607	6.19353261	-1.85933957
C	0.70054257	5.27968153	-1.55024884
H	1.26136514	6.18830590	-1.78632247
C	1.43026297	4.09488269	-1.20831264
C	2.84005743	4.01137607	-1.19621764
C	3.45545972	2.81551266	-0.87166256
H	4.54295219	2.72295706	-0.89500835
C	2.65582337	1.69829997	-0.54301860
C	0.71728222	2.90787512	-0.88867347
C	-0.72565696	2.90590013	-0.95507612
C	-3.19869468	0.29172446	-0.50745572
C	3.17070490	0.28205781	-0.36566053
Eu	-0.02134918	-0.56702745	-0.47340562

N	0.03186170	-0.79218241	-3.37201426
O	-0.00824614	-1.81040574	-2.57870706
O	0.08372849	0.36250418	-2.78724632
O	0.02324998	-0.90694851	-4.58436303
N	-0.13742403	-3.20495061	0.75275605
O	-1.06685111	-2.31033385	0.91180807
O	0.83875078	-2.84750753	-0.00310925
O	-0.19592370	-4.29792130	1.28770598
N	0.29124161	0.23053123	2.36081422
O	0.41224411	0.55250643	3.53316606
O	1.22924978	-0.37341858	1.70930332
O	-0.78218105	0.48316377	1.68578136
H	3.43590122	4.88832348	-1.46381221
H	-3.40439558	4.89429496	-1.67336417
C	-4.88973167	1.01813933	1.17223095
C	-4.85242057	-1.31284654	0.28672385
C	-4.52076886	0.52770137	2.57922254
H	-5.98530202	1.06726614	1.04514129
H	-4.47241196	2.01826682	1.00033554
C	-4.52331676	-1.83417454	1.69746217
C	-5.02499444	-0.90186442	2.80836539
H	-4.95689440	1.22225615	3.31766859
H	-3.42145733	0.56717464	2.68703550
H	-4.92890084	-2.85265234	1.81220279
H	-3.42513276	-1.93277768	1.75530837
H	-4.67216789	-1.27143632	3.78577616
H	-6.12939945	-0.89791173	2.84216039
C	4.82733704	-1.34560805	0.36672234
C	4.85199875	0.94822613	1.35343625
C	4.54335194	-1.92597597	1.76347081
C	4.54477321	0.38797638	2.74941170
H	5.94167187	1.04105936	1.19818446
H	4.39751142	1.94109446	1.23998714
C	5.08211153	-1.04032326	2.89489057
H	4.94522545	-2.95052190	1.82171109
H	3.44710433	-2.01122796	1.85690896
H	4.99708091	1.05807666	3.50039197
H	3.45085813	0.39229598	2.89861213
H	4.77511775	-1.45776321	3.86847574
H	6.18676079	-1.02320832	2.88127048
N	-4.35625493	0.08667503	0.16084506
N	4.31758914	0.05198852	0.31286575
H	-4.24800900	-1.88784198	-0.43457790
H	4.20551537	-1.89456663	-0.36059625
C	-6.31365433	-1.37873539	-0.15403032
C	-6.70696664	-0.72837865	-1.33404314
C	-7.28247545	-2.12083204	0.53281102
C	-8.01652547	-0.81051406	-1.80258889
H	-5.96894372	-0.15239921	-1.90007723
C	-8.59379584	-2.20362663	0.06004093
H	-7.01964167	-2.65052632	1.45085275
C	-8.98802196	-1.55218789	-1.11503304
H	-8.29053321	-0.29367873	-2.72777821

H	-9.32797541	-2.78959815	0.62189951
C	-10.39712156	-1.67163118	-1.63923058
H	-10.50918325	-2.57781814	-2.25946371
H	-11.12590785	-1.74407420	-0.81702406
H	-10.66645472	-0.80741774	-2.26555688
C	6.27639303	-1.38526955	-0.11587181
C	7.26359702	-2.15899266	0.50531766
C	6.63760846	-0.67519012	-1.27241907
C	8.56247498	-2.21481490	-0.00665965
H	7.02641791	-2.73565153	1.40182513
C	7.93320053	-0.73075377	-1.77979087
H	5.88351669	-0.07469776	-1.78958939
C	8.92430258	-1.50417860	-1.15645352
H	9.31222251	-2.82721187	0.50401081
H	8.18068229	-0.16794907	-2.68558324
C	10.31821448	-1.58908038	-1.72613709
H	10.35742171	-2.30843177	-2.56237074
H	10.65217683	-0.61484842	-2.11656209
H	11.04127761	-1.92318452	-0.96659624

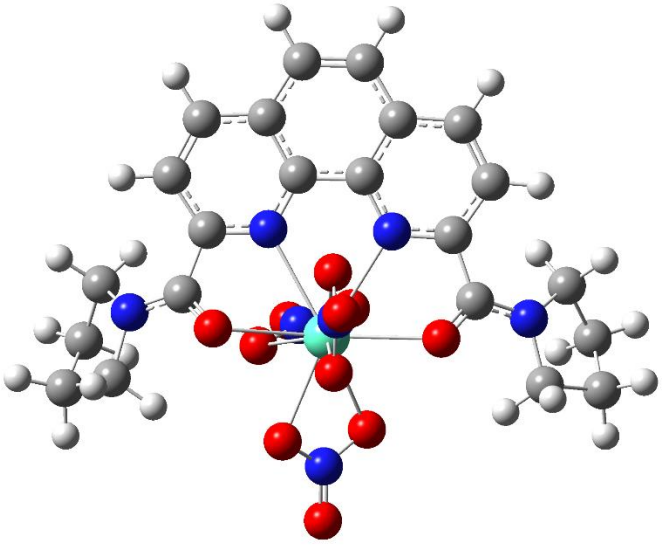

Figure S16. Optimized structure of **L3·Eu(NO$_3$)$_3$**

H	-4.46550131	3.31566811	-0.71893531
H	-3.47777200	-2.93646646	-3.32435012
N	-1.43908632	1.10169768	0.28113699
N	-0.09651148	3.87951303	2.05691862
N	-1.04306889	-1.34770739	-0.74998987
N	1.14012742	-4.09135866	-1.15178239
O	0.00474465	1.65450573	2.42379069
O	0.45450643	-3.00597119	0.72052002
C	-1.57537961	2.32275724	0.79217076
C	-2.66493487	3.15514207	0.45539644
H	-2.78638363	4.13066244	0.92747664
C	-3.60137677	2.69935250	-0.45642841
C	-3.44572496	1.42707205	-1.04806089
C	-4.35266447	0.87243551	-2.00892830
H	-5.21439075	1.46940374	-2.32000923
C	-4.15618086	-0.37824497	-2.52655125
H	-4.86018515	-0.79058945	-3.25470877

