Electronic Supplementary Material (ESI) for Photochemical & Photobiological Science

Photophysics of 1,8-naphthalimide / Ln(III) dyads (Ln = Eu, Gd): napthalimide ⟶ Eu(III) energy-transfer from both singlet and triplet states. Supplementary information DFT calculations

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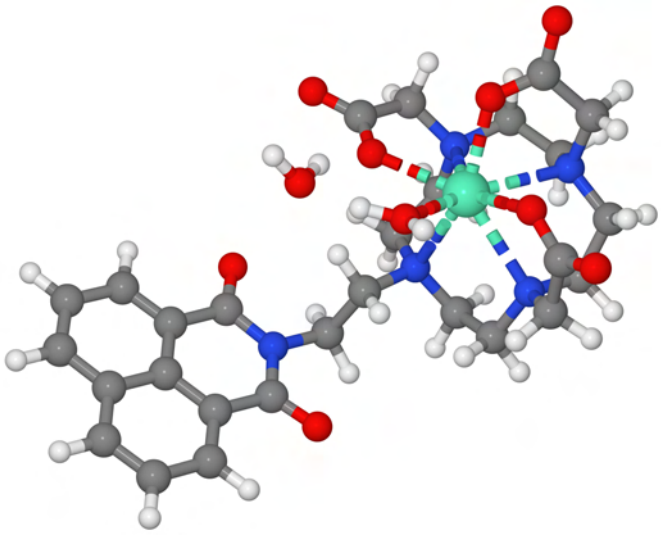
S1. EU·L UNBOUND STRUCTURE



SMILES	:	c1cc2cccc3c2c(c1)C(=O)N(C3=O)CC[N]45CC[N]67[Eu]4891([N](CC6)(CC[N]8(CC5)CC(=O)O9)CC(=O)O1)(OC(=O)C7)[OH2].O
Formula	:	$C_{28}H_{36}EuN_5O_{10}$
Charge	:	0
Multiplicity	:	1
Dipole	:	21.5360 Debye
Energy	:	-2825.03099634 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

80

C	-1.07745814	0.23644286	0.97559452
H	-1.07695115	1.17263854	0.40939188
H	-1.22637975	-0.57878888	0.26403868
H	5.54098320	0.80589169	-1.29237151
C	5.35274315	-0.09518553	-0.69878560
N	4.43779373	0.25857851	0.43415073
C	4.76537371	-1.12980354	-1.67933023
H	6.32510328	-0.45762399	-0.33696607
C	4.62520599	-0.67584866	1.59769058
C	4.65314817	1.68187690	0.87553585
O	5.54424047	-1.73742139	-2.47111654
O	3.45543003	-1.27328479	-1.64976597
C	4.01929331	-2.06664634	1.37758911
C	3.46374249	2.25259495	1.66001451
N	2.53213954	-2.03048182	1.14283669
N	2.17997527	2.30419779	0.87495530
O	2.85584903	1.74112892	-1.73515463
O	0.56076336	-1.90476918	-0.80761999
O	-1.33334756	-1.27614975	-2.43974185
C	1.80169976	-1.81595027	2.44004726
C	2.08535576	-3.29014468	0.47210732
C	1.00535333	2.45354605	1.80467522
C	2.21336937	3.42396092	-0.12174109

