

Electronic Supplementary Information:

Alkyl chain elongation and acyl group effects in a series of Eu/Tb complexes with hexadentate π -electronic skeletons and their enhanced luminescence in solutions

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14. References

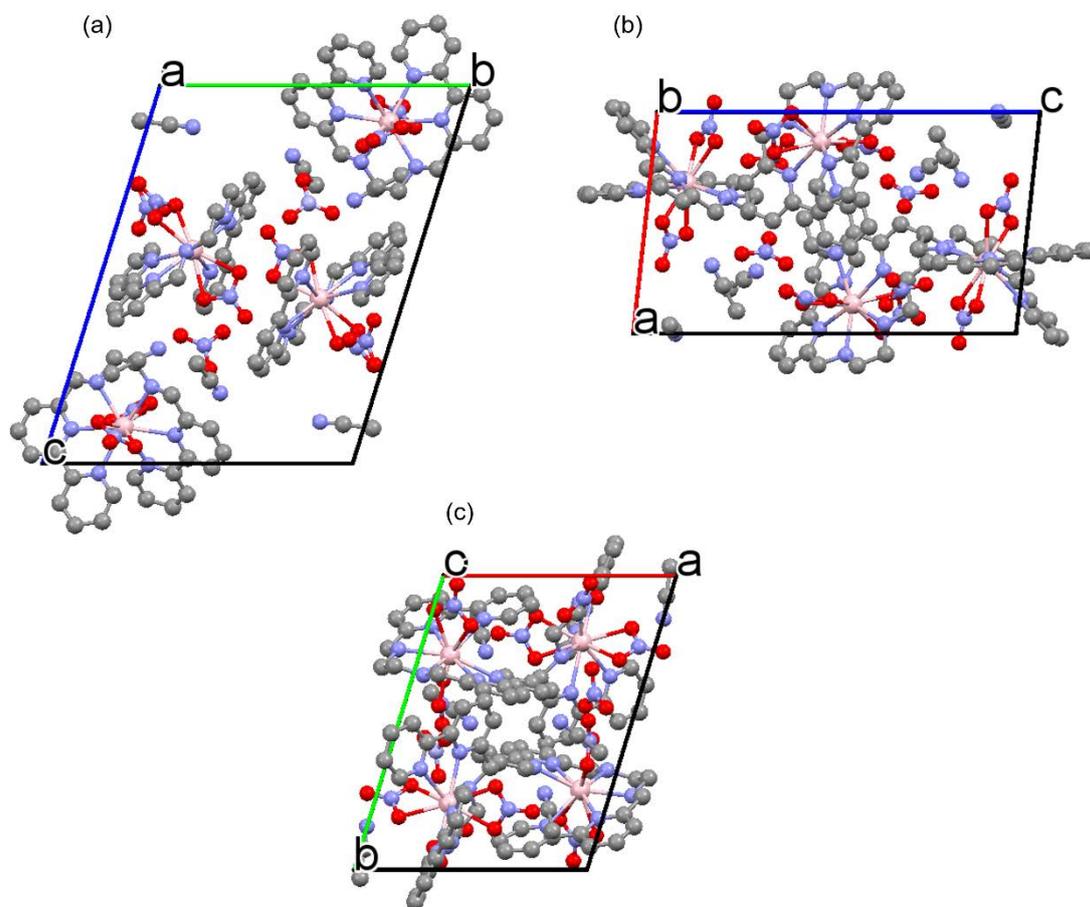


Fig. S1 Molecular packing structure of EuLH projected from *a*- (a), *b*- (b), and *c*- axis (c). Colouring atoms in grey, blue, red, and pink show carbon, nitrogen, oxygen, and europium, respectively. Hydrogen atoms are omitted for clarity.

Table S1. Selected bond lengths and bond angles for EuLH.

EuLH	
Eu(1)-N(1)	2.613(3)
Eu(1)-N(2)	2.589(3)
Eu(1)-N(3)	2.531(2)
Eu(1)-N(4)	2.553(3)
Eu(1)-N(5)	2.585(3)
Eu(1)-N(6)	2.608(2)
Eu(1)-O(1)	2.532(2)
Eu(1)-O(2)	2.567(2)
Eu(1)-O(4)	2.490(2)
Eu(1)-O(5)	2.563(2)
C(1)-C(24)	3.276(4)
Eu(2)-N(10)	2.577(2)
Eu(2)-N(11)	2.583(3)
Eu(2)-N(12)	2.551(3)
Eu(2)-N(13)	2.533(2)
Eu(2)-N(14)	2.597(3)
Eu(2)-N(15)	2.596(3)
Eu(2)-O(10)	2.543(2)
Eu(2)-O(11)	2.531(3)
Eu(2)-O(13)	2.543(2)
Eu(2)-O(14)	2.552(2)
C(25)-C(48)	3.370(5)
N(1)-Eu(1)-N(2)	62.27(8)
N(2)-Eu(1)-N(3)	62.94(8)
N(3)-Eu(1)-N(4)	66.67(9)
N(4)-Eu(1)-N(5)	62.46(8)
N(5)-Eu(1)-N(6)	62.31(8)
O(1)-Eu(1)-O(2)	50.07(7)
O(4)-Eu(1)-O(5)	50.55(7)
N(10)-Eu(2)-N(11)	62.94(8)
N(11)-Eu(2)-N(12)	62.00(9)
N(12)-Eu(2)-N(13)	66.8(1)
N(13)-Eu(2)-N(14)	62.67(9)
N(14)-Eu(2)-N(15)	62.26(8)
O(10)-Eu(2)-O(11)	50.55(7)
O(13)-Eu(2)-O(14)	50.10(7)

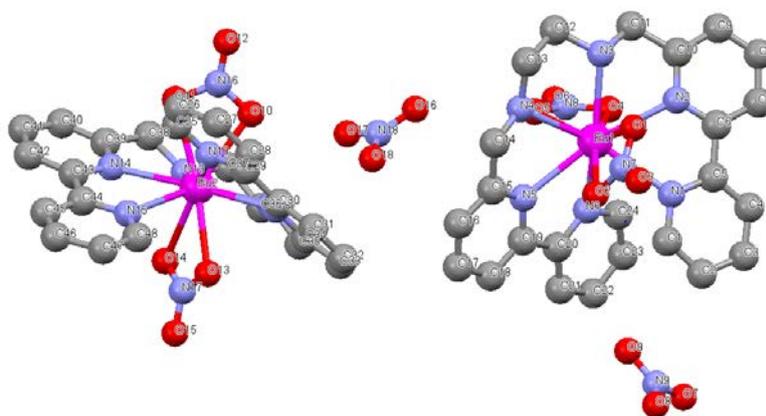
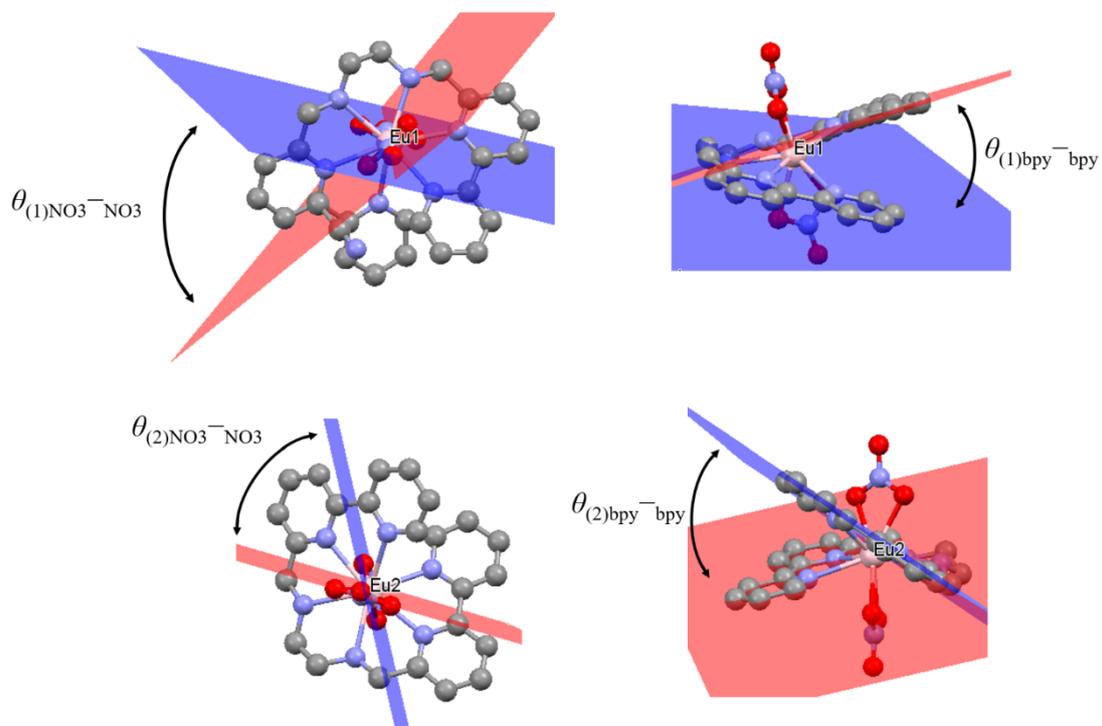


Table S2. Selected mean interatomic distances and angles between skeletons for EuLH. See inset figure in Table S1 for atomic labels.

	EuLH
mean Eu(1)-N _{py} (Å)	2.598
mean Eu(1)-N _{en} (Å)	2.542
mean Eu(1)-O (Å)	2.538
mean Eu(2)-N _{py} (Å)	2.588
mean Eu(2)-N _{en} (Å)	2.542
mean Eu(2)-O (Å)	2.542
$\theta_{(1)\text{NO}_3^- \text{NO}_3}$ (deg)	62.5
$\theta_{(1)\text{bpy}^- \text{bpy}}$ (deg)	61.7
$\theta_{(2)\text{NO}_3^- \text{NO}_3}$ (deg)	60.2
$\theta_{(2)\text{bpy}^- \text{bpy}}$ (deg)	48.8