C	-3.03545403	-1.17832196	-2.12908316
C	-2.78728628	-2.48377657	-2.60739779
C	-1.68441975	-3.18630314	-2.15259719
H	-1.49161768	-4.20509481	-2.49367356
C	-0.82680196	-2.57773733	-1.21232629
C	-2.11075902	-0.65626663	-1.18405664
C	-2.32205319	0.66253537	-0.63045710
C	-0.50147909	2.61691833	1.81507170
C	0.31842276	-3.25502968	-0.49092472
C	-0.32318369	5.08302116	1.23179710
H	-1.17905378	5.66545773	1.62102389
C	0.98265141	5.87068892	1.40443599
H	1.74423826	5.47596550	0.71204609
H	0.84606218	6.94355392	1.20380008
C	1.37364972	5.56131411	2.85769820
H	0.76911783	6.16803026	3.55247116
H	2.43543386	5.75470686	3.06763482
C	1.03089523	4.07467985	3.00404787
H	1.86190414	3.41274118	2.70464277
H	0.72535068	3.78362036	4.02072620
C	2.33286715	-4.60076857	-0.42656657
H	2.03907943	-5.38820791	0.28486159
H	2.76637888	-3.76819158	0.15326577
C	3.26154923	-5.09045839	-1.54572880
C	2.87176800	-4.20515823	-2.73983335
C	1.34482014	-4.13359213	-2.61431026
H	3.19026375	-4.61072016	-3.71152997
H	3.28748059	-3.19185615	-2.61602426
H	3.06846285	-6.15170765	-1.77656448
H	4.31932974	-4.98734331	-1.26308525
H	0.91987622	-3.23890662	-3.09081101
Eu	0.53357255	-0.48613361	1.22236919
N	-1.28251946	-1.44405508	3.28205419
O	-0.00619730	-1.34024012	3.45067334
O	-1.71440721	-1.11681283	2.10575938
O	-2.02984881	-1.82220221	4.16698837
N	3.27523971	-0.45313212	2.19890356
O	2.65627742	0.61963916	1.81135619
O	2.58467698	-1.53761828	2.13545275
O	4.42875528	-0.42766666	2.59214926
N	1.91109276	0.15764186	-1.31937385
O	2.48145866	0.44676176	-2.36070538
O	2.01010513	-1.01043797	-0.77776301
O	1.15511322	1.00084960	-0.69458401
H	0.87114209	-5.03514814	-3.04580545
H	-0.52217209	4.80689049	0.18630683

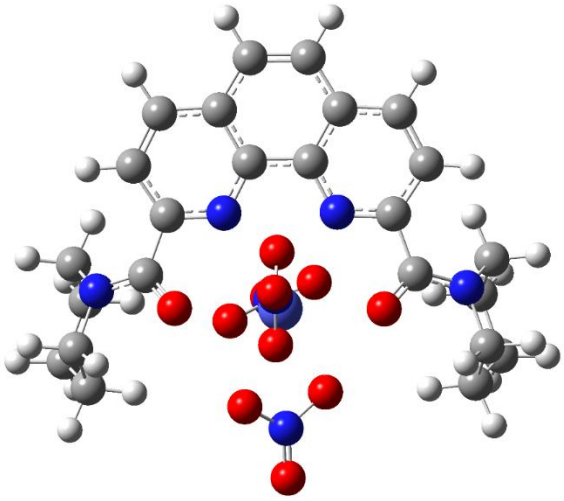

Figure S17. Optimized structure of **L1·Am(NO$_3$)$_3$**

N	-1.38734865	1.26914593	-0.93282690
N	1.29137935	1.30312736	-0.81347646
O	-2.48616974	-1.08864184	-1.38165637
O	2.46571726	-0.99489754	-1.40278712
C	-2.71973875	1.20583825	-0.93757935
C	-3.51882307	2.35198442	-1.14516755
H	-4.60417320	2.25739194	-1.21164151
C	-2.90460014	3.57997090	-1.30873998
C	-1.49477576	3.67641156	-1.24828207
C	-0.76652461	4.89650767	-1.40398118
H	-1.32515515	5.82394719	-1.55683029
C	0.60396877	4.91062770	-1.37989171
H	1.14772247	5.84945393	-1.51663403
C	1.35482754	3.70860778	-1.18799217
C	2.76779334	3.64697522	-1.20010782
C	3.40365900	2.43045852	-1.02695583
H	4.49154564	2.35858641	-1.08072481
C	2.62913328	1.26908687	-0.82120301
C	0.66281580	2.48013209	-1.00331829
C	-0.77896970	2.46264060	-1.05236511
C	-3.21208549	-0.21414920	-0.85860661
C	3.15738925	-0.14192948	-0.80570917
Am	-0.01706041	-0.99296514	-0.92295222
N	-0.01227018	-0.99903970	-3.83622893
O	0.02539949	-2.07378498	-3.11089685
O	-0.03401715	0.10972505	-3.16026165
O	-0.02460741	-1.02605826	-5.05020527
N	-0.08075021	-3.72413818	0.08230098
O	-1.01183629	-2.85560695	0.35167879
O	0.86012807	-3.27711991	-0.68407414
O	-0.09672163	-4.85687597	0.51995597
N	0.32007846	-0.49208516	1.98082872
O	0.42908063	-0.29731660	3.17885097
O	1.25400099	-1.03812834	1.27333626
O	-0.74313911	-0.15310980	1.31848246
H	3.34726819	4.55813898	-1.37094355
H	-3.49944971	4.47794838	-1.49586761

C	-4.96384076	0.27419351	0.84227498
C	-4.87159205	-1.90096789	-0.31891363
C	-4.62987839	-0.41085031	2.17717225
H	-6.05810478	0.33966240	0.69867157
H	-4.55112760	1.29106226	0.82843182
C	-4.54052450	-2.63588132	0.98408052
H	-5.96514698	-1.86329867	-0.47727959
H	-4.39772442	-2.38366981	-1.18421048
C	-5.09903890	-1.87148045	2.19163407
H	-5.10281040	0.16321478	2.99262331
H	-3.53574516	-0.36399779	2.32549968
H	-4.96502963	-3.65283037	0.93384470
H	-3.44426927	-2.74334576	1.05952025
H	-4.78060709	-2.35717717	3.12901331
H	-6.20567025	-1.90237055	2.17307007
C	4.85214031	-1.81493660	-0.33888738
C	4.91933357	0.32617561	0.89574925
C	4.61453208	-2.59641380	0.95701821
H	5.93407769	-1.74529281	-0.55750292
H	4.33827298	-2.28491874	-1.18794894
C	4.68570430	-0.41774167	2.22043582
H	6.00159546	0.45593827	0.70743477
H	4.45422577	1.31981641	0.93774988
C	5.21757349	-1.85490120	2.15669455
H	5.05544096	-3.60171961	0.84996456
H	3.52687830	-2.72374404	1.09390932
H	5.17633940	0.15015190	3.02946369
H	3.60040906	-0.43393857	2.42330147
H	4.97554342	-2.38483033	3.09294328
H	6.32124928	-1.84054031	2.06986739
N	-4.40079425	-0.50233347	-0.27658052
N	4.34489722	-0.43389358	-0.22657188

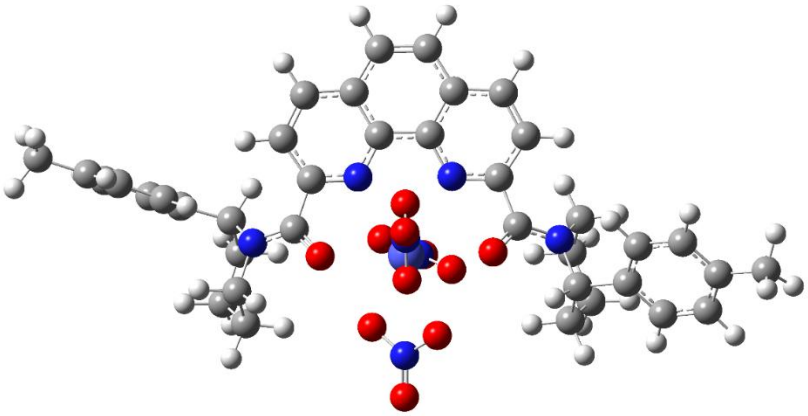

Figure S18. Optimized structure of **$L2_{rac}$•$Am(NO_3)_3$**

N	-1.25364216	1.35415863	-0.67107193
N	1.42253158	1.15869997	-0.76200901
O	-2.54983981	-0.92419314	-1.02652416
O	2.37166727	-1.28879810	-0.92752621
C	-2.59115980	1.39366937	-0.69117920