C	2.85565901	3.02921891	-1.46582890
C	0.82610077	-3.13314438	-0.38717857
C	0.36350706	-1.29963934	2.28458762
H	1.92256963	-4.10140419	1.19582808
H	2.87290740	-3.61698413	-0.21562116
C	0.65599436	1.15012085	2.53266454
H	1.18420279	3.72631454	-0.34935322
H	2.72825170	4.30815792	0.27873787
O	3.28822589	3.93811154	-2.23496127
O	0.14338222	-4.14995527	-0.69605994
N	0.27940106	0.03695942	1.59552348
H	-0.70389140	-1.78174555	-1.82595170
H	-1.58804214	-1.77808607	-3.23447680
H	4.18189764	-0.21296510	2.48328137
H	5.69909286	-0.79718012	1.81349695
H	4.48700571	-2.54455805	0.51371658
H	4.25864124	-2.68859553	2.25500178
H	2.38060212	-1.11153185	3.04361868
H	1.76664579	-2.75761509	3.01148582
H	-0.07310033	-1.24635792	3.29375577
H	-0.24205813	-2.00838828	1.71479785
H	1.50590384	0.81386173	3.13236856
H	-0.15242577	1.35875177	3.24807191
H	0.14830954	2.79074645	1.21421742
H	1.20087099	3.23351383	2.55752730
H	3.29255176	1.65953660	2.56144977
H	3.73170424	3.26560354	2.00121617
H	4.84362507	2.28920627	-0.01195095
H	5.54911947	1.75796664	1.51202607
Eu	1.96500278	0.00262658	-0.49252373
C	-2.26539469	0.24947949	1.97367096
H	-2.24465370	-0.63309342	2.61465812
H	-2.26526856	1.15032339	2.58829641
C	-4.14963770	1.46169364	0.90117353
C	-4.08344173	-1.04260707	0.89509016
C	-5.44203901	1.41727304	0.18194635
C	-5.37550879	-1.06511068	0.17617410
C	-6.02406645	0.16020647	-0.16152333
C	-6.08931303	2.60755420	-0.16017516
C	-5.95791483	-2.28736019	-0.16962230
C	-7.27840042	0.12782793	-0.85853589
C	-7.33112240	2.57986212	-0.84881330
H	-5.63114595	3.55451035	0.10749209
C	-7.19976902	-2.32374525	-0.85763168
H	-5.44921780	-3.20907211	0.09517553
C	-7.91605234	1.36275685	-1.19197881
C	-7.84885359	-1.13838029	-1.19649673
H	-7.82142305	3.51343656	-1.10611236
H	-7.63972950	-3.28128171	-1.11787355
H	-8.79902935	-1.16461527	-1.72364485
H	-8.86642647	1.34003925	-1.71911359
N	-3.55234504	0.22383007	1.23223972
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O	-3.45502877	-2.08912563	1.21568632
O	0.29984793	0.61240858	-2.11074805
H	-0.45347142	-0.01473666	-2.40952229
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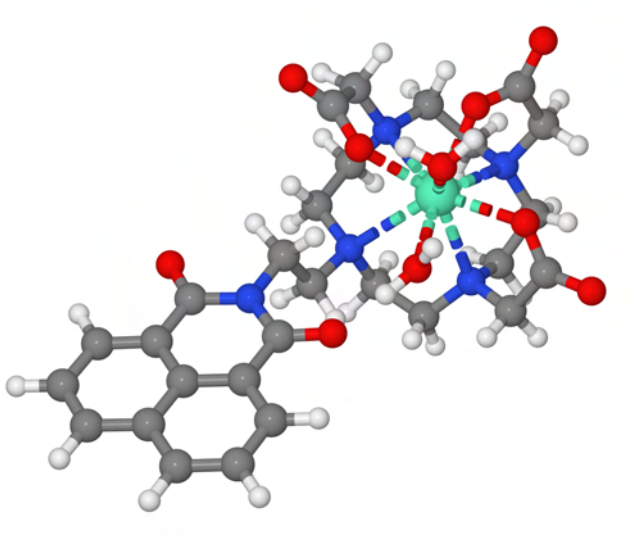
S2. EU·L SEMI-BOUND STRUCTURE



SMILES	:	c1cc2cccc3c2c(c1)C(=O)N(C3=O)CC[N]45CC[N]67[Eu]4891([N](CC6)(CC[N]8(CC5)CC(=O)O9)CC(=O)O1)(OC(=O)C7)([OH2])[OH2]	
Formula	:	$C_{28}H_{36}EuN_5O_{10}$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	26.3365	Debye
Energy	:	-2825.02609019	a.u.
Number of imaginary frequencies	:	0	

Cartesian Co-ordinates (XYZ format)

80

C	-1.36566484	-0.45820266	1.41192734
H	-1.90946567	-0.91902816	2.25453711
H	-1.52843678	0.61931860	1.47232044
H	5.44641161	1.34942198	-0.68769801
C	5.31625843	0.29103112	-0.43838081
N	4.34303331	0.18413337	0.69610941
C	4.83938885	-0.38837233	-1.73458993
H	6.30363798	-0.10687933	-0.16404028
C	4.55389738	-1.08812308	1.46656966
C	4.47005653	1.37407112	1.60775781
O	5.69161606	-0.67175573	-2.63042140
O	3.54351568	-0.58043075	-1.83715498
C	4.03717804	-2.33852053	0.74377948
C	3.23364258	1.58516693	2.48862863
N	2.55320930	-2.29878640	0.48572922
N	1.95895004	1.78936446	1.71553123
O	2.79847646	2.23553443	-0.88774174
O	0.69483227	-1.54891479	-1.46471584
O	1.19820046	0.59950691	-2.87667251
C	1.80849743	-2.61372232	1.75265205
C	2.18662000	-3.25964165	-0.60495085
C	0.77389491	1.51980782	2.60358906
C	1.89177811	3.17801952	1.15360570