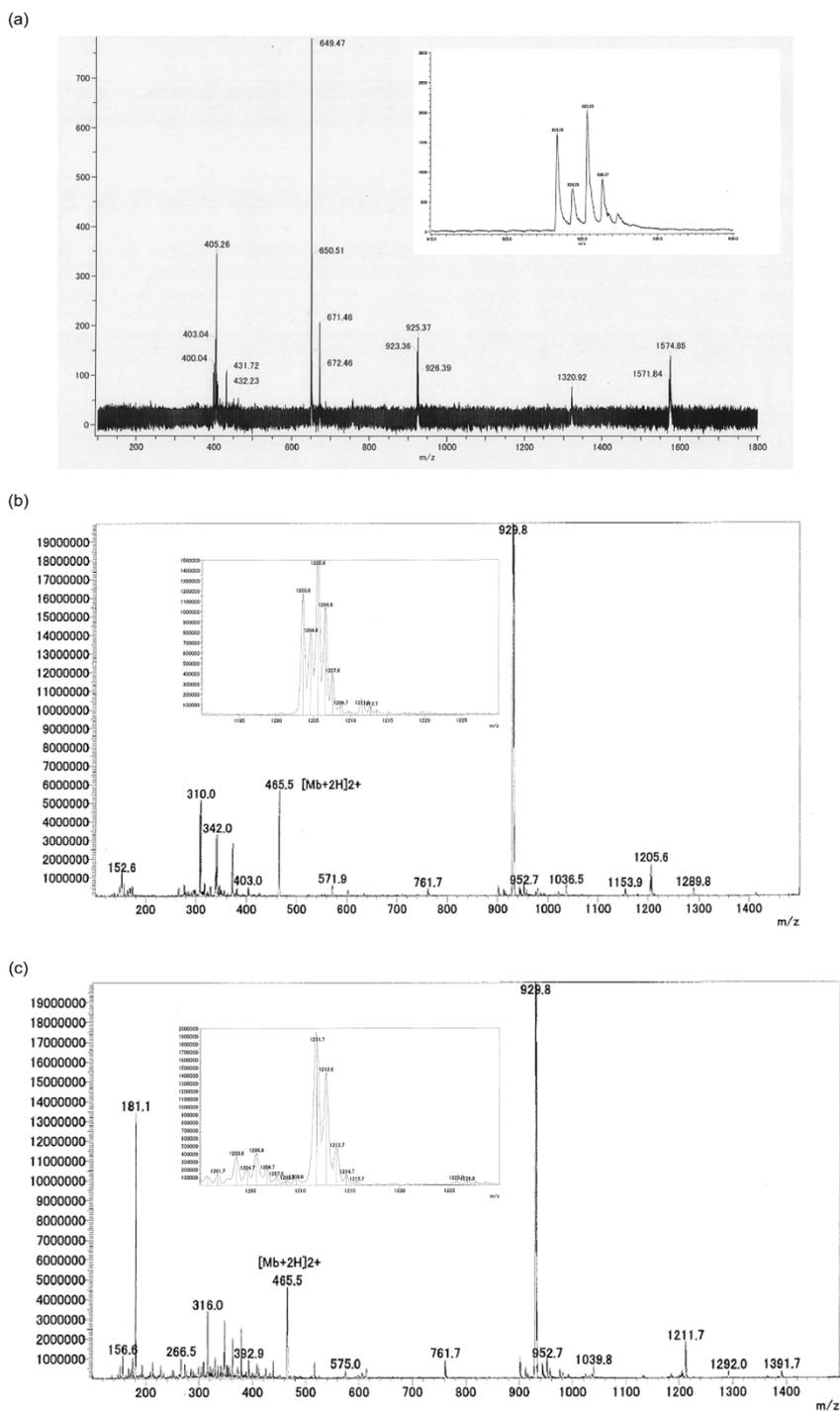


Fig. S2 LC-MS spectra of EuLC₈ in acetonitrile (a) EuLC₁₈ (b) and TbLC₁₈ (c) in chloroform. Each bottom figure is extended view. The peak at m/z = 1574.85 will suggest another component consisting of 1:2 of Eu and LC₈. The Eu and Tb complex as 1:2 with LC₁₈ calculated as m/z = 2134.84 and 2141.80, respectively, were out of limit in the observation, but many larger m/z species than the 1:1 were observed.

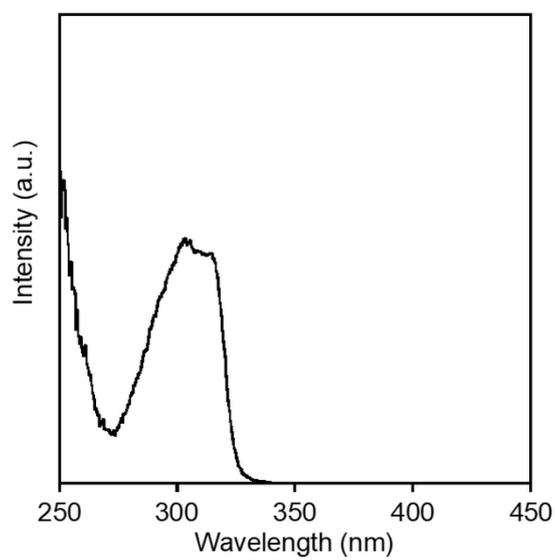


Fig. S3 Excitation spectrum of EuLH in acetonitrile. $\lambda_{\text{mon}} = 618$ nm.

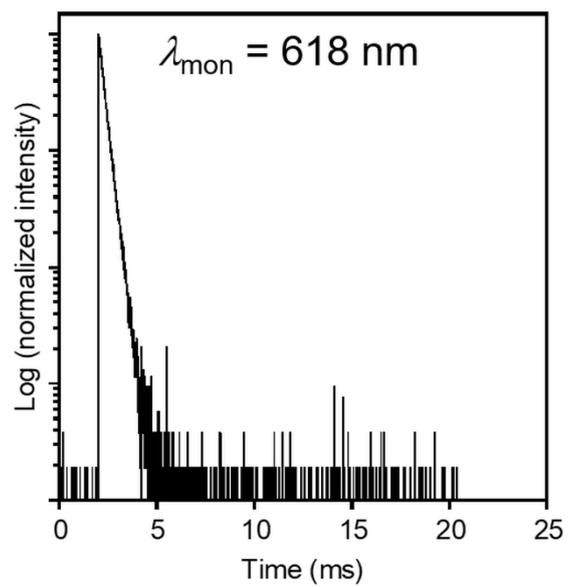


Fig. S4 Luminescence decay curve of EuLH in acetonitrile (30 μM). $\lambda_{\text{ex}} = 280 \text{ nm}$.

Calculation of rate constants of energy relaxation for Eu complexes

The total luminescence quantum yield of Eu sensitized by the organic ligand moiety (ϕ_{L-Ln}) is determined by using following equation.¹

$$\phi_{L-Ln} = \phi_{ISC} \times \eta_{EnT} \times \phi_{Ln-Ln} \quad (1)$$

Here, ϕ_{ISC} , η_{EnT} , and ϕ_{Ln-Ln} represents the triplet yield of the ligand, the efficiency of energy transfer and the efficiency of metal-centered luminescence.

The $n\pi^*$ character of the ligand and heavy-atom effect should result in the value of ϕ_{ISC} is approximately 1.^{2,3} The efficiency of metal-centered luminescence can be calculated from the observed emission lifetime τ_{obs} ,

$$\phi_{Ln-Ln} = k_R / k_R + k_{NR} = k_R \times \tau_{obs} \quad (2)$$

The radiative rate constant can be calculated from equation (3).⁴⁻⁶

$$k_R = A_{MD} \times n^3 \times (I_{tot} / I_{MD}) \quad (3)$$

Where, A_{MD} is the spontaneous emission probability of the $^5D_0 \rightarrow ^7F_1$ transition of Eu ion in vacuo, n is the refractive index, I_{tot} / I_{MD} represents the ratio of the total integrated intensity of the corrected Eu luminescence spectrum to the integrated intensity of the magnetic-dipole transition.

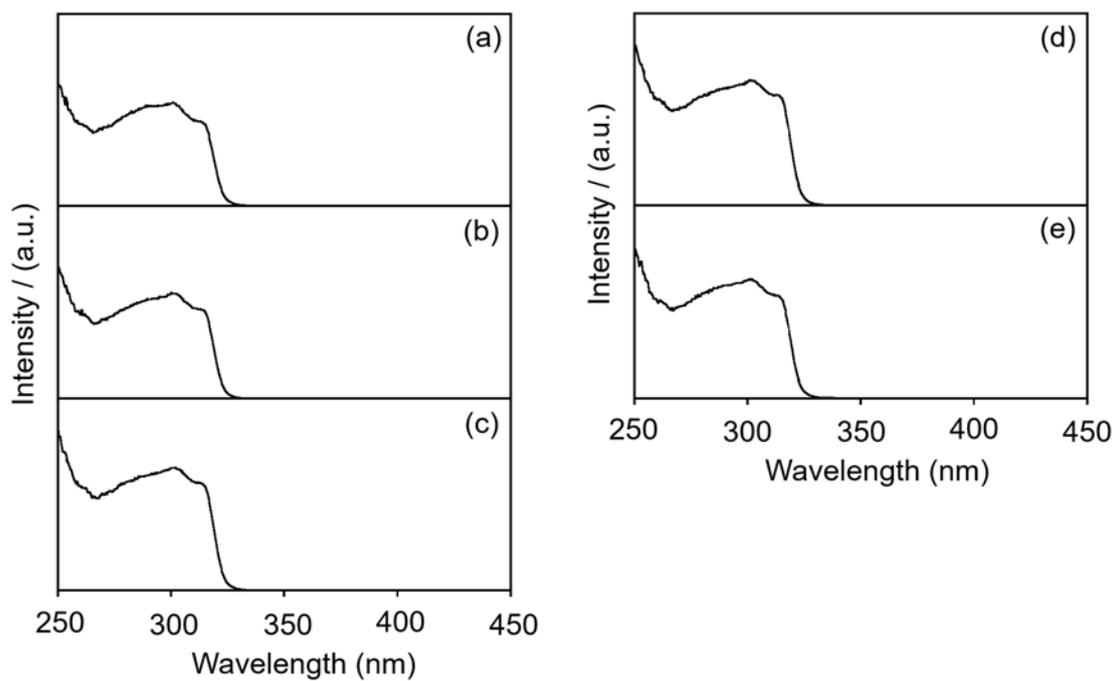


Fig. S5 Excitation spectra of EuLC₈ (a), EuLC₁₂ (b), EuLC₁₄ (c), EuLC₁₈ (d), and EuLC₂₂ (e) in chloroform. $\lambda_{\text{mon}} = 616$ nm.

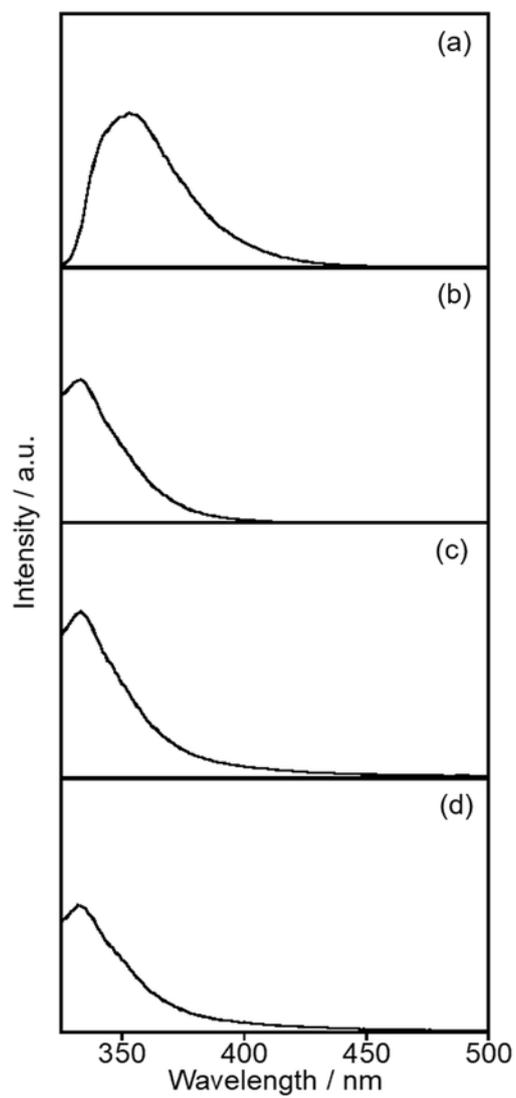


Fig. S6 Fluorescence spectra of GdL (a), GdLH (b) in acetonitrile, GdLC₈ (c), and GdLC₁₈ (d) in chloroform (30 μ M). $\lambda_{\text{ex}} = 315$ nm for GdL, $\lambda_{\text{ex}} = 303$ nm for GdLH, and $\lambda_{\text{ex}} = 290$ nm for GdLC₈ and GdLC₁₈.