C	-3.29768230	2.56726335	-1.03035478
H	-4.38751535	2.55131787	-1.08963059
C	-2.59281168	3.72120928	-1.32241217
C	-1.17877402	3.70588509	-1.29806620
C	-0.36131710	4.83833134	-1.60519968
H	-0.85136382	5.78590374	-1.84537621
C	1.00631122	4.74650716	-1.61110343
H	1.61725582	5.62068469	-1.85213465
C	1.66414049	3.51105146	-1.32166866
C	3.06680049	3.33327956	-1.35217318
C	3.61327706	2.09775032	-1.05730944
H	4.69432256	1.94619727	-1.09304601
C	2.75027908	1.02257674	-0.74644012
C	0.88117659	2.36482836	-1.00972424
C	-0.55783328	2.46733692	-0.97720798
C	-3.19969922	0.02346946	-0.53291662
C	3.15741593	-0.40867785	-0.51105748
Am	-0.07608041	-1.00561419	-0.51454417
N	-0.06772692	-1.33339425	-3.41060757
O	-0.16156601	-2.31846731	-2.57251916
O	0.00570659	-0.15927610	-2.86049260
O	-0.05145206	-1.49409918	-4.61441717
N	-0.17352823	-3.60487696	0.79116188
O	-1.08067697	-3.19676424	-0.03562276
O	0.80417650	-2.76603646	0.97281665
O	-0.22732420	-4.67897285	1.35566845
N	-0.40791745	-0.16425421	2.30868696
O	-0.51650980	0.17118347	3.47514036
O	0.67625707	0.04295401	1.62659121
O	-1.36341576	-0.74018074	1.65517422
H	3.71219225	4.17494254	-1.61702417
H	-3.11863755	4.63982243	-1.59586604
C	-4.95391817	0.77761622	1.07109981
C	-5.00071414	-1.50425648	0.06258349
C	-4.75565635	0.18901126	2.47535727
H	-6.02645944	0.92933883	0.85600254
C	-4.82469114	-2.11396054	1.46477897
C	-5.37454874	-1.20981476	2.57597700
H	-5.21209495	0.87593369	3.20849243
H	-3.67283930	0.13428576	2.68462024
H	-5.28549247	-3.11476597	1.48921176
H	-3.74141873	-2.26304869	1.61431346
H	-5.14391072	-1.65130060	3.55988619
H	-6.47428452	-1.13284878	2.50312886
C	4.70499351	-2.13768175	0.21113471
C	4.98667938	0.19492953	1.06894493
C	4.42003607	-2.68021997	1.61309204
H	5.78245793	-2.20860404	-0.01700729
C	4.71133950	-0.34535490	2.49380449
H	4.46147378	1.16190429	1.00285055
C	5.11826814	-1.81217172	2.66580633
H	4.77426295	-3.72359066	1.66352964
H	3.32798701	-2.69588256	1.77623919

H	5.21747035	0.29862599	3.23039072
H	3.62579617	-0.24119844	2.67098287
H	4.84906537	-2.14997153	3.68041395
H	6.21508833	-1.91159091	2.56870093
N	-4.40896573	-0.13826436	0.05272651
N	4.32972279	-0.71069799	0.09842283
H	-4.37495843	-2.08354050	-0.63695066
H	-4.44198787	1.74535095	0.99526973
H	4.13400480	-2.68130654	-0.55298490
C	-6.42221010	-1.45436392	-0.49499921
C	-6.68346819	-0.70309138	-1.65194752
C	-7.48100434	-2.18526669	0.05725462
C	-7.95207637	-0.67814529	-2.22656156
H	-5.87259814	-0.13278685	-2.11442534
C	-8.75189939	-2.16034793	-0.52188130
H	-7.32252578	-2.79078085	0.95212611
C	-9.01409869	-1.40863138	-1.67314855
H	-8.12163819	-0.08412536	-3.13027708
H	-9.55917027	-2.74036486	-0.06374095
C	-10.37872559	-1.40949871	-2.31543319
H	-10.44469067	-2.18771128	-3.09550452
H	-11.16885739	-1.61436122	-1.57685053
H	-10.59635296	-0.44313211	-2.79619649
C	6.45260584	0.44002983	0.71432665
C	7.35247811	0.95518779	1.65846957
C	6.92231644	0.24461525	-0.59259995
C	8.66957975	1.25204670	1.30877914
H	7.02689274	1.13903577	2.68508197
C	8.24110260	0.54092055	-0.93880306
H	6.24296531	-0.15243078	-1.35228521
C	9.14365469	1.04649921	0.00568998
H	9.34610814	1.65536884	2.06867220
H	8.57497755	0.37406959	-1.96769793
C	10.57810353	1.33445110	-0.35892105
H	11.21163089	0.44635759	-0.19105014
H	10.67319394	1.61115876	-1.42012303
H	10.98996457	2.15295534	0.25121367

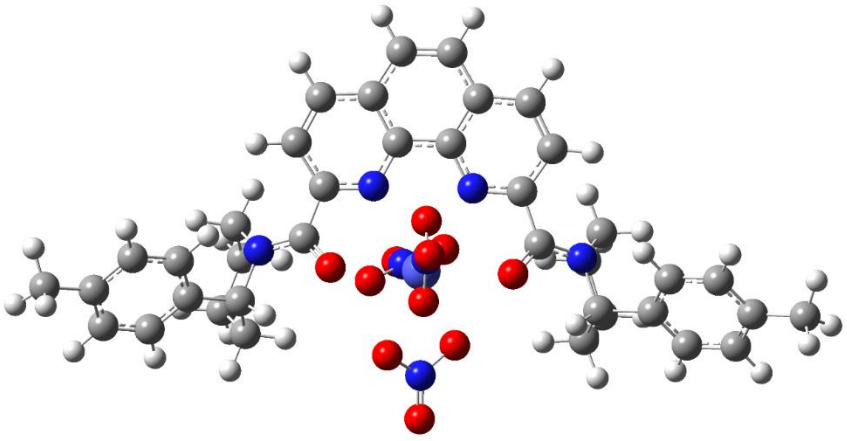

Figure S19. Optimized structure of **$L2_{meso}$•$Am(NO_3)_3$**

N	-1.35055762	1.74975850	-0.65682595
N	1.32839220	1.76125137	-0.50397570
O	-2.47464824	-0.62846444	-0.84229374
O	2.47487671	-0.60239247	-0.81771089
C	-2.68357584	1.70319951	-0.67936127
C	-3.46118545	2.82473159	-1.04430155
H	-4.54649107	2.73803826	-1.12127914
C	-2.82541655	4.01545499	-1.34401070
C	-1.41584981	4.10134898	-1.26636190
C	-0.66754981	5.28446449	-1.55497163
H	-1.21007832	6.19338095	-1.82894268
C	0.70237081	5.28378017	-1.50873248
H	1.26225691	6.19190352	-1.74858704
C	1.43200632	4.10373723	-1.16167942
C	2.84393534	4.02229059	-1.14699538
C	3.45977202	2.82662118	-0.82287479
H	4.54714496	2.73526377	-0.85211824
C	2.66551402	1.70849849	-0.49061854
C	0.71934251	2.91570060	-0.84109060
C	-0.72174470	2.91153775	-0.91068278
C	-3.19659574	0.30871666	-0.43229324
C	3.17344463	0.30084553	-0.30729503
Am	-0.01229183	-0.51409374	-0.37232233
N	0.02758932	-0.84514445	-3.26685193
O	0.03678397	-1.83258648	-2.42644188
O	0.01606355	0.33243565	-2.71840876
O	0.03110100	-1.00631457	-4.47049461
N	-0.12424951	-3.11620262	0.92691539
O	-1.04871805	-2.21390870	1.08422275
O	0.83155286	-2.76679370	0.12869734
O	-0.15845062	-4.19251256	1.48815997
N	0.30154639	0.29964788	2.46033657
O	0.40368063	0.62537003	3.62998431
O	1.23284060	-0.33719921	1.82836111
O	-0.74907948	0.57948301	1.75248258
H	3.43872426	4.89897693	-1.41671212
H	-3.40315855	4.89111933	-1.65153269
C	-4.97360566	1.04237763	1.15262577
C	-4.87297340	-1.29896274	0.30587802
C	-4.65188308	0.57758298	2.58001238
H	-6.06404964	1.07298809	0.98380102
H	-4.56527502	2.04615863	0.98294678
C	-4.58618094	-1.79633743	1.73455628
C	-5.14233205	-0.85610930	2.81240746
H	-5.12545278	1.27641082	3.29085105
H	-3.55835138	0.63577640	2.72943547
H	-4.98023497	-2.81917027	1.85009612
H	-3.48925660	-1.87595568	1.83263322
H	-4.82147083	-1.20587055	3.80786817
H	-6.24703698	-0.86845417	2.80412048
C	4.84405603	-1.34367994	0.35509258
C	4.92812462	0.94670530	1.34257374
C	4.58917770	-1.92490500	1.75726687