C	2.61873937	3.33790779	-0.19592284
C	0.97783840	-2.83687711	-1.45965660
C	0.33505821	-2.19236231	1.74348009
H	2.00873685	-4.26992416	-0.21024974
H	3.02604532	-3.32663989	-1.30558741
C	0.53227848	0.02274729	2.83780241
H	0.84242135	3.42154908	0.95631438
H	2.28004193	3.92035913	1.86514342
O	2.95038414	4.50207853	-0.57729769
O	0.37337497	-3.71268535	-2.14562583
N	0.10976540	-0.71120435	1.58867848
H	0.84201366	-0.32410207	-2.90850401
H	2.02458000	0.66939545	-3.39382172
H	4.06243753	-0.98837644	2.43792892
H	5.62697411	-1.22985923	1.67552638
H	4.54623270	-2.45179796	-0.21561028
H	4.29981089	-3.21983576	1.35092688
H	2.33157063	-2.13650870	2.58472466
H	1.84595788	-3.69791150	1.94733727
H	-0.12243412	-2.54575419	2.68349504
H	-0.18467170	-2.70044303	0.92880321
H	1.43725801	-0.44397238	3.23083687
H	-0.23565668	-0.09154348	3.61992097
H	-0.10426328	1.97393012	2.13686943
H	0.90577078	2.01001883	3.58142471
H	3.10013318	0.72614628	3.15078545
H	3.41800547	2.45362663	3.14149213
H	4.64480305	2.25678468	0.98962504
H	5.34606791	1.26631355	2.26779962
Eu	1.89936948	0.15753283	-0.38084596
C	-1.98245144	-0.97507167	0.09454188
H	-1.45031226	-0.59349126	-0.77432340
H	-1.98212481	-2.06296110	0.05024959
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C	-3.68442845	0.77129436	-0.34736821
C	-5.81770182	-1.08633709	0.23297660
C	-5.09391880	1.18820369	-0.44554678
C	-6.12875366	0.25017256	-0.15509300
C	-6.84442520	-1.99235702	0.51641911
C	-5.41328669	2.49702239	-0.82028449
C	-7.50049496	0.65908515	-0.25164083
C	-8.20319366	-1.59293711	0.41962662
H	-6.58958101	-3.00561047	0.81079346
C	-6.76934576	2.90483761	-0.91723180
H	-4.61215687	3.19667482	-1.03619421
C	-8.52673912	-0.29067075	0.04283651
C	-7.79492044	2.00306416	-0.63844121
H	-8.98849678	-2.30852199	0.64125162
H	-7.00222540	3.92365742	-1.20971966
H	-8.83370018	2.31430888	-0.71217686
H	-9.56667519	0.01676577	-0.03057771
N	-3.41046739	-0.55183035	0.02032792
O	-4.06459570	-2.67562866	0.68863571
O	-2.72889233	1.57339227	-0.58343112
O	-0.08824786	1.56233442	-0.81548661
H	0.10958225	1.70206559	-1.77052093
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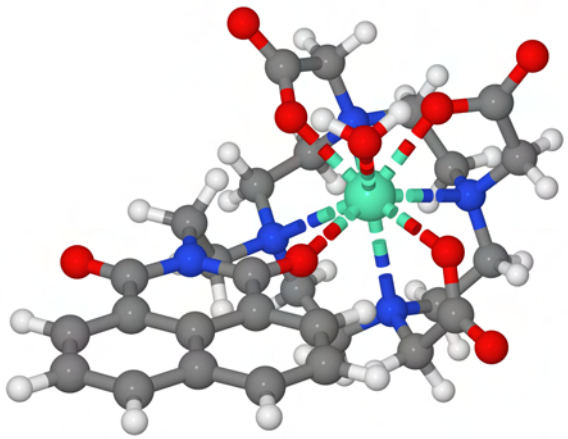
S3. EU·L BOUND STRUCTURE



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Formula	:	$C_{28}H_{34}EuN_5O_9$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	22.4941	Debye
Energy	:	-2748.58135236	a.u.
Number of imaginary frequencies	:	0	

Cartesian Co-ordinates (XYZ format)