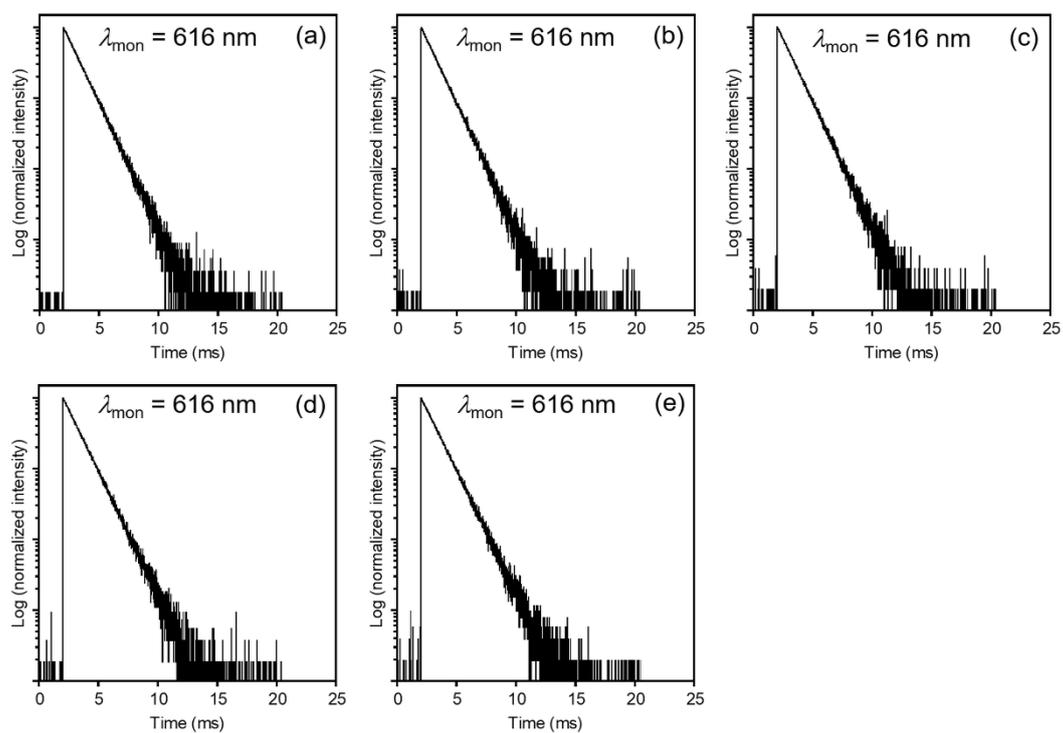


Fig. S7 Luminescence decay curves of EuLC₈ (a), EuLC₁₂ (b), EuLC₁₄ (c), EuLC₁₈ (d), and EuLC₂₂ (e) in chloroform. (30 μM). $\lambda_{\text{ex}} = 280 \text{ nm}$.

Cartesian coordinates of critical points shown in Fig. 2 and 7

Eu(LC₂)(NO₃)₂ (Fig 2(b) left)

Electronic energy = -2158.310252331633/ Gibbs free energy = -2157.828350517548 (hartree)

C	0.666892565210	-3.831115364851	0.386443884797
C	-0.361825514157	-4.733473605192	0.993063741648
H	-0.624963746556	-5.548399132491	0.303289438594
H	0.022001787497	-5.167031987152	1.926375615267
C	2.312713973020	-5.624081056577	0.396871233893
H	3.046046292330	-5.957631852202	-0.349497573412
H	1.467989380224	-6.322890442280	0.331697180642
C	2.915303370997	-5.661700641221	1.794820350294
C	3.796355087303	-6.674239021327	2.165805267873
H	4.088003227975	-7.451293393219	1.457382605113
C	4.292340486333	-6.660716903189	3.468729932698
H	4.983190533459	-7.436080229709	3.803289719998
C	3.908247723644	-5.642828751604	4.332298989003
H	4.274117540341	-5.574627816295	5.355324124338
C	3.024893546006	-4.663113080137	3.865438008409
C	2.607654668239	-3.530761602936	4.742161024496
C	1.742274232993	-2.532717658361	4.285804318014
H	1.343302105514	-2.574140025680	3.272671702668
C	1.396983521735	-1.499339216127	5.152605048534
H	0.721205078096	-0.710720528732	4.822230102667
C	1.927438781141	-1.503322553551	6.438645903383
H	1.681915082327	-0.718743655283	7.154661302944
C	2.785893205869	-2.542222886731	6.798945820092
H	3.224079144626	-2.579196281426	7.799877225645
C	2.856425215915	-3.352384856963	-0.504603899199
H	2.361098879126	-2.678422777587	-1.213825085683
H	3.585180398163	-3.934583137614	-1.079689395716
C	3.556370729887	-2.541332839062	0.606087261961
H	2.814134142496	-2.126280267937	1.298323784417
H	4.216551350383	-3.183575898821	1.199942772450
C	5.751204493049	-1.730480022704	-0.281480520638
H	6.165347827973	-2.407132429868	0.478023121727
H	6.338213602125	-0.804161379541	-0.222983406006
C	5.877362536148	-2.341735396315	-1.670001264847
C	6.987275614436	-3.109069880973	-2.013423273920
H	7.778946616704	-3.305551428012	-1.288445349270
C	7.053017817658	-3.615477270685	-3.310645133835
H	7.906619411316	-4.218471576533	-3.624291402853
C	6.015235502217	-3.353807650480	-4.195780647754
H	6.007826515891	-3.732909029245	-5.216191726891
C	4.934841728127	-2.580562151432	-3.755648623066
C	3.781168526852	-2.296614818725	-4.657478719692
C	2.677332961185	-1.557409165504	-4.223163547603
H	2.646942497698	-1.160989103431	-3.208647517895
C	1.629913200035	-1.335167736188	-5.113013533351
H	0.758162297650	-0.760663173919	-4.799767114903
C	1.726452864489	-1.856370783004	-6.399193261823
H	0.934154356975	-1.704380768436	-7.132665823312
C	2.867774069175	-2.584122663505	-6.736615044664
H	2.978855056866	-3.011576011933	-7.736807355284

C	3.770618988074	-0.314736295767	-0.298808728471
C	4.543839832045	0.807912764135	-0.917495269959
H	5.020279846455	0.466236864450	-1.846367347475
H	5.321240824718	1.175284160709	-0.231944316045
H	-1.258006424456	-4.142155099236	1.206220054409
H	3.848465241048	1.623190951488	-1.140586136137
Eu	0.291024297352	-0.372545911609	0.030702632412
N	1.864679526672	-4.287889635523	0.025925319652
N	2.532842457315	-4.686941436213	2.619123672535
N	3.125186162052	-3.534147575400	5.977288477050
N	4.366404132042	-1.446370418602	0.072627156995
N	4.880452779467	-2.077994081074	-2.514452842026
N	3.873879959201	-2.806131558681	-5.892559471392
N	-0.888422121995	-0.056421952401	2.589220744751
N	-0.125143268890	0.732433138727	-2.546813445581
O	0.383380218961	-2.614128692262	0.197275430331
O	2.528003578280	-0.176037625786	-0.114499079603
O	-1.568710797142	-0.179475006389	1.508810973221
O	0.383839639255	-0.017488815868	2.406896627679
O	-1.389103373386	0.008522200605	3.665898073617
O	-0.130929877824	1.428401903759	-1.469148054521
O	0.014048368128	-0.530939906411	-2.354990730490
O	-0.232155692092	1.214579675043	-3.628741791943

Eu(LC₂)(NO₃)₂ (Fig 2(b) right)

Electronic energy = -2158.338933094079/ Gibbs free energy = -2157.846276895414 (hartree)

Eu	-0.314507050149	0.054811436443	-0.037489058520
N	-1.733531544232	2.138650017648	-0.330062548941
N	0.326420224570	1.608821861217	-2.016752243641
N	1.565067066060	-1.051702616101	-1.912148347184
N	-0.604573436249	-2.505729354161	-0.598211521395
N	0.123369152038	-1.584399245120	1.967823719044
N	-0.478597753376	1.063859403077	2.424491930891
C	1.786932064588	3.621443913989	-3.229952264149
H	2.387797374603	4.416674087158	-3.671879865697
C	2.137780149714	2.287086399585	-3.415742514473
H	2.997576772502	2.012927266604	-4.027063604540
C	1.375926019419	1.303944739701	-2.795976202385
C	1.592417503754	-0.162077375231	-3.086416558247
H	2.510277335742	-0.300604343827	-3.679319757371
H	1.359066868941	-2.579754359269	-3.367380155207
C	-2.949035083283	2.210245940176	0.226107892601
H	-3.227155976998	1.383661596356	0.885372943547
C	-3.822228881584	3.264689276895	0.002887218691
H	-4.802527238607	3.275153726755	0.477454038149
C	-3.408907339128	4.288847712419	-0.843883103446
H	-4.063987382953	5.135379169451	-1.053182471825
C	-2.160060170555	4.205398536984	-1.447810858218
H	-1.841462601260	4.968961031980	-2.155317551571
C	-1.347393938682	3.105511737798	-1.180129548056
C	-0.066117477257	2.888396273730	-1.905896122035
C	0.655726183557	3.929896452262	-2.487885723171
H	0.358605096980	4.965848375562	-2.336358027542
C	1.191370819783	-2.446399591697	-2.287969466718
H	1.882493928876	-3.124065334800	-1.775332709292

C	-0.254392861179	-2.822464369300	-1.995159524734
H	-0.913450940777	-2.238387009490	-2.647063847404
C	0.044220729754	-3.421555910748	0.361024496419
H	1.087734169087	-3.529061936766	0.039796717155
C	0.087993118907	-2.910530151815	1.775977427073
C	0.138384365019	-3.823584929690	2.825614491921
H	0.098754745643	-4.894153535679	2.623268552180
C	0.225166265753	-3.343607664360	4.125027719300
H	0.255984118995	-4.031053887938	4.971076165123
C	0.236575149336	-1.970903268796	4.331093882763
H	0.247513736363	-1.568086685402	5.342185793908
C	0.183143256329	-1.118211359255	3.227704152314
C	0.120693794500	0.355484174776	3.405852634282
C	0.641285776355	0.957443631508	4.549161816862
H	1.169172987979	0.364624379796	5.294516621396
C	0.505803403392	2.331870482770	4.719106272367
H	0.913303173185	2.821467719090	5.604367848027
C	-0.147303196805	3.057752660513	3.735668927877
H	-0.282104727069	4.135720185331	3.811719094668
C	-0.603367716092	2.385633457906	2.606970407894
H	-1.072980281602	2.941379719416	1.801259211537
H	-0.387920293468	-3.896820682045	-2.215332710010
H	0.738135367750	-0.456575462590	-3.715369923353
H	-0.427974434578	-4.419595521175	0.332295306400
C	2.689074384975	-1.044664959915	-1.015579740642
O	2.652180021764	-1.801487404208	-0.067284448129
C	-2.019228838880	-2.374345750862	-0.323694368576
O	-2.329168971530	-1.577005551522	0.544273627295
C	3.847574263020	-0.141707270929	-1.297591546061
H	3.574750093980	0.909803092316	-1.129769803666
H	4.641852828325	-0.396554950172	-0.587775827200
H	4.212707796993	-0.268731815411	-2.327313489464
C	-2.999897495011	-3.187164556231	-1.095814228476
H	-3.969911914785	-3.167614386682	-0.588180281896
H	-3.109043453493	-2.718085868380	-2.085677236770
H	-2.650313383413	-4.218128609514	-1.243988837555
N	-1.997573978796	0.156857076518	-2.996036353602
O	-1.849532576864	-0.316905734282	-1.791778318925
O	-2.560940813499	1.220615138122	-3.139046754680
O	-1.559602093529	-0.525933614221	-3.922566596626
N	2.032720190319	2.411800779186	0.417300924179
O	1.646930087450	1.167346319779	0.448368416515
O	1.199191309414	3.279214860400	0.658779740784
O	3.193186544998	2.643141792471	0.138769371282