C	4.65209853	0.38783666	2.74587036
H	6.01400342	1.02215004	1.15596789
H	4.48640884	1.94650691	1.24387867
C	5.17067191	-1.04898493	2.87509441
H	4.97907544	-2.95466591	1.80271861
H	3.49463889	-1.99708704	1.87881307
H	5.13444817	1.04963609	3.48542183
H	3.56281777	0.40902853	2.92557441
H	4.88457614	-1.46349635	3.85618845
H	6.27459819	-1.04811210	2.83092316
N	-4.38896690	0.10427410	0.17563351
N	4.34889682	0.05986294	0.31758729
H	-4.23814752	-1.87874503	-0.38451933
H	4.19844536	-1.88533865	-0.35645416
C	-6.31727902	-1.38982708	-0.18346084
C	-6.67975945	-0.75411874	-1.38106668
C	-7.29780411	-2.14125336	0.47632885
C	-7.97135713	-0.85957701	-1.89300824
H	-5.93158058	-0.17041052	-1.92534743
C	-8.59085596	-2.24736484	-0.03994348
H	-7.05880545	-2.65986939	1.40712512
C	-8.95443840	-1.61082654	-1.23305939
H	-8.22142228	-0.35392772	-2.83103475
H	-9.33502151	-2.84003636	0.50137472
C	-10.34318082	-1.75544068	-1.80321484
H	-10.42807927	-2.68079017	-2.39890773
H	-11.10054306	-1.80785088	-1.00561072
H	-10.59468016	-0.91225197	-2.46451479
C	6.27995251	-1.39791409	-0.16374096
C	7.27102679	-2.19151516	0.42539630
C	6.62279030	-0.68048496	-1.32134417
C	8.55602498	-2.26019016	-0.11900522
H	7.04786042	-2.77381348	1.32188054
C	7.90472138	-0.74874435	-1.86085385
H	5.86511753	-0.06292907	-1.81247118
C	8.89960138	-1.54265161	-1.27014060
H	9.30936588	-2.88798152	0.36704252
H	8.13809399	-0.17956844	-2.76637268
C	10.27775459	-1.64108397	-1.87486286
H	10.28640735	-2.35311208	-2.71817740
H	10.61528198	-0.66789813	-2.26474886
H	11.01469022	-1.99193173	-1.13651796

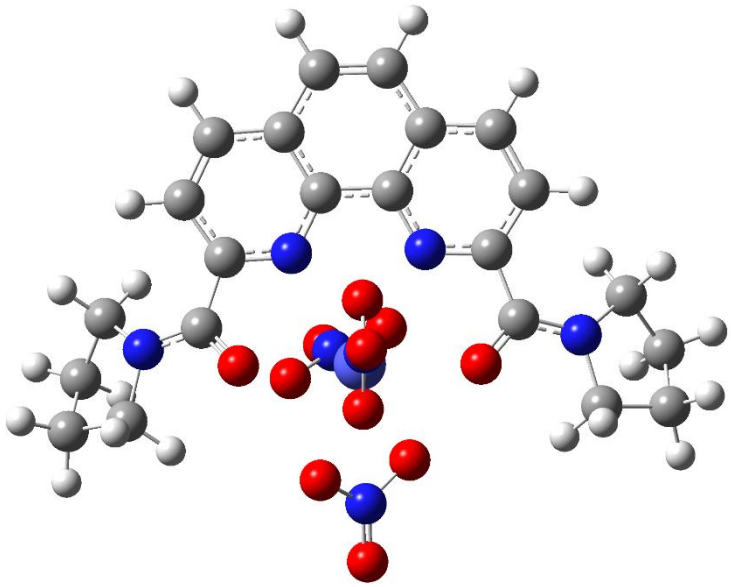

Figure S20. Optimized structure of **L3•Am(NO$_3$)$_3$**

N	-1.35877688	0.99580267	-0.65072305
N	-4.40032959	-0.76373141	0.04158066
N	1.33059525	1.04852409	-0.63442641
N	4.39756316	-0.65484223	-0.05792650
O	-2.38395830	-1.41332550	-0.73258916
O	2.48362129	-1.28705958	-1.08973563
C	-2.69495671	0.92530588	-0.63554731
C	-3.49884476	2.06233006	-0.87262674
H	-4.58431134	1.97422740	-0.91849626
C	-2.89283806	3.28600842	-1.08685418
C	-1.48302326	3.39015093	-1.05705388
C	-0.76760895	4.60932303	-1.26206726
H	-1.33668624	5.52737093	-1.43239643
C	0.60345545	4.63538046	-1.26062403
H	1.13751825	5.57418048	-1.43153116
C	1.36534364	3.44440987	-1.05187919
C	2.77877523	3.39554485	-1.07942586
C	3.43022642	2.18882016	-0.89495464
H	4.51851204	2.13277908	-0.95055152
C	2.66932384	1.02340375	-0.67109568
C	0.68616028	2.21396488	-0.82702730
C	-0.75883369	2.18435884	-0.83512503
C	-3.17081560	-0.48300690	-0.43909234
C	3.19856185	-0.38167110	-0.60624408
C	-5.32708551	0.13418717	0.75820030
H	-6.06849568	0.56685493	0.06065506
C	-6.01843188	-0.80441046	1.75672674
H	-5.38228578	-0.92730335	2.64860807
H	-6.99811135	-0.41780289	2.07416524
C	-6.10151109	-2.12533056	0.97693098
H	-6.92709367	-2.08578204	0.24675975
H	-6.25802349	-2.99921173	1.62556978
C	-4.75056655	-2.18997824	0.25694983
C	4.79577525	-2.07998688	0.06388561

C	6.00070583	-2.04005056	1.01128473
C	5.71736676	-0.80886547	1.88602972
C	5.16076038	0.19996096	0.87288472
H	6.60655651	-0.42457301	2.40735711
H	4.93884366	-1.04181363	2.63082940
H	6.93622676	-1.89874993	0.44421818
H	6.08835554	-2.96935846	1.59256830
Am	0.05754594	-1.24452161	-0.44240777
N	-0.09728063	-1.58873097	-3.33260684
O	-0.01162514	-2.57160047	-2.49100172
O	-0.09840224	-0.40938289	-2.79000775
O	-0.17007987	-1.75723648	-4.53358422
N	0.08271838	-3.82832855	0.89410476
O	-0.83107102	-2.93377223	1.12425719
O	0.95939192	-3.48358656	0.00601554
O	0.11103048	-4.89895669	1.46797015
N	0.64215105	-0.38605329	2.32645728
O	0.84426449	-0.03214019	3.47417073
O	1.50691736	-1.05133940	1.63464703
O	-0.46121734	-0.10527124	1.70072377
H	5.98412557	0.71455715	0.34285651
H	4.50435653	0.95212043	1.33379895
H	-4.77710766	0.95076909	1.24824615
H	-3.96358141	-2.66149898	0.87092500
H	3.94556622	-2.64677035	0.48092982
H	3.34639422	4.31071734	-1.26766936
H	-4.78126566	-2.72155716	-0.70658413
H	5.02096031	-2.49882732	-0.92905060
H	-3.49545051	4.17537544	-1.28940104