77

C	0.85984123	2.13518786	1.87395108
H	0.87555695	3.03627014	2.50749207
H	1.41303253	1.36710978	2.41845345
H	-3.67634416	-2.90695310	-0.90627509
C	-4.10543013	-1.89983475	-0.86793077
N	-3.59070373	-1.20993173	0.35769615
C	-3.69684768	-1.22618878	-2.18802786
H	-5.19900942	-2.00891495	-0.84217173
C	-4.53529835	-0.12786761	0.79916519
C	-3.38764548	-2.20873475	1.46414161
O	-4.35038567	-1.48177791	-3.24253631
O	-2.62976909	-0.45610175	-2.13005257
C	-4.48197699	1.12861669	-0.07712359
C	-2.46905279	-1.69375157	2.57655573
N	-3.12314582	1.77850926	-0.10106407
N	-1.08363557	-1.32909358	2.11549497
O	-0.93422127	-2.40466046	-0.41946718
O	-0.71567494	1.88977551	-1.45069945
O	-0.03979275	-0.41508546	-2.56239319

C	-2.90822434	2.56970286	1.16049075
C	-3.00061202	2.65689135	-1.30792367
C	-0.44117251	-0.42406094	3.13100648
C	-0.25431854	-2.55852914	1.90181553
C	-0.41855502	-3.18301535	0.50223148
C	-1.55766177	2.84043074	-1.80026460
C	-1.44247472	2.88995862	1.49151659
H	-3.45479155	3.64359784	-1.13880920
H	-3.53703547	2.18386388	-2.13757086
C	-0.95359755	1.01853335	3.04293323
H	0.80386150	-2.28956294	1.99363935
H	-0.46109584	-3.32495904	2.66255856
O	-0.00536974	-4.36854029	0.31242549
O	-1.27095723	3.82980275	-2.53749704
N	-0.57917726	1.68123496	1.74370503
H	0.18705580	0.53400093	-2.69076920
H	-0.90956938	-0.58598924	-2.99978375
H	-4.30515909	0.12921423	1.83626330
H	-5.57091856	-0.50599337	0.79669917
H	-4.75474262	0.87709844	-1.10447657
H	-5.24259329	1.83688188	0.28919676
H	-3.36335039	2.01988959	1.98803055
H	-3.45092869	3.52676606	1.09421420
H	-1.44100547	3.54469705	2.38025427
H	-0.98617148	3.46169972	0.67946267
H	-2.03868675	1.04061711	3.15692639
H	-0.54661781	1.58986104	3.89338923
H	0.63893306	-0.44681552	2.96530962
H	-0.61610013	-0.80077624	4.15147114
H	-2.91464543	-0.81482506	3.04887795
H	-2.40932226	-2.46753573	3.35921979
H	-2.97121406	-3.11726356	1.02528012
H	-4.35301590	-2.48453355	1.91922045
Eu	-1.21677780	-0.11035576	-0.28552267
C	1.59542346	2.43315768	0.54666048
H	0.90861255	2.39037752	-0.30108294
H	2.05431128	3.42053652	0.58116150
C	4.05178928	1.97392654	0.29514149
C	2.38222551	0.14899077	0.03584730
C	5.12993908	1.00519001	0.00563957
C	3.45660424	-0.80461562	-0.27349240
C	4.81054115	-0.35508186	-0.27736136
C	6.46341467	1.42797971	0.00285671
C	3.15421152	-2.13941312	-0.56519085
C	5.86241198	-1.28446341	-0.57168263
C	7.50812674	0.51080698	-0.28276449
H	6.68944931	2.46723580	0.21987861
C	4.19242811	-3.05962110	-0.86108088
H	2.11967874	-2.46486807	-0.57080203
C	7.21413994	-0.82188314	-0.56674975
C	5.52245903	-2.64206719	-0.86172700
H	8.53755474	0.85441887	-0.28074613
H	3.94376802	-4.09140158	-1.08716083
H	6.31781006	-3.34799695	-1.08635473
H	8.01307964	-1.52447546	-0.78866756
N	2.71586061	1.47689092	0.28200984
O	4.26621532	3.18808222	0.54611301
O	1.16502869	-0.20524916	0.09711342

S4. WATER

SMILES	:	O
Formula	:	H_2O
Charge	:	0
Multiplicity	:	1
Dipole	:	2.6959 Debye
Energy	:	-76.42448812 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

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3

O -0.08857159 -1.10425389 0.00000000
H  0.88866001 -1.10137820 0.00000000
H -0.41206738 -0.18211494 0.00000000
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