Eu(LC₂)₂(NO₃)₂

S0 (same structure as Fig2(a))

Electronic energy = -3720.915571896388 / Gibbs free energy = -3719.938162419136 (hartree)

C	0.491176500262	-3.350403576481	0.709440449100
C	-0.495154950753	-3.874922984853	1.713110667723
H	-0.917641178661	-4.838094826818	1.390544321026
H	-0.010237732168	-4.006951615706	2.690334073883
C	2.067258875021	-5.163972320162	1.224551621778
H	2.551999667335	-5.834691875762	0.500076939290
H	1.166183912131	-5.684802037506	1.572576810468

C	2.991897520234	-4.908769321317	2.400634262894
C	4.001088391868	-5.813143459179	2.723565676513
H	4.159197549663	-6.710734402482	2.123480205750
C	4.798147136988	-5.537659586672	3.833691119516
H	5.594876089470	-6.223843132627	4.125431882980
C	4.574149558016	-4.372872459104	4.553911615235
H	5.172701384140	-4.097018668696	5.420443445961
C	3.545728828850	-3.515584988882	4.143711581784
C	3.300984495349	-2.230495019242	4.860449903121
C	2.318180614533	-1.340490489150	4.425328622295
H	1.708529352061	-1.572362007204	3.555386905016
C	2.143277218896	-0.148862195469	5.120712556810
H	1.370967159001	0.548990300337	4.797756017338
C	2.953553095851	0.108689510569	6.221521783444
H	2.853202006719	1.027739440902	6.800023498328
C	3.908632367728	-0.844764583366	6.576832738232
H	4.564639390718	-0.678765615483	7.436012443102
C	2.666858478003	-3.283572615939	-0.313798909628
H	2.158323873316	-2.850922428478	-1.184298889457
H	3.364348511834	-4.046662621488	-0.680128600703
C	3.414861531215	-2.172926847374	0.456374282685
H	2.699618211402	-1.574557597772	1.034087690027
H	4.133156166287	-2.602770955876	1.164772349134
C	5.522903391174	-1.634277280590	-0.770033817569
H	6.043066215552	-1.891836436793	0.163684683902
H	6.033063587646	-0.751115643802	-1.175055971273
C	5.624178776049	-2.780036054859	-1.760634295576
C	6.652414730793	-3.714626210000	-1.670219251838
H	7.396104176133	-3.651723895751	-0.874144453988
C	6.701810797216	-4.729383469253	-2.625127707699
H	7.493214345367	-5.479957386481	-2.593863895593
C	5.722832659604	-4.781687485283	-3.607271657880
H	5.701926028861	-5.555836613070	-4.372000019798
C	4.718526899890	-3.805068641481	-3.608936840300
C	3.623705453923	-3.846337714209	-4.621310886506
C	2.566702823633	-2.934875030960	-4.582456151878
H	2.520078050664	-2.171486562103	-3.809045331481
C	1.568462988237	-3.030684754814	-5.546669017714
H	0.744435442217	-2.317538214763	-5.531678692148
C	1.664152056629	-4.027928073194	-6.511566445343
H	0.909218359897	-4.139867049813	-7.290765338121
C	2.758850006612	-4.891874353431	-6.464136755386
H	2.868756577040	-5.688119633731	-7.205880655080
C	3.485457054858	-0.293079277163	-1.049522383505
C	4.143570509860	0.536754684827	-2.114005321312
H	4.527814553274	-0.114598534106	-2.911459716018
H	4.976080453245	1.127107696070	-1.704086197988
H	-1.304779812713	-3.140855247653	1.794048485475
H	3.388234104344	1.218511168404	-2.519691997261
Eu	-0.005747643625	-0.106792184769	-0.550311057540
N	1.674028273968	-3.950509597063	0.526235279709
N	2.761502427972	-3.792281227812	3.093084314487
N	4.087410715487	-1.988769200191	5.919012836003
N	4.150068993671	-1.285263349407	-0.441844414371

N	4.683137393212	-2.817054575975	-2.705575105801
N	3.719032952855	-4.813444700601	-5.544829973701
N	-0.460237705169	-0.165065595449	2.347628520896
N	0.524485114697	-0.050071298044	-3.422999437614
O	0.207572605916	-2.333460897685	0.039872830942
O	2.301234887420	-0.056091012663	-0.728894716560
O	-1.412636759794	-0.272476469023	1.515062875643
O	0.698477628514	-0.025227504677	1.850013633879
O	-0.646604791025	-0.195636205359	3.541718637436
O	0.326112574071	1.010518076598	-2.753979044397
O	0.427132993719	-1.138886093706	-2.778155903333
O	0.795401394040	-0.024597860955	-4.600674571677
C	-0.854112712462	3.102342556858	0.606773897124
C	-0.208013650931	3.598793752395	1.867978799916
H	0.282311965472	4.570778724644	1.710128657202
H	-0.960885571448	3.703796897462	2.661649327674
C	-2.512077578576	4.913907455859	0.677232627436
H	-2.770866562253	5.597887046869	-0.144183276893
H	-1.748859458660	5.427847381155	1.275437833279
C	-3.733335491191	4.646031672536	1.537201624812
C	-4.777243173090	5.566867698785	1.589146273998
H	-4.747069148718	6.479323355186	0.991148995254
C	-5.855900956434	5.289827360946	2.427152751271
H	-6.690645944270	5.988632872498	2.502345289208
C	-5.859523658315	4.107858235030	3.154152434834
H	-6.676857312175	3.829541757898	3.817130893492
C	-4.772202116608	3.234806296322	3.024748762691
C	-4.756927613925	1.934940716303	3.756347773968
C	-3.724188540779	1.014495693246	3.570411430032
H	-2.906734010613	1.231906962218	2.886887271619
C	-3.770091777108	-0.187343300419	4.268919382617
H	-2.963771398094	-0.909754191879	4.142800620493
C	-4.840362110729	-0.424166308897	5.125075040333
H	-4.919015907161	-1.350168578376	5.695859148501
C	-5.823239672754	0.559392857184	5.242608381936
H	-6.679218917517	0.411432488208	5.907046476767
C	-2.637359371456	3.068166288162	-1.007026014862
H	-1.897701789591	2.661927143019	-1.708021955582
H	-3.208580085605	3.840012682473	-1.536900129903
C	-3.563642696023	1.936429568939	-0.512349692862
H	-3.032042916062	1.314082513967	0.217933446445
H	-4.450068947212	2.345475438994	-0.013553422299
C	-5.247050622896	1.451280179066	-2.294280334415
H	-5.994748481338	1.724689862781	-1.536379666521
H	-5.645980604045	0.572438078032	-2.817587834057
C	-5.062236724397	2.591476095469	-3.281290745476
C	-6.096280829479	3.489671671203	-3.536079478828
H	-7.052025600041	3.401915815105	-3.016767344798
C	-5.872564996760	4.499156132825	-4.470883300357
H	-6.656925102609	5.221432595986	-4.702732024200
C	-4.634224137844	4.583544744686	-5.092338054192
H	-4.396212116003	5.355570193521	-5.821878032513
C	-3.651060351794	3.643267289333	-4.761777818287
C	-2.293182958869	3.718643268288	-5.373824070961

C	-1.276887039631	2.841906754680	-4.989027889620
H	-1.458042451790	2.081948338468	-4.231286854131
C	-0.025818827541	2.967861406911	-5.584823036051
H	0.770962256276	2.280732518871	-5.300779784636
C	0.160770884381	3.960391108380	-6.541288182717
H	1.121312917997	4.095874643808	-7.039412820900
C	-0.916981371234	4.788912062848	-6.855849489457
H	-0.808595724644	5.580532632883	-7.602706165666
C	-3.204900534173	0.115299498797	-2.048959163067
C	-3.552569373831	-0.683811385770	-3.271337181961
H	-3.701018620040	-0.009568813279	-4.126404469501
H	-4.469800887306	-1.270939950172	-3.118770097077
H	0.547594878260	2.862872903939	2.164371771502
H	-2.719209013446	-1.364985255458	-3.473639887366
N	-1.933376619790	3.711860424704	0.100275017280
N	-3.722693355589	3.511353184667	2.238416460255
N	-5.793191499410	1.712700992783	4.577419399573
N	-4.020164725751	1.082846331438	-1.607052745506
N	-3.872782933044	2.659680389780	-3.879770901673
N	-2.117812654274	4.680661534249	-6.290587916727
O	-0.385323147400	2.099417410205	0.026406774483
O	-2.142412060821	-0.127303548429	-1.437697508439

T1

Electronic energy = -3720.800494732568 (hartree)

C	0.465159812806	-3.459505935992	0.720250434192
C	-0.459887428111	-4.208246935163	1.635599656701
H	-0.831788607580	-5.127697840380	1.160108586851
H	0.059890827953	-4.474316568196	2.566281519815
C	2.115645223069	-5.262450703713	0.866393303307
H	2.713030683538	-5.736300908925	0.074460174339
H	1.253915289685	-5.923089711894	1.032335585708
C	2.931936210126	-5.164289514260	2.145679793019
C	3.813280768949	-6.184736160214	2.500338810577
H	3.951441748474	-7.052874476636	1.853561067390
C	4.508963629273	-6.060932400438	3.700581543033
H	5.205109738698	-6.838865396036	4.018206907054
C	4.318026665259	-4.927791746142	4.481444736309
H	4.843505202966	-4.770051547533	5.421495039991
C	3.423533587096	-3.949335179423	4.035625712905
C	3.219372459415	-2.692638824092	4.812854226335
C	2.366459180757	-1.686482675219	4.353206524245
H	1.822038278384	-1.807663521270	3.418403774225
C	2.234570362096	-0.526487733854	5.110272080991
H	1.561149661745	0.259307912898	4.769040068050
C	2.952970888944	-0.417696373990	6.296657610887
H	2.879701618587	0.469649746044	6.926478608386
C	3.775806057877	-1.479886999072	6.672106048088
H	4.353099578775	-1.433004841677	7.599893267722
C	2.573029474299	-3.154116727238	-0.405238262728
H	2.008276744930	-2.640152655700	-1.192887870825
H	3.289015628054	-3.819590500206	-0.899849391109
C	3.302075947678	-2.122482010359	0.478516855659
H	2.574586756428	-1.568474296114	1.084955137090
H	3.990666619017	-2.620157752045	1.170092858304