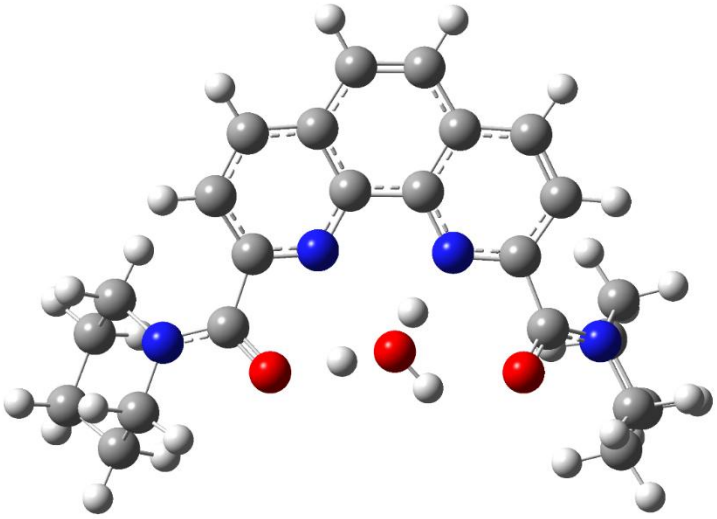

Figure S21. Optimized structure of **[L1•H_3O]$^+$**

O	-0.20374949	-3.38064721	-0.12778957
O	2.92492495	0.50242438	0.38998701
N	-0.86054230	-0.96881654	-1.33484026
N	0.80122871	1.11847281	-1.10701520
C	-1.69607889	-2.00832987	-1.37758856
C	-2.67429859	-2.11758060	-2.39196648
H	-3.30936879	-3.00351515	-2.44300660

C	-2.78413506	-1.12036989	-3.34604866
H	-3.51209161	-1.20931728	-4.15722071
C	-1.93716779	0.00917914	-3.28514123
C	-1.94241817	1.07581412	-4.24461644
H	-2.68348693	1.05097640	-5.04807777
C	-1.02210875	2.08815226	-4.18884166
H	-1.02131700	2.87228701	-4.95086538
C	-0.03791339	2.13365132	-3.14784938
C	1.00666205	3.08394801	-3.06675620
H	1.10242510	3.85008971	-3.84099331
C	1.92874735	3.01681168	-2.03353861
H	2.77341226	3.70745811	-2.01005316
C	1.77032871	2.01907300	-1.04115881
C	-0.05484231	1.13657502	-2.13600547
C	-0.98802439	0.03404266	-2.23102499
C	2.74340380	1.70833546	0.08506458
C	-1.38750389	-3.10669684	-0.36158150
H	2.13222042	-0.59396640	-0.10039785
O	1.59041613	-1.40961256	-0.54437004
H	1.44749912	-2.22745946	-0.01043289
H	0.59238538	-1.11541206	-0.76079302
N	3.42475319	2.69610221	0.69909929
C	4.50773847	2.35278157	1.64425320
C	3.04147845	4.11893207	0.71027364
C	4.15623076	2.76792637	3.07540571
H	5.41186264	2.89119969	1.30595439
H	4.68247095	1.27293355	1.56216222
C	2.67586832	4.57128366	2.13250430
H	3.89274844	4.71295332	0.32966600
H	2.18453912	4.27019989	0.04277824
C	3.79110669	4.25544311	3.13461731
H	5.02048532	2.54928007	3.72399005
H	3.31265094	2.15234625	3.43372298
H	2.46813608	5.65395974	2.10229510
H	1.74216218	4.06571126	2.43627667
H	3.47436908	4.53432059	4.15255115
H	4.68346026	4.86452249	2.89917532
N	-2.43395832	-3.77383958	0.19681325
C	-3.81809611	-3.28405052	0.29128568
C	-2.14984573	-4.95625579	1.03101339
C	-4.20493227	-3.01171054	1.75335595
H	-4.49245465	-4.04784273	-0.13978151
H	-3.92200058	-2.36346270	-0.29728413
C	-2.50084815	-4.70793053	2.50089208
H	-2.75641910	-5.79132986	0.63439059
H	-1.08590151	-5.19346482	0.90019739
C	-3.95275779	-4.23569721	2.64084557
H	-5.26810074	-2.71919502	1.77942516
H	-3.61741067	-2.15230458	2.12258092
H	-2.33614668	-5.64116841	3.06448115
H	-1.81241595	-3.94956746	2.91357440
H	-4.18085621	-3.99483011	3.69182167
H	-4.63652308	-5.05281321	2.34458505

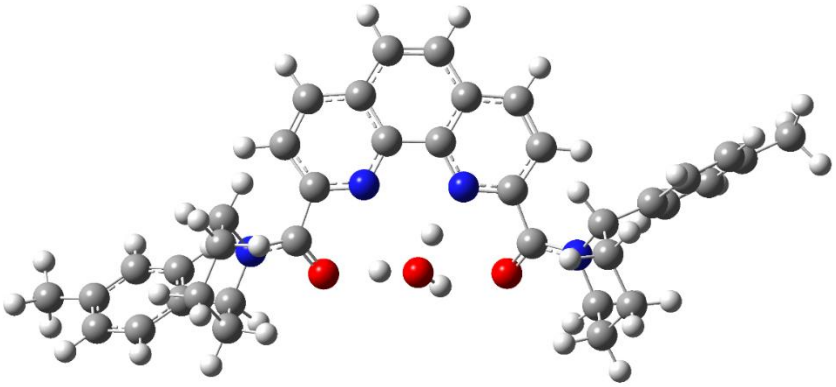

Figure S22. Optimized structure of **[L2$_{rac}$•H$_3$O]$^+$**

N	-1.29092197	1.16406895	-0.23718132
N	1.37702495	0.87141297	-0.39276356
O	-2.53425119	-1.18951058	-0.36989435
O	2.40183283	-1.65694139	-0.98952787
C	-2.61357740	1.18472239	-0.31818829
C	-3.31234193	2.31953676	-0.79718253
H	-4.39533733	2.29851632	-0.93021618
C	-2.59301358	3.45403741	-1.13619607
C	-1.18146206	3.44910548	-1.05219454
C	-0.34436768	4.54584072	-1.43826781
H	-0.81272094	5.48632107	-1.74094184
C	1.01746827	4.41555519	-1.45946070
H	1.64636993	5.25205818	-1.77557590
C	1.65204930	3.17629103	-1.11536163
C	3.03853579	2.94038609	-1.24512013
C	3.55566298	1.68698258	-0.97012928
H	4.62107073	1.48416010	-1.10141822
C	2.68761704	0.65753476	-0.54272587
C	0.85609797	2.08735598	-0.67247099
C	-0.58344029	2.23610324	-0.61473830
C	-3.21882692	-0.18781101	-0.05394848
C	3.11069966	-0.80726788	-0.42789146
H	3.69473217	3.74353469	-1.59170841
H	-3.10895339	4.34403344	-1.50669447
C	-5.18461519	0.74607230	1.18806482
C	-5.12260167	-1.64311974	0.45366811
C	-5.36164951	0.31985840	2.65242669
H	-6.16750907	0.91155271	0.71348331
C	-5.30746831	-2.08369979	1.91660286
C	-6.05571515	-1.04131873	2.75640281
H	-5.94631383	1.10006022	3.16796338
H	-4.36871522	0.27814526	3.13464256
H	-5.81775004	-3.05952907	1.93898093
H	-4.30170251	-2.24773568	2.34106665
H	-6.09544194	-1.36606067	3.80895482
H	-7.09814555	-0.94690000	2.40739282
C	4.71986554	-2.51283181	0.23578220
C	4.98145151	-0.17613862	1.12499567

C	4.71375746	-3.09654283	1.64963809
H	5.74459027	-2.53738657	-0.17165687
C	4.98795277	-0.77384284	2.55404836
H	4.37291926	0.74283759	1.17511521
C	5.52623554	-2.20638052	2.59471046
H	5.13397711	-4.11492065	1.60701212
H	3.67307121	-3.18407599	2.00885317
H	5.57279772	-0.11526336	3.21370359
H	3.94831545	-0.75896336	2.92639023
H	5.47710857	-2.59087505	3.62642306
H	6.58928138	-2.21479443	2.29504159
N	-4.47394630	-0.29971973	0.42982882
N	4.26180484	-1.10623028	0.22720435
H	-4.38692563	-2.31255464	-0.01936132
H	-4.60917078	1.67827073	1.14365058
H	4.05161820	-3.06173719	-0.44051766
C	-6.38133089	-1.62242467	-0.41518574
C	-6.34251133	-1.00391017	-1.67459910
C	-7.56974263	-2.26222054	-0.04095349
C	-7.44981933	-1.01747616	-2.52016251
H	-5.42644567	-0.50703104	-2.00696075
C	-8.67670007	-2.27637340	-0.89167809
H	-7.64807581	-2.76647612	0.92445718
C	-8.64153308	-1.65606523	-2.14675807
H	-7.38737249	-0.52647207	-3.49606378
H	-9.59119013	-2.78228859	-0.56785312
C	-9.82875668	-1.70036600	-3.07389034
H	-9.79631656	-2.60524048	-3.70475777
H	-10.77502937	-1.72459835	-2.51251082
H	-9.84588422	-0.82947598	-3.74639597
C	6.36159962	0.20726181	0.58662814
C	7.25502023	0.93298258	1.38904685
C	6.74923656	-0.06834198	-0.73239855
C	8.49090446	1.34760826	0.89542053
H	6.98670130	1.19523550	2.41574481
C	7.98942164	0.34557986	-1.22230237
H	6.07427963	-0.61673505	-1.39522143
C	8.88923020	1.05584493	-0.41739409
H	9.16300867	1.91462092	1.54641273
H	8.26222998	0.10889260	-2.25518955
C	10.24230830	1.47087372	-0.93404678
H	10.98550071	0.67362952	-0.76142629
H	10.21581776	1.66699005	-2.01664209
H	10.60589418	2.37597679	-0.42470506
H	0.42878763	-0.30761059	-0.09244304
O	-0.01759749	-1.28494475	0.00105044
H	0.58009643	-1.79871705	-0.60694468
H	-1.02875464	-1.22093047	-0.28299041

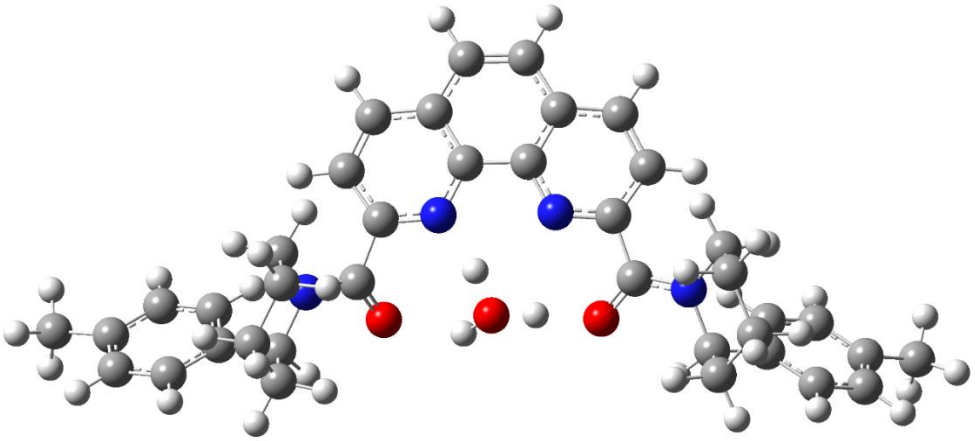

Figure S23. Optimized structure of **[L2$_{meso}$•H$_3$O]$^+$**

N	-1.32168287	1.49359408	-0.25021644
N	1.35513818	1.61578700	-0.07845622
O	-2.53175915	-0.98920387	-0.76722228
O	2.43637906	-0.82039848	-0.10208056
C	-2.63891962	1.35418808	-0.41431772
C	-3.43172292	2.40727899	-0.92245156
H	-4.50172440	2.25515047	-1.07664545
C	-2.83335415	3.60934574	-1.25512390
C	-1.43749435	3.76728471	-1.10288641
C	-0.71917960	4.94405566	-1.49806812
H	-1.28738511	5.80188099	-1.86744045
C	0.64799548	4.98727606	-1.46004613
H	1.18030185	5.87890159	-1.80227589
C	1.40708095	3.85991050	-1.00651462
C	2.81666600	3.76681596	-1.07207843
C	3.45447308	2.60436566	-0.67028545
H	4.53487101	2.50486000	-0.78813275
C	2.67658332	1.54287975	-0.14660839
C	0.72549821	2.71330908	-0.51620573
C	-0.71951264	2.65651953	-0.58716443
C	-3.16812943	-0.06640100	-0.23216002
C	3.18383622	0.14508656	0.18389525
H	3.39505167	4.60104634	-1.47835173
H	-3.42904333	4.42917425	-1.66598883
C	-4.95445968	0.74907556	1.33044472
C	-4.95851406	-1.59080567	0.44805076
C	-4.92341276	0.24193317	2.77833055
H	-5.99695096	0.91332499	1.00491556
H	-4.41200414	1.70019756	1.25147431
C	-4.95488397	-2.11708158	1.89473379
C	-5.58690265	-1.13475294	2.88992179
H	-5.43937868	0.97900589	3.41607342
H	-3.87348715	0.18758422	3.11755899
H	-5.45843323	-3.09634871	1.92451097
H	-3.90304355	-2.29876554	2.17664664
H	-5.48195256	-1.52358872	3.91596825
H	-6.66762033	-1.03263712	2.69257576
C	4.97288826	-1.41396486	0.79134477

C	5.19423294	0.99754463	1.41258681
C	5.10617419	-1.79505744	2.27649128
C	5.31930899	0.63204802	2.89863097
H	6.19300548	1.06795428	0.94772863
H	4.68873966	1.96537315	1.31351997
C	5.91344788	-0.76775369	3.07966748
H	5.54682186	-2.80156379	2.35328595
H	4.08554956	-1.86858982	2.69067146
H	5.94981962	1.39364548	3.38722360
H	4.31882586	0.68371465	3.36405535
H	5.91438130	-1.04315303	4.14691823
H	6.96506886	-0.76330600	2.74592757
N	-4.33896384	-0.23622168	0.42662379
N	4.42057318	-0.03114057	0.69381058
H	-4.27320275	-2.21253091	-0.15100058
H	4.19842796	-2.05236631	0.33778717
C	-6.31189858	-1.55357316	-0.26290674
C	-6.41242503	-0.92142355	-1.51222965
C	-7.45694033	-2.18182389	0.24243129
C	-7.61196142	-0.90887386	-2.22075866
H	-5.53189107	-0.44045487	-1.94837983
C	-8.65729482	-2.16916535	-0.47082045
H	-7.42732870	-2.69879220	1.20382510
C	-8.76130850	-1.53363504	-1.71436521
H	-7.65733658	-0.41030116	-3.19377540
H	-9.53462463	-2.66671967	-0.04667112
C	-10.05086382	-1.54992788	-2.49415330
H	-10.12209068	-2.46312230	-3.10962320
H	-10.92427164	-1.53624013	-1.82455804
H	-10.12041399	-0.68712429	-3.17356903
C	6.24124561	-1.52270617	-0.05639096
C	7.37963717	-2.21717339	0.36979660
C	6.25875122	-0.97116346	-1.34773256
C	8.49427788	-2.34857856	-0.46176109
H	7.41250284	-2.67383301	1.36115253
C	7.37262282	-1.10166551	-2.17335043
H	5.38097327	-0.43528614	-1.72046597
C	8.51584505	-1.79527732	-1.74729767
H	9.36923828	-2.89537188	-0.09792270
H	7.35402254	-0.66132205	-3.17498193
C	9.70828532	-1.96176778	-2.65357723
H	9.54574382	-2.79128599	-3.36288766
H	9.89028369	-1.05313938	-3.24801465
H	10.61908474	-2.18916110	-2.08000325
H	-0.46188979	0.26532211	0.10385419
O	-0.08429239	-0.73675585	0.23402617
H	-0.70725881	-1.23337159	-0.36227756
H	0.93355379	-0.75076641	-0.03626387