C	5.476744147816	-1.440128077508	-0.557249777531
H	5.900328234899	-1.885337223056	0.354760554590
H	6.020332626653	-0.497276755673	-0.712341691549
C	5.726333449261	-2.363650699365	-1.739346071194
C	7.009625608184	-2.985051241069	-1.852837941861
H	7.776827889571	-2.803442531333	-1.098955539346
C	7.250549830511	-3.822901254220	-2.962817707591
H	8.223409545863	-4.299869733096	-3.089447610296
C	6.247660572442	-4.033310885132	-3.870264442099
H	6.364261900057	-4.674934544394	-4.741332915869
C	4.952842932833	-3.382556554103	-3.672951373006
C	3.889738568225	-3.613038945225	-4.518950937809
C	2.593261024939	-2.956945721405	-4.329642702291
H	2.476836415827	-2.238340571101	-3.521335519509
C	1.556267089812	-3.257505816157	-5.172055749790
H	0.596462341045	-2.758239780206	-5.041951721146
C	1.771422387857	-4.188936203566	-6.206123825066
H	0.982245192239	-4.459661071395	-6.907459401113
C	3.073876882130	-4.769233914719	-6.343969337141
H	3.250442353426	-5.480169938384	-7.159038318784
C	3.421505847633	-0.164669933679	-0.919443359446
C	4.145928617348	0.770275200704	-1.843366494299
H	4.643195903992	0.203324267510	-2.642278954759
H	4.901767896029	1.357197386244	-1.301011022946
H	-1.308525928746	-3.553582119968	1.860169338164
H	3.406320343832	1.451101446245	-2.277553871066
Eu	-0.089045365508	-0.138574380292	-0.404991298751
N	1.648276540556	-3.980050232963	0.369291761582
N	2.733996553148	-4.079871913856	2.893040615936
N	3.914656160841	-2.593045790258	5.954444836276
N	4.073378675703	-1.164444468580	-0.311887657634
N	4.752170856017	-2.514921962992	-2.586641842101
N	4.090759832888	-4.517403570756	-5.573409774540
N	-0.424345048992	0.023218817227	2.497846571904
N	0.156795489419	-0.301537434116	-3.314129234273
O	0.123033561141	-2.340530682883	0.282163760333
O	2.200180142200	-0.001939555305	-0.711772832509
O	-1.407800984266	-0.129332112575	1.710346611321
O	0.721741864480	0.066721966778	1.951984513093
O	-0.570601695041	0.128602773572	3.692400707732
O	0.046028503403	0.808081746179	-2.710857642881
O	0.213064106735	-1.332765667753	-2.572236131761
O	0.196971422818	-0.378194677917	-4.519163840462
C	-0.864513669061	3.170985282324	0.523407034131
C	-0.202970651673	3.763641918404	1.733925056188
H	0.293979914351	4.715092797075	1.493793097974
H	-0.948795023273	3.940287024975	2.521455148662
C	-2.483094914827	5.015428587140	0.442892761580
H	-2.771397451102	5.617083246347	-0.431457689621
H	-1.695619522416	5.580846727384	0.958309573108
C	-3.671426643709	4.842960133994	1.372159832823
C	-4.683585940983	5.799626607108	1.413318299590
H	-4.655175576619	6.670304159334	0.755837274053
C	-5.727594353235	5.611631054695	2.317233576634

H	-6.535987055498	6.341379971481	2.386242670345
C	-5.731741425411	4.478481546288	3.118757735569
H	-6.523518900451	4.270125632872	3.836322323437
C	-4.679936932157	3.562960515364	2.994004900761
C	-4.665617876342	2.312370794523	3.806566985532
C	-3.663003489429	1.355820984727	3.639513040659
H	-2.868644123150	1.506012599033	2.911982034638
C	-3.705281037984	0.203615657062	4.417386021603
H	-2.920965674669	-0.544891873484	4.305678043392
C	-4.742656271602	0.050925918750	5.331193281485
H	-4.816030423707	-0.832119349900	5.967085409709
C	-5.697928044516	1.064114965476	5.422913532841
H	-6.527082570869	0.981624187723	6.131324178404
C	-2.648962776191	3.040563520699	-1.084825546328
H	-1.919812642590	2.549593134571	-1.741583178822
H	-3.192767719769	3.779059834594	-1.685824676852
C	-3.613728358369	1.987867589941	-0.496452795303
H	-3.106112863270	1.418687768532	0.292131803973
H	-4.489552804207	2.468835784621	-0.044812290342
C	-5.312403485451	1.387021983671	-2.227359080092
H	-6.068342755348	1.685120391708	-1.486744327741
H	-5.699810495684	0.485786470061	-2.719221805207
C	-5.125318965320	2.488703876147	-3.254962014342
C	-6.131378483162	3.422284005681	-3.491813122701
H	-7.068107916330	3.387597115232	-2.933047702804
C	-5.905052941477	4.399056575320	-4.460553203850
H	-6.668914767331	5.146648133169	-4.680619019475
C	-4.689452991640	4.418445559634	-5.129754967834
H	-4.448450672407	5.164745179709	-5.884588944241
C	-3.732136754689	3.446040072040	-4.813693115370
C	-2.394727753381	3.456455538947	-5.473968893852
C	-1.406113311596	2.538833067453	-5.114590485084
H	-1.594136295495	1.793150420831	-4.345582430471
C	-0.170931488079	2.606860690125	-5.750703437997
H	0.605061897379	1.889476079853	-5.483679881983
C	0.029081898486	3.584119972876	-6.720246047735
H	0.978816619656	3.676386283118	-7.248416183108
C	-1.022183605148	4.455662815811	-7.007974516784
H	-0.903631639310	5.236688508661	-7.764488390794
C	-3.303384780513	0.023697375765	-1.857295915385
C	-3.653087786376	-0.855292405261	-3.023560054399
H	-3.782713071619	-0.244701995193	-3.928067105845
H	-4.580353985921	-1.417033334378	-2.838412543151
H	0.547946403933	3.047554441483	2.085695690700
H	-2.829528701074	-1.563152510533	-3.166714410240
N	-1.929069043320	3.760192700018	-0.036502466368
N	-3.662756660293	3.754820560133	2.142700108753
N	-5.670780866432	2.170670641931	4.682366813319
N	-4.088588140347	1.054418063770	-1.515685104228
N	-3.958601132872	2.491793279710	-3.901439436830
N	-2.208158712887	4.403261644251	-6.404567241511
O	-0.421643263092	2.108808218203	0.036166686668
O	-2.265130670458	-0.208128048300	-1.201820618881

Minimum energy crossing (MEX) between T1 and S0

Electronic energy = -3720.776443862325 (hartree)

C	0.466163946928	-3.440827662152	0.733984010347
C	-0.461520994047	-4.201034043874	1.637050287344
H	-0.827099643710	-5.117642306304	1.151503468611
H	0.054276340706	-4.473934713391	2.568232967161
C	2.123678276402	-5.241853940915	0.871418911622
H	2.720261731597	-5.706995606682	0.073459959916
H	1.263609918362	-5.905714156865	1.031839502312
C	2.941498309552	-5.151842267438	2.150108864059
C	3.822745583948	-6.173624695569	2.501156775839
H	3.959392899914	-7.040885949200	1.852738001359
C	4.517200853175	-6.053682066459	3.702839993349
H	5.211942441282	-6.833673991746	4.018613312941
C	4.327946937412	-4.922047681576	4.486557922714
H	4.852821277423	-4.768963366541	5.427720900244
C	3.435107617986	-3.941267145756	4.042350538242
C	3.230771318209	-2.684946462127	4.819733895720
C	2.377379483649	-1.679649630575	4.358763426524
H	1.833709806311	-1.801523564642	3.423629910438
C	2.239958103247	-0.521435061113	5.117395894667
H	1.564942201947	0.262889946263	4.775752987494
C	2.956668492247	-0.412046586737	6.304749533873
H	2.878207381848	0.473184728815	6.936849481501
C	3.782203902524	-1.472282427090	6.680121964347
H	4.359224439968	-1.424099226578	7.607953482968
C	2.580820986640	-3.120492133695	-0.371243294292
H	2.023474341521	-2.603558741417	-1.162389096002
H	3.299236731282	-3.785574797716	-0.862191782364
C	3.303911713655	-2.089275129162	0.520407779532
H	2.573712455616	-1.532052304791	1.119908143964
H	3.985824453073	-2.586186681896	1.219266668583
C	5.480289010407	-1.455375977912	-0.522787241462
H	5.916985894380	-1.848755560687	0.406302509130
H	6.044416363772	-0.541160799396	-0.760238353531
C	5.641965393955	-2.464207026804	-1.638682751314
C	6.739719089224	-3.478719616426	-1.667667446808
H	6.415412857024	-4.423184574155	-1.187579994328
C	7.305443863363	-3.665585766724	-3.032319744066
H	8.373841278173	-3.745548564456	-3.233779651717
C	6.335826055018	-3.806777114521	-3.967195987530
H	6.529518519800	-4.102452366790	-5.000585819998
C	4.982108017639	-3.404247148280	-3.628578572552
C	3.860295665583	-3.666978061086	-4.512187014442
C	2.610586489550	-3.046277367653	-4.320152417689
H	2.470326174575	-2.334502946187	-3.508575664164
C	1.571945807472	-3.343993436470	-5.192243077838
H	0.609131431947	-2.847929929031	-5.065495559985
C	1.803888939838	-4.255147177627	-6.220342093597
H	1.018087450208	-4.528971694305	-6.926207519047
C	3.080980217472	-4.816728158697	-6.336658179251
H	3.297887486828	-5.528608694193	-7.138687711460
C	3.438513353291	-0.146136657129	-0.899976192969
C	4.167402255110	0.761476206329	-1.847195996264
H	4.666060165223	0.170295532483	-2.627464834772

H	4.921194567085	1.364205445861	-1.319697710623
H	-1.314121116909	-3.552108045909	1.863152493580
H	3.429637976096	1.428476989711	-2.305196788852
Eu	-0.077079426599	-0.120934226387	-0.409720517191
N	1.654144983280	-3.954787358422	0.388819237633
N	2.745714809401	-4.068762297062	2.899582389949
N	3.925867076592	-2.584055456704	5.961142572721
N	4.085251861744	-1.136317905075	-0.268419428097
N	4.743244068599	-2.535642545323	-2.557432185737
N	4.089516026745	-4.541789726044	-5.517193878217
N	-0.419363383618	0.032418488185	2.493025797011
N	0.192448388645	-0.314903759228	-3.315467703861
O	0.124230991018	-2.319988898549	0.301537811731
O	2.218676943101	0.025387813133	-0.695344336109
O	-1.401128882591	-0.109342034341	1.701584904026
O	0.727612931885	0.085740036857	1.949617643353
O	-0.567954650668	0.118771453165	3.688719415140
O	0.078956704103	0.801302689482	-2.723979068202
O	0.246814358103	-1.337833088379	-2.560918376663
O	0.236550807171	-0.405487354438	-4.518788579753
C	-0.863879184698	3.183334765960	0.517163990170
C	-0.205856680546	3.773534117973	1.730698436571
H	0.291750905925	4.725416747785	1.493609878926
H	-0.953603702535	3.948520397636	2.516749875802
C	-2.489977453142	5.021559656684	0.442388980886
H	-2.780259038216	5.623040012919	-0.431430396298
H	-1.703344874335	5.588496977608	0.957426570010
C	-3.677261950370	4.845992605234	1.372431162489
C	-4.690043869824	5.801934399205	1.415582684538
H	-4.663165247464	6.673021100964	0.758584478302
C	-5.732958717042	5.612266219468	2.320368020551
H	-6.541592813634	6.341593491578	2.391128098152
C	-5.734756807538	4.478913988709	3.121608033204
H	-6.525795234481	4.269327991427	3.839620691205
C	-4.683111639058	3.563639016633	2.993871795070
C	-4.665932867460	2.313561060332	3.807168257832
C	-3.663416562487	1.357284344341	3.637715660134
H	-2.869539310194	1.508940992964	2.909895825315
C	-3.703435805310	0.205231946500	4.415967591062
H	-2.918770201840	-0.542773736928	4.303075129625
C	-4.740465994842	0.050702404503	5.329889445457
H	-4.812222362718	-0.832421591965	5.965857189822
C	-5.696079245265	1.063385108371	5.423438311893
H	-6.524898634637	0.979626480033	6.132097514407
C	-2.650926072976	3.047987375870	-1.087493298184
H	-1.921084467998	2.560172821381	-1.745706843203
H	-3.198219987648	3.785148628728	-1.686890845277
C	-3.610910979840	1.991602906470	-0.498306549917
H	-3.100057873637	1.423764524790	0.289016426526
H	-4.487412798193	2.469206326718	-0.044456527893
C	-5.310982559234	1.386907684880	-2.225428525124
H	-6.065473738132	1.685430772022	-1.483555656698
H	-5.699006226539	0.485254689921	-2.715969852523
C	-5.125274615589	2.488503957505	-3.253574770112

C	-6.131420304292	3.421799085193	-3.491019279008
H	-7.067922247909	3.387948326803	-2.931817922173
C	-5.904811257219	4.398494124957	-4.459850538900
H	-6.668620972703	5.146031445778	-4.680360994589
C	-4.689489918883	4.417175490044	-5.129652920710
H	-4.448395737403	5.163425863638	-5.884533150415
C	-3.731920298030	3.445213138447	-4.812766493769
C	-2.394727351339	3.454016548634	-5.473487529520
C	-1.407005454118	2.534631878935	-5.115529563443
H	-1.595829794968	1.787837834936	-4.347638505733
C	-0.172135347614	2.601466978255	-5.752402101998
H	0.602965485760	1.882476665854	-5.486975995457
C	0.028766897022	3.579991381029	-6.720588391573
H	0.978250051148	3.671601636886	-7.249301455892
C	-1.021105678544	4.453899574225	-7.006170586920
H	-0.901771563528	5.236029936297	-7.761436372057
C	-3.294793629506	0.031793707373	-1.863897368649
C	-3.649525928455	-0.852316047385	-3.024598104319
H	-3.781523874758	-0.245189820369	-3.931123247781
H	-4.577175749826	-1.411606734588	-2.834095092752
H	0.544440390847	3.056879526812	2.082701151670
H	-2.827587435887	-1.561832583665	-3.168379384242
N	-1.932552528278	3.768423220475	-0.038791127018
N	-3.666406370131	3.757397742043	2.142313453549
N	-5.671084155845	2.169803124915	4.682607652312
N	-4.085102560267	1.056428001834	-1.516032014897
N	-3.959058328351	2.490856492560	-3.900895139297
N	-2.206848266615	4.402360700835	-6.402201283867
O	-0.414123583017	2.126541357340	0.023946857274
O	-2.248940007628	-0.191525931276	-1.216891166113

MEX between T1 and ⁵D₀

Electronic energy = -3720.799113316789 (hartree)

C	0.496429464094	-3.344182185860	0.699237706828
C	-0.498358233186	-3.863876514776	1.697209383060
H	-0.922356698246	-4.825978644842	1.373459731108
H	-0.019809157326	-3.996429007102	2.677539553713
C	2.059254745901	-5.167024294569	1.223190127841
H	2.543726329486	-5.839048195253	0.499677638720
H	1.152827712646	-5.682824400902	1.564612138850
C	2.978989988966	-4.921754255045	2.405226977641
C	3.977784929321	-5.835697403127	2.733806274086
H	4.130849392594	-6.734873096937	2.134786461536
C	4.771491577418	-5.567464508910	3.848066831078
H	5.559876646356	-6.261231795583	4.144480014795
C	4.555181111004	-4.400124315903	4.566749413914
H	5.152804155330	-4.129775202607	5.435625393161
C	3.536564098497	-3.533788355139	4.151487800018
C	3.297853441562	-2.246228614667	4.865578045809
C	2.308517708989	-1.360772596689	4.436367967847
H	1.690554849382	-1.598520529856	3.574236062994
C	2.137161622605	-0.166667603859	5.128015148088
H	1.359316335633	0.527476611234	4.810007792055
C	2.958404745219	0.098323654060	6.218901744838
H	2.861818292805	1.019862512433	6.794066416754

C	3.919462897790	-0.851233726577	6.568921625509
H	4.583979593656	-0.679046651539	7.420320614064
C	2.681260203393	-3.286584482494	-0.305868442648
H	2.180028332872	-2.843754113189	-1.175374126499
H	3.372774867810	-4.054011487845	-0.674661325431
C	3.437458462390	-2.187136957405	0.473072877827
H	2.727174296866	-1.592959108517	1.060909766344
H	4.158882011592	-2.626692110385	1.172406852485
C	5.539466428456	-1.637786650573	-0.760796499604
H	6.067008496351	-1.897735380014	0.168211773314
H	6.045014069560	-0.752344870896	-1.166640528832
C	5.635823889595	-2.779881612686	-1.755958249457
C	6.662545347996	-3.717008307096	-1.673268925027
H	7.409800855971	-3.658516901080	-0.880216982630
C	6.705726599596	-4.728689570792	-2.631799106209
H	7.495860369275	-5.480815219259	-2.606596522907
C	5.722254483991	-4.775954662141	-3.609876084393
H	5.696152002823	-5.548022229097	-4.376589901865
C	4.720512799403	-3.796896368864	-3.604036734190
C	3.620658337072	-3.830130953788	-4.611117559872
C	2.576455911210	-2.904467064537	-4.570009906103
H	2.544339928963	-2.137592979117	-3.799921518987
C	1.572346161218	-2.989686862211	-5.528727709343
H	0.758196690963	-2.265175035362	-5.512095506340
C	1.648868045072	-3.992034157136	-6.490089773004
H	0.888408776265	-4.097151963193	-7.264879024635
C	2.732083445494	-4.870639225275	-6.445051286804
H	2.826886846214	-5.671018782191	-7.184385636563
C	3.501049587065	-0.290199331646	-1.009982345893
C	4.145772576670	0.543437909923	-2.079704242727
H	4.524224644856	-0.104997187650	-2.882220057761
H	4.980144946010	1.136165339996	-1.676955146879
H	-1.306311395383	-3.127329082932	1.772402894142
H	3.384233597617	1.223591883592	-2.477015003378
Eu	0.013073425919	-0.089389258187	-0.528166456973
N	1.678492423796	-3.949082268552	0.525636731131
N	2.755203690339	-3.803786945644	3.096961946287
N	4.094253197105	-1.998252433279	5.915189708542
N	4.168662296207	-1.291740149064	-0.420924709863
N	4.691349953948	-2.811773009740	-2.697372530548
N	3.698644740255	-4.801626227782	-5.531629058665
N	-0.477789854467	-0.209243259445	2.361608605394
N	0.639908797307	0.016299326927	-3.380885185489
O	0.220969235412	-2.327131905949	0.026318694448
O	2.323584272715	-0.049276261159	-0.668018613446
O	-1.421233560489	-0.289204324323	1.515602413430
O	0.686321687551	-0.057224834653	1.880911816016
O	-0.675860869071	-0.277086701475	3.552267565502
O	0.403861983492	1.066607645531	-2.708480764213
O	0.496634826719	-1.082166277843	-2.762286002485
O	0.992716964499	0.057768912173	-4.536695893968
C	-0.832492959644	3.098719468684	0.684302903327
C	-0.204451482671	3.562457492331	1.966846674362
H	0.289917044047	4.536962125491	1.840425703986

H	-0.969349853960	3.649377416911	2.751113206038
C	-2.487309027899	4.913902347007	0.767921255207
H	-2.727305733953	5.617079991028	-0.042842090803
H	-1.734747670205	5.410308333039	1.393722213724
C	-3.726436902252	4.631440799846	1.596406936120
C	-4.783246744430	5.538300461440	1.622369358968
H	-4.750364181188	6.450355141662	1.023921697984
C	-5.878224626018	5.248076463090	2.434598696163
H	-6.723795643199	5.935784435947	2.488017491510
C	-5.882871534991	4.067683706984	3.163687878554
H	-6.711313045369	3.780790377649	3.809011919088
C	-4.782253090394	3.207650787498	3.059639592198
C	-4.769152052667	1.909407073266	3.793970487205
C	-3.741970272629	0.983297596191	3.604754132379
H	-2.928549815661	1.194917116869	2.914303830516
C	-3.789619312949	-0.215936109038	4.307787893253
H	-2.988215271523	-0.943267592995	4.178587763393
C	-4.855940278403	-0.444458967907	5.171220355302
H	-4.935051252357	-1.367889450644	5.746090942025
C	-5.834507703844	0.543141661116	5.289572618779
H	-6.687680676411	0.401239040081	5.958906294051
C	-2.590624500997	3.104339579769	-0.956331864957
H	-1.840182955195	2.705505513355	-1.648893942654
H	-3.147184765696	3.887199675846	-1.484989279973
C	-3.528028961531	1.967462851120	-0.497826762297
H	-3.008486341597	1.328482292510	0.226917648117
H	-4.418222628678	2.371662793945	-0.001835551639
C	-5.194772552329	1.522456176642	-2.304896124487
H	-5.924906963228	1.843605269259	-1.548364885578
H	-5.632260870392	0.642377894071	-2.795613472866
C	-4.997481936645	2.626523073483	-3.333238292743
C	-6.105744050774	3.425949901602	-3.693461354096
H	-7.077583613034	3.267661748292	-3.223812371448
C	-5.914107117176	4.434108698814	-4.654318956429
H	-6.745931479082	5.073282250845	-4.954441564462
C	-4.664601396901	4.616037028801	-5.195981046287
H	-4.450275048934	5.397066488313	-5.923071232459
C	-3.582229882859	3.756239417317	-4.777292302965
C	-2.303492988248	3.911750432608	-5.277733877136
C	-1.180133381208	3.011891776273	-4.883565453253
H	-1.236421050414	2.444602830596	-3.956882130029
C	-0.142543165988	2.863467344362	-5.749534330299
H	0.656913685558	2.156932119681	-5.524434176454
C	-0.119227600226	3.656109981902	-6.930849494759
H	0.691933144565	3.580521151607	-7.655067812648
C	-1.094897456605	4.724363467964	-7.058150448866
H	-0.942312654211	5.478969209536	-7.839256092599
C	-3.163678551298	0.174095106657	-2.065701687938
C	-3.514217324867	-0.604109491274	-3.300173081947
H	-3.643697110050	0.085626555696	-4.145843942109
H	-4.443639785111	-1.175487078574	-3.162515226886
H	0.545289590314	2.817492247562	2.255629329940
H	-2.691898725659	-1.297258137989	-3.506028443612
N	-1.902372258268	3.722184451962	0.175474434283