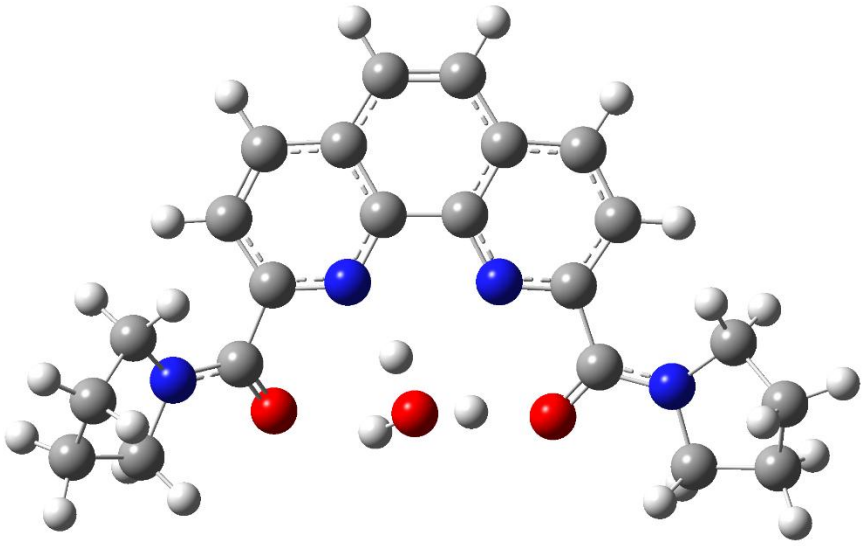

Figure S24. Optimized structure of **[L3•H_3O]$^+$**

H	-4.25572992	3.11864498	-0.24002127
H	-3.05365614	-2.97686466	-3.08613396
N	-0.97362093	1.15023035	0.39938294
N	0.08359670	3.88912059	2.41914737
N	-0.50323071	-1.23959481	-0.74482591
N	1.60686649	-4.11705783	-1.07208946
O	0.26925391	1.67158667	2.84794541
O	1.40457357	-2.55910535	0.53317422
C	-1.21988690	2.27748881	1.07225768
C	-2.40568735	3.01298841	0.85967652
H	-2.60693042	3.90999585	1.44608016
C	-3.32739330	2.56606412	-0.07088553
C	-3.08667837	1.36985616	-0.78131676
C	-4.00971394	0.79858701	-1.71906372
H	-4.92597770	1.34872298	-1.94938837
C	-3.77439077	-0.42003394	-2.29412496
H	-4.50142476	-0.85168361	-2.98736176
C	-2.59232917	-1.16605777	-1.97845059
C	-2.33138282	-2.47739083	-2.43473143
C	-1.18596751	-3.14182543	-2.02534584
H	-1.02386346	-4.17276767	-2.33753462
C	-0.27278962	-2.47351537	-1.17548390
C	-1.62177130	-0.60178042	-1.10633179
C	-1.87487403	0.68771742	-0.49278103
C	-0.21647565	2.59474429	2.17541491
C	0.97402799	-3.05988059	-0.53352843
C	-0.17251256	5.07247514	1.56860595
H	-1.11423999	5.56836866	1.86559060
C	1.02114852	5.98508492	1.87877568
H	1.89342555	5.68036777	1.27784549
H	0.79759573	7.03894763	1.65895440
C	1.27145019	5.71322196	3.37028378
H	0.53608259	6.25729986	3.98489789
H	2.27722646	6.01016524	3.69909936
C	1.05602620	4.19982409	3.49566167
H	1.98205502	3.62749520	3.31747697

H	0.65278860	3.88779357	4.47081787
C	2.80806347	-4.65314894	-0.38145436
H	2.53999358	-4.98139181	0.63362471
H	3.55497775	-3.84700357	-0.28808700
C	3.28338901	-5.78509023	-1.29795174
C	2.83430107	-5.32072547	-2.69114477
C	1.45107822	-4.71666968	-2.41620862
H	2.78280780	-6.13501055	-3.42799731
H	3.51313011	-4.54312213	-3.07736575
H	2.78452560	-6.73070830	-1.03067872
H	4.36916948	-5.93850941	-1.22519024
H	1.15966890	-3.95430413	-3.15269341
H	0.68642072	-5.51391603	-2.39511940
H	-0.23922550	4.78717628	0.50886629
H	0.31940491	0.29397252	0.70702470
O	1.18296216	-0.12870340	1.15829579
H	1.02412328	0.16246697	2.09865803
H	1.16961923	-1.17454555	0.96573229

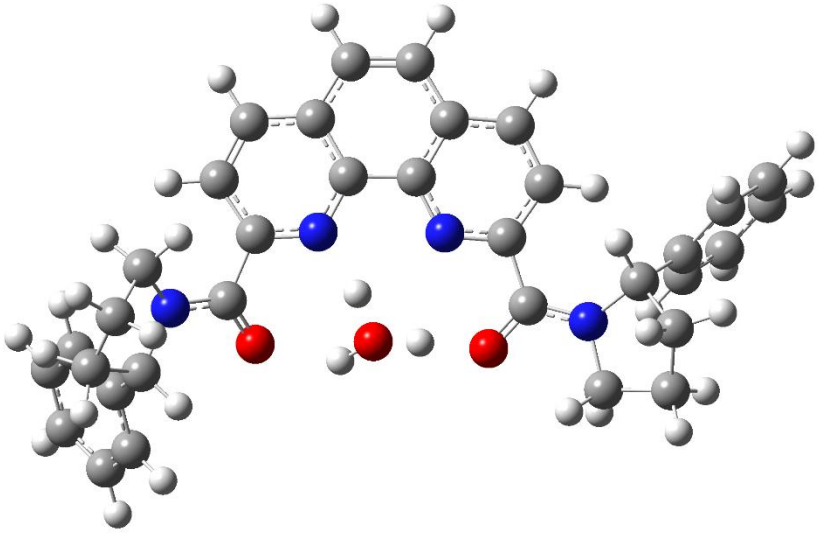

Figure S25. Optimized structure of **[L4$_{rac}$•H$_3$O]$^+$**

O	-3.09198290	-0.72143299	-0.32928751
O	1.72686243	-1.90481215	-0.10055252
N	-1.26284409	1.30545235	0.28285617
N	1.35927111	0.69248052	0.20173066
N	-4.68262785	0.42345924	0.82720094
N	3.91794336	-1.81384775	0.38051911
C	-2.57447059	1.55012998	0.22100299
C	-3.06723713	2.85405959	0.00037406
H	-4.14107741	3.02346946	-0.08619961
C	-2.17685354	3.90332689	-0.14323315
C	-0.78706511	3.65880850	-0.09251778
C	0.20830876	4.67221979	-0.29092996
H	-0.12073370	5.70574588	-0.42799025
C	1.53896434	4.35951638	-0.34039409
H	2.28243018	5.14122316	-0.51847758
C	1.98258675	3.00496851	-0.19270395
C	3.32180569	2.58347205	-0.34735001
C	3.64714496	1.23980874	-0.24659175