N	-3.718790850720	3.495953775284	2.297163882003
N	-5.802552524040	1.694002702155	4.620319194444
N	-3.976110999818	1.138598817655	-1.614341243579
N	-3.791627121044	2.755467137750	-3.835479091926
N	-2.092901380107	4.907050611599	-6.263182494882
O	-0.357078340129	2.108292041611	0.087137425467
O	-2.105210619742	-0.084939349693	-1.452815370549

MEX between T1 and 5D_1

Electronic energy = -3720.800472953143 (hartree)

C	0.492656575002	-3.364902855931	0.690320258726
C	-0.498267626085	-3.882298254599	1.693397452008
H	-0.922402051890	-4.845880198390	1.374211920724
H	-0.016803776852	-4.011080275557	2.672785642538
C	2.062041649607	-5.179804417342	1.222530403248
H	2.550477441894	-5.851024456074	0.500896932366
H	1.156470277561	-5.698634765751	1.561805840937
C	2.978191988569	-4.931935117506	2.407036829994
C	3.966173276115	-5.853482334624	2.747558877234
H	4.113309309570	-6.758673688294	2.156133207668
C	4.756423028311	-5.585408937619	3.864157648682
H	5.536328268621	-6.284785882812	4.169673954180
C	4.547840636043	-4.410913380417	4.573438550738
H	5.143102474730	-4.139961867283	5.443776871433
C	3.540099747185	-3.537657629020	4.146677064507
C	3.310415411623	-2.243370324276	4.851570551847
C	2.335816223801	-1.348035378388	4.409167911880
H	1.722882721930	-1.581879840529	3.542307065934
C	2.171980314059	-0.149262985529	5.094631177168
H	1.405001645686	0.552573891284	4.767203817841
C	2.986126863760	0.110813565640	6.192053450412
H	2.894759484120	1.035693684284	6.762733809461
C	3.932706050176	-0.848359109860	6.554955597398
H	4.590945262431	-0.680669981707	7.412108287747
C	2.678514806611	-3.301233673991	-0.311865595808
H	2.177332243504	-2.868259485419	-1.186266167330
H	3.377035323749	-4.066008091331	-0.672935399314
C	3.423240229420	-2.191266171773	0.462750268367
H	2.705417370966	-1.596657914447	1.041013027937
H	4.141541252035	-2.621233945023	1.171025946960
C	5.530794444122	-1.642513304260	-0.760887479861
H	6.051221404709	-1.904609922602	0.171401018350
H	6.039284262142	-0.755912429585	-1.160606342485
C	5.633681173803	-2.781999269234	-1.758678825271
C	6.664643079525	-3.714543743544	-1.678014956760
H	7.411845942258	-3.654565917077	-0.885018635771
C	6.711812416340	-4.723997085828	-2.638743103355
H	7.504954615084	-5.473021815576	-2.615093968456
C	5.728439774688	-4.773575186192	-3.616866564901
H	5.705570659049	-5.544231093111	-4.385089793400
C	4.722587183835	-3.798707311755	-3.609099628066
C	3.622989871618	-3.833647338664	-4.616388757900
C	2.573746235419	-2.913383174181	-4.573702106785
H	2.536711573684	-2.148765686607	-3.801120769772
C	1.570572898788	-3.001344411612	-5.533364134141

H	0.752988000210	-2.280830394884	-5.515400317311
C	1.653563816753	-4.000545230487	-6.497516288058
H	0.894412278708	-4.107113127860	-7.273352297524
C	2.741161547175	-4.873652866420	-6.453941483969
H	2.840776802237	-5.671671122013	-7.195226157747
C	3.488125331960	-0.308610075197	-1.038479030205
C	4.143218476023	0.526726824357	-2.100489505168
H	4.525885891293	-0.121109165898	-2.901591919549
H	4.976405483098	1.115747804458	-1.690172882955
H	-1.306811382116	-3.146409528519	1.768769710653
H	3.386310433025	1.209589511000	-2.501381132388
Eu	-0.006980813413	-0.119151433684	-0.555287928708
N	1.678071653152	-3.964782104597	0.521674987462
N	2.761499372059	-3.807098197230	3.089719354704
N	4.099702524475	-2.000150026771	5.907655893997
N	4.157104803364	-1.298268920023	-0.431274580669
N	4.689370304597	-2.815961668986	-2.700119008875
N	3.706455257008	-4.802322761561	-5.539333222578
N	-0.466168774303	-0.221001858079	2.340770150357
N	0.556084865056	-0.007565719508	-3.419107628736
O	0.211092787666	-2.354651821817	0.009602772049
O	2.302178339069	-0.078786073932	-0.719495899122
O	-1.418517705794	-0.307151410804	1.505225354007
O	0.693387390617	-0.077047100588	1.846647067137
O	-0.652293542555	-0.275972948844	3.533913906364
O	0.349034158057	1.040456015996	-2.731445679090
O	0.437549412610	-1.108622657886	-2.799259893580
O	0.855555482468	0.042700846313	-4.588539405717
C	-0.826180769864	3.091309899594	0.632684438020
C	-0.184429067569	3.581298687492	1.898655740616
H	0.309513540860	4.552475821500	1.747819329661
H	-0.941814827542	3.685405045048	2.688222928913
C	-2.469745158527	4.916997706031	0.690117438677
H	-2.718001359263	5.603524434561	-0.132359282246
H	-1.709226774354	5.425547651771	1.296268789182
C	-3.700596001514	4.654038393611	1.537843214337
C	-4.752960320197	5.566234101011	1.562999875412
H	-4.721781746736	6.470730717818	0.953059110222
C	-5.841780135961	5.290498402529	2.388492370086
H	-6.684024865897	5.982394091857	2.440723887685
C	-5.845892340908	4.118269600461	3.130773462153
H	-6.670585336259	3.842011547958	3.785476690792
C	-4.749676375371	3.252628501265	3.027646802383
C	-4.736643922582	1.961582755975	3.774601852642
C	-3.714673723903	1.029434382579	3.586475028146
H	-2.904982257859	1.231889710030	2.888826698464
C	-3.762730228797	-0.163607516938	4.299958572730
H	-2.965285754004	-0.895416347315	4.171636991901
C	-4.824163694598	-0.380006433659	5.172564172496
H	-4.903384487984	-1.298055836525	5.755951207137
C	-5.797705185660	0.612807002148	5.288698360755
H	-6.646933940012	0.480412644373	5.965003407437
C	-2.596344361248	3.072669743277	-0.995943111395
H	-1.855425061206	2.660619835037	-1.691536314590

H	-3.157835024331	3.847061028590	-1.531850097785
C	-3.531643485751	1.949723765381	-0.499978267751
H	-3.001129042534	1.317941628049	0.223045711023
H	-4.407154041869	2.368156475605	0.009929553332
C	-5.239903071423	1.489737256493	-2.262466125507
H	-5.944148439465	1.851848252198	-1.499481768392
H	-5.711031012594	0.605269657813	-2.713644000092
C	-5.045969809446	2.554668226704	-3.331290054702
C	-6.167262219657	3.347513984054	-3.712547533820
H	-7.135225948508	3.200007575209	-3.231764019087
C	-5.986898870586	4.317782338917	-4.720113841678
H	-6.824731697669	4.937776973379	-5.042131146782
C	-4.746653821891	4.475592280511	-5.280433121916
H	-4.539843409596	5.211147464110	-6.055194512924
C	-3.646106992421	3.634853633052	-4.829564888264
C	-2.370729691428	3.771695699413	-5.345712860713
C	-1.263995280475	2.922415283966	-4.901208892789
H	-1.447605201519	2.168672662450	-4.138822050583
C	-0.021832663294	3.089159748725	-5.453708173023
H	0.796744994996	2.442382821258	-5.138900810352
C	0.154403274030	4.081995267260	-6.436230604603
H	1.119953564182	4.252718618666	-6.912322346764
C	-0.975854520118	4.877908376527	-6.814469767188
H	-0.842860186334	5.652718378797	-7.578087732864
C	-3.213866015553	0.128399129122	-2.044331187144
C	-3.601866036155	-0.676590189235	-3.250243861281
H	-3.778723202499	-0.009258918297	-4.104943994217
H	-4.514638446592	-1.260395524834	-3.060735664171
H	0.566891003564	2.841486436213	2.196084196983
H	-2.777887574227	-1.361411693493	-3.476599814191
N	-1.894243441651	3.711761164819	0.115910879062
N	-3.691444821887	3.527663884003	2.253042782035
N	-5.765568056307	1.757818754250	4.609420551416
N	-4.011664020513	1.104917507272	-1.590994029788
N	-3.853053756396	2.660308440991	-3.845772636607
N	-2.173437158682	4.758554479651	-6.322175187747
O	-0.364519277079	2.081631225925	0.058078918084
O	-2.140590833218	-0.121980453416	-1.454769944198

MEX between T1 and ⁵D₂

Electronic energy = -3720.798989448296 (hartree)

C	0.491163574330	-3.341403690745	0.677093402064
C	-0.501650854500	-3.874788158665	1.670696536777
H	-0.917781383615	-4.837502016154	1.337798295622
H	-0.024130099169	-4.012415022190	2.650733489849
C	2.067638426699	-5.146935861191	1.215082703533
H	2.572725913205	-5.811818819634	0.499302816683
H	1.163072182484	-5.676130566392	1.540607010076
C	2.963658276958	-4.895587588744	2.415008394013
C	3.935736065509	-5.824601226101	2.780145328667
H	4.084520721127	-6.735834874599	2.198243688104
C	4.706388627274	-5.559148612875	3.911166357255
H	5.472529550988	-6.265091384884	4.235876721492
C	4.493886433468	-4.379842624612	4.610781006622
H	5.071910340207	-4.109707023559	5.493225828219