H	4.67133676	0.91533221	-0.43594013
C	2.62162454	0.31037480	0.04792361
C	1.03078871	1.98246587	0.07163953
C	-0.38021745	2.31416221	0.11825662
C	-3.46704046	0.31404886	0.23740966
C	-5.07119429	1.38223287	1.88436089
H	-5.71803144	2.17801391	1.47241644
H	-4.18395243	1.84665354	2.33715455
C	-5.86550328	0.50754798	2.86183923
H	-5.17359628	-0.04985233	3.51393892
H	-6.53690621	1.10590113	3.49501789
C	-6.61373248	-0.44210945	1.91844333
H	-7.48660728	0.06458949	1.47596547
H	-6.96888784	-1.35866996	2.40975736
C	-5.58775378	-0.76705446	0.80919459
H	-4.97790392	-1.64425155	1.08844841
C	-6.20296595	-1.02902185	-0.55097600
C	-6.85941875	-0.00986164	-1.25521133
H	-6.90032803	1.00214892	-0.84052231
C	-7.46263214	-0.27214460	-2.48509402
H	-7.97002481	0.53112768	-3.02500505
C	-7.42458014	-1.56150849	-3.02331812
H	-7.90155946	-1.76858923	-3.98422732
C	-6.77398571	-2.58226641	-2.32842140
H	-6.73741546	-3.59188544	-2.74462872
C	-6.16183169	-2.31404688	-1.10230840
H	-5.64153465	-3.11337080	-0.56622493
C	2.74551762	-1.20485814	0.10999928
C	3.91766367	-3.29678327	0.49991151
H	3.71927932	-3.75552128	-0.48070735
H	3.09890749	-3.59113270	1.17687119
C	5.30055085	-3.62733599	1.07009078
H	6.02388863	-3.80156564	0.25871679
H	5.27294256	-4.52347659	1.70555319
C	5.67170894	-2.35822866	1.84714675
H	6.74820699	-2.26642415	2.04686646
H	5.12713029	-2.31418359	2.80473278
C	5.16904535	-1.22592261	0.91846959
H	4.92105488	-0.32706611	1.50667501
C	6.19517398	-0.86727649	-0.15005672
C	7.30248045	-0.08912700	0.22333734
H	7.39515366	0.26477781	1.25549874
C	8.28737067	0.23793532	-0.70834228
H	9.14361827	0.84422275	-0.40286866
C	8.17916794	-0.20812315	-2.02880733
H	8.95099350	0.04653420	-2.75881277
C	7.07897065	-0.97695651	-2.40956784
H	6.98530753	-1.32693150	-3.44046256
C	6.09065461	-1.30317499	-1.47621080
H	5.22607805	-1.89457363	-1.78852405
H	4.09696508	3.31864530	-0.58025735
H	-2.54113203	4.91812646	-0.32558729
H	-0.73564811	-0.15634156	0.44844811

O	-0.63391518	-1.21915155	0.47414176
H	-1.40646274	-1.46325536	-0.10553461
H	0.33275576	-1.46084590	0.11193577

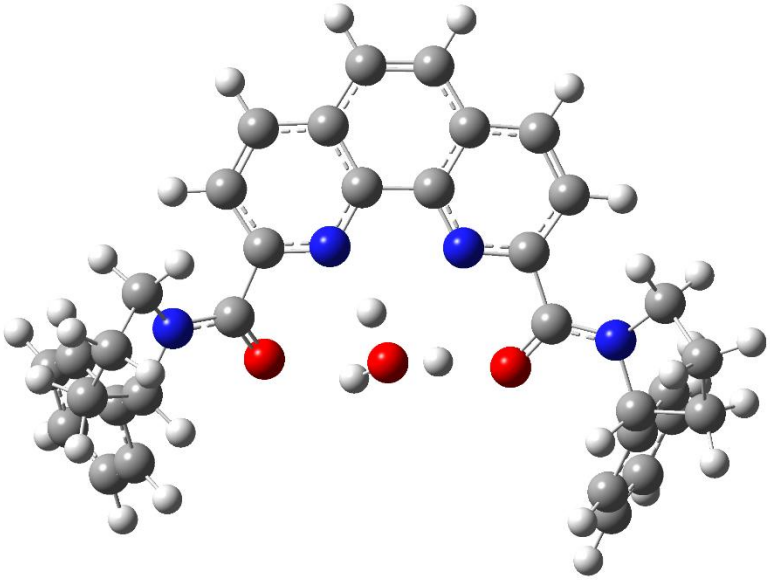

Figure S26. Optimized structure of **[L4$_{meso}$•H$_3$O]$^+$**

N	-1.31264404	1.60980583	0.00348644
N	-4.36614648	-0.11983493	0.67177641
N	1.36614531	1.82017284	0.13984002
N	4.54218615	0.33701280	0.89337250
O	-2.41227508	-0.95875354	-0.13916048
O	2.50980505	-0.55040973	0.47354830
C	-2.62676056	1.42513446	-0.14579302
C	-3.45221037	2.43205833	-0.69131443
H	-4.51615257	2.24331304	-0.83894492
C	-2.89342220	3.63882908	-1.07272815
C	-1.50301681	3.84435220	-0.93498121
C	-0.82630233	5.03433137	-1.36309846
H	-1.42393692	5.85913976	-1.76029609
C	0.53720007	5.13307868	-1.31236913
H	1.03769069	6.03706398	-1.66985548
C	1.33516130	4.04845571	-0.82263367
C	2.74786269	4.02163610	-0.85122686
C	3.43049655	2.89921418	-0.41042636
H	4.51660079	2.86092470	-0.49270546
C	2.69202984	1.80598131	0.10160741
C	0.69568074	2.88194242	-0.32103208
C	-0.74866120	2.77310719	-0.38674375
C	-3.12132426	0.01395075	0.15180005
C	3.25173531	0.45662896	0.52042902
C	-5.11131676	0.88928331	1.45555018
H	-5.91943478	1.33711999	0.84909668
C	-5.70557473	0.05999447	2.60030294
H	-4.94533458	-0.09900591	3.38223903
H	-6.57681974	0.55365936	3.05521678
C	-6.05666232	-1.25914064	1.90147409
H	-6.99400306	-1.15426158	1.33153104

H	-6.17559931	-2.10421397	2.59378358
C	-4.88283467	-1.50019719	0.92542004
C	5.06575647	-1.02466445	1.23526295
C	6.39709170	-0.71485654	1.95370020
C	6.19359262	0.68734069	2.53758169
C	5.42461798	1.40164791	1.42014760
H	7.13771195	1.19920022	2.77447342
H	5.57787702	0.64841118	3.45074537
H	7.21951636	-0.71179807	1.22015400
H	6.62303240	-1.47716490	2.71215931
H	6.12357727	1.74928388	0.63794201
H	4.83350733	2.25521725	1.77958193
H	-4.44202469	1.69029750	1.79962643
H	-4.07399754	-2.06481579	1.42179152
H	4.34467942	-1.48349089	1.93404354
H	-3.51595863	4.42473015	-1.50924153
H	3.29644328	4.87730997	-1.25417928
C	5.20904554	-1.93190079	0.02991744
C	5.86609935	-1.49637883	-1.12919156
C	4.73080114	-3.24551501	0.08492523
C	6.04002945	-2.35874878	-2.21160482
H	6.24432621	-0.47135643	-1.19124302
C	4.91375943	-4.11431742	-0.99280475
H	4.20755484	-3.59128818	0.98147851
C	5.56740744	-3.67230543	-2.14423977
H	6.55167329	-2.00689299	-3.11078111
H	4.53958837	-5.13920079	-0.93404111
H	5.70889278	-4.34964432	-2.98974007
C	-5.26772715	-2.23617359	-0.34243717
C	-4.80353180	-3.53681904	-0.56559043
C	-6.12491703	-1.65123153	-1.28512172
C	-5.19566034	-4.24715519	-1.70210380
H	-4.12461709	-3.99749976	0.15817024
C	-6.50990725	-2.35417611	-2.42658006
H	-6.49691538	-0.63393665	-1.12847198
C	-6.04866222	-3.65686332	-2.63595056
H	-4.82860091	-5.26397258	-1.86088703
H	-7.17741578	-1.88669642	-3.15464624
H	-6.35428367	-4.20982246	-3.52732607
H	-0.39001299	0.44112080	0.52413142
O	0.00943322	-0.50604827	0.79755818
H	-0.60195190	-1.09343598	0.27495446
H	1.03800781	-0.51676238	0.53067165