C	3.499547499405	-3.501574079681	4.162290479127
C	3.257826359428	-2.212228006395	4.871082341082
C	2.269310166561	-1.327549440779	4.439305473894
H	1.655567279032	-1.563515785206	3.573863258017
C	2.089575989288	-0.137150816058	5.136070083612
H	1.310498113912	0.555899757788	4.818157889450
C	2.902988812214	0.125630803311	6.233173736767
H	2.799286274311	1.044171854928	6.812026403919
C	3.863717926513	-0.823418596725	6.585341395877
H	4.520425931382	-0.655000733546	7.443456067758
C	2.677755246894	-3.269784946004	-0.324057145570
H	2.169678800366	-2.822653883439	-1.187388402402
H	3.365728171875	-4.035696682781	-0.702233988558
C	3.439447404485	-2.174951009178	0.454859741800
H	2.731964184362	-1.578900938953	1.044438099677
H	4.159176421024	-2.618958467115	1.153005645379
C	5.546373700585	-1.631849117382	-0.773117550575
H	6.070535324709	-1.890833136117	0.158028700320
H	6.055163272121	-0.748569857923	-1.179546174742
C	5.642244121029	-2.776910797154	-1.765221165539
C	6.666743605039	-3.716069815130	-1.678736783718
H	7.413333950590	-3.656906399449	-0.885112029125
C	6.708344511011	-4.730774456425	-2.634193060551
H	7.496860398677	-5.484493493142	-2.605889767757
C	5.725336670785	-4.779137696303	-3.612684333551
H	5.697921302266	-5.553795995191	-4.376773591037
C	4.725442145232	-3.798127949581	-3.610404521284
C	3.625004621044	-3.833033457994	-4.616750324530
C	2.581041643824	-2.907029210055	-4.576308676952
H	2.550340688517	-2.139146455465	-3.807053259967
C	1.576116256992	-2.993322212648	-5.534107746122
H	0.762588580267	-2.268154779313	-5.518457290449
C	1.651685820094	-3.997496871536	-6.493671771976
H	0.890961792501	-4.103248196942	-7.268098531343
C	2.734350517313	-4.876710283004	-6.447665970763
H	2.828093042086	-5.678609899800	-7.185505051968
C	3.509584096310	-0.284542405051	-1.035638607392
C	4.162939400492	0.552740623177	-2.097047892822
H	4.544190190156	-0.092651763799	-2.900702926006
H	4.996907333874	1.140351048303	-1.686114867677
H	-1.315537895526	-3.145534007400	1.751070288821
H	3.406047873670	1.237309570902	-2.495322032595
Eu	0.018033340912	-0.087002424426	-0.564349659974
N	1.680336468878	-3.934929423795	0.511252006816
N	2.741881384273	-3.766449301075	3.089213025884
N	4.045806573486	-1.966634014548	5.927634490654
N	4.175029881237	-1.282377491720	-0.438475340283
N	4.698484816170	-2.809651492221	-2.707276067403
N	3.701690783578	-4.806695783629	-5.535051478371
N	-0.466248787188	-0.228683600492	2.322778911263
N	0.622404875007	0.022697703667	-3.418783692136
O	0.206534739074	-2.328778476550	0.001255913644
O	2.326965412597	-0.049349258478	-0.706959668259
O	-1.412439428911	-0.287666495603	1.478748074925

O	0.697448998574	-0.077982226034	1.843480169911
O	-0.662552100500	-0.317403089114	3.512922392782
O	0.397161632232	1.072844261368	-2.742365523291
O	0.487050339801	-1.076757779799	-2.798297319489
O	0.951911978433	0.064616741777	-4.580900634763
C	-0.817407742784	3.101070738547	0.664382496468
C	-0.196197016668	3.580386695466	1.944812573620
H	0.285445618349	4.560358605407	1.810176905832
H	-0.962261453393	3.664201346863	2.728247363451
C	-2.497330714196	4.888881522811	0.755860735737
H	-2.781874022999	5.578894212151	-0.051848093222
H	-1.747523891304	5.418127182760	1.358177433285
C	-3.704771273428	4.579554812170	1.625480724337
C	-4.732965622152	5.546542138388	1.735443416519
H	-4.670416844409	6.484114129386	1.181655121990
C	-5.827509566712	5.264766509367	2.574138758342
H	-6.632786928444	5.991214843005	2.691319633324
C	-5.867975658623	4.062054097966	3.234466676448
H	-6.689732380990	3.778179995527	3.888970782447
C	-4.785354993176	3.120782576873	3.062345981018
C	-4.795011818187	1.888818028614	3.716610795601
C	-3.707842917378	0.925247634431	3.565437140871
H	-2.911718640150	1.126726199302	2.852889982110
C	-3.705187978602	-0.208458209905	4.336548016446
H	-2.879235753102	-0.913781071258	4.250547248006
C	-4.766617720608	-0.422428001945	5.234887697775
H	-4.803702629680	-1.298771674746	5.882223934954
C	-5.833429649951	0.534438888907	5.267616085266
H	-6.689606343677	0.350128226474	5.925919698829
C	-2.577632668216	3.089375440880	-0.976210251423
H	-1.824317532922	2.683873486513	-1.662687398041
H	-3.128919752788	3.870940984016	-1.513322506061
C	-3.522802029043	1.963303235970	-0.509096488140
H	-3.004822509763	1.323408327440	0.215581693812
H	-4.405201550346	2.377429220025	-0.009105323525
C	-5.219434017897	1.514890791677	-2.286421546592
H	-5.944047405956	1.809963828251	-1.514474404407
H	-5.645623771484	0.635087041078	-2.786785848210
C	-5.047612734282	2.637132804222	-3.296850364672
C	-6.108065846837	3.490935728188	-3.594440253692
H	-7.069158791732	3.385363243019	-3.088186504259
C	-5.905020570977	4.476898783178	-4.557965613562
H	-6.709536944017	5.164538344705	-4.823980564852
C	-4.665114001546	4.574951240767	-5.175275546631
H	-4.446260188212	5.323812470589	-5.934328567557
C	-3.660628676408	3.670686221876	-4.811764506295
C	-2.320050817409	3.722065162108	-5.463588255196
C	-1.281800478928	2.881508679479	-5.055060001283
H	-1.421797541441	2.190161188012	-4.225755429310
C	-0.067321089248	2.945010265280	-5.731168428158
H	0.743582747113	2.278833403017	-5.436220538145
C	0.065014520908	3.846563701770	-6.782871478907
H	0.992293785305	3.922829466225	-7.351940887711
C	-1.023697913053	4.658978552587	-7.100200451787

H	-0.954763570632	5.386926808270	-7.913480050005
C	-3.172582220294	0.177401748476	-2.085217497830
C	-3.533701104002	-0.602476311936	-3.315285243118
H	-3.683675582826	0.085691526610	-4.158803776022
H	-4.454858085675	-1.183715096872	-3.164243807891
H	0.564087997095	2.848994899139	2.240112608595
H	-2.707199194959	-1.286565535742	-3.534170054571
N	-1.891222020308	3.715403946532	0.152079318282
N	-3.700107349378	3.425247723456	2.248759485323
N	-5.880683640560	1.623406893693	4.557200423882
N	-3.984128891478	1.136929159021	-1.621044758562
N	-3.856412460635	2.719172304882	-3.888778413806
N	-2.191574292846	4.606578727215	-6.462141289270
O	-0.334496957932	2.109911495734	0.074800068745
O	-2.103971373612	-0.073588263752	-1.487100571777

EuLH(NO₃)₂

S0

Electronic energy = -1853.145856220905 (hartree)

Eu	-0.008576304444	0.001975075776	0.013497147226
N	-1.444548264419	2.209347932031	-0.000680718914
N	0.364302590683	1.768083925375	-1.900116498423
N	1.665694294772	-0.682350752130	-1.875775154908
N	-0.136764837541	-2.546889517666	-0.547023443208
N	-0.435458436419	-1.621266559172	2.047168383764
N	-0.111053730974	0.987972508345	2.462443013668
C	1.251576997481	3.708633184773	-3.665993385177
H	1.610610147821	4.476454453717	-4.352122319835
C	1.569292908438	2.371870247872	-3.874652240968
H	2.172301733067	2.062933176746	-4.728662872881
C	1.098381362296	1.427398907495	-2.966054092820
C	1.336610489323	-0.049701181634	-3.156596419182
H	2.117792986697	-0.219950640088	-3.917196406492
H	2.342941675700	-2.440438832372	-2.895686142118
C	-2.445944947485	2.349798685272	0.877328831682
H	-2.827825007734	1.420088145065	1.304801545336
C	-2.981720634812	3.583168052605	1.225513733147
H	-3.801011232619	3.641898246963	1.941033214531
C	-2.436816238428	4.722410535365	0.643323042540
H	-2.809173107729	5.714493190158	0.902189166101
C	-1.422806456840	4.581934766154	-0.298829880482
H	-1.007270485017	5.464684030686	-0.781250707091
C	-0.964076308496	3.303590529225	-0.620728851621
C	0.010259178466	3.050097847678	-1.722759553960
C	0.450176800152	4.055254425524	-2.584514481308
H	0.164810861845	5.094437453849	-2.434396048149
C	1.846077775212	-2.142301596022	-1.956090841057
H	2.508805348143	-2.429377312117	-1.127567073795
C	0.509737323254	-2.860709700085	-1.832489777076
H	-0.175690173003	-2.524702576587	-2.623250898823
C	0.317724496524	-3.377812624877	0.572242159671
H	1.402069705260	-3.228813992711	0.700719828554
C	-0.352297276678	-2.942722013365	1.851697513799

C	-0.807579925499	-3.861695091626	2.793842465470
H	-0.732111857979	-4.931977943395	2.601579776347
C	-1.352374564905	-3.381977680824	3.979033530548
H	-1.725748439284	-4.072612370611	4.735951433119
C	-1.395559554230	-2.010580375464	4.199847624268
H	-1.783687641300	-1.625586388403	5.140755161456
C	-0.913697174442	-1.153297931368	3.209989292055
C	-0.791133616552	0.320106186088	3.413135143242
C	-1.271315728275	0.965742468204	4.553608795855
H	-1.849863078107	0.425991307875	5.301060835757
C	-0.990744069412	2.315587051615	4.738764373783
H	-1.355954338769	2.833094628060	5.626798668816
C	-0.221658950879	2.982380624081	3.791193984440
H	0.053818095572	4.029284153039	3.912624555514
C	0.186982406448	2.277604699832	2.666123232550
H	0.786603292579	2.748558321815	1.884396676247
H	0.658937184104	-3.947113062919	-1.960866549965
N	-2.650206968093	-0.507465183985	-1.116412409821
O	-1.610603737276	-0.411746362365	-1.848572526209
O	-2.413757330568	-0.597696051346	0.139979476868
O	-3.760385251517	-0.514602214435	-1.563252599152
N	2.684906987855	0.411515289057	1.059458818386
O	2.165111458698	-0.749919170248	0.974719871992
O	2.041566796475	1.331929304728	0.442237286367
O	3.694647255184	0.628190722800	1.664201466164
H	0.398868632446	-0.489852336657	-3.532904829982
H	0.143042617971	-4.451919990773	0.390099368043
H	-1.141577166063	-2.696037112445	-0.652205858738
H	2.540698693268	-0.273140982191	-1.544654925086

T1

Electronic energy = -1853.034858801863 (hartree)

Eu	0.072407649106	0.016206681899	0.093243498466
N	-1.342770864841	2.235053851078	0.048517020458
N	0.544667006570	1.777720180486	-1.764940810149
N	1.657686777827	-0.668433871227	-1.879653169086
N	-0.125514750018	-2.524063099236	-0.517039250954
N	-0.412024179105	-1.641747864022	2.086420426736
N	-0.082636437704	0.959115986135	2.538404068674
C	1.138223233218	3.761814002053	-3.711895612600
H	1.489989378640	4.494293360000	-4.438932764222
C	1.215477245472	2.377269839573	-4.005391890588
H	1.571754667874	2.020707229105	-4.971642629932
C	0.992970110535	1.432206332869	-2.931880970111
C	1.312242228182	-0.024189089734	-3.146213443865
H	2.105083386837	-0.137483968521	-3.906888344111
H	2.299939801015	-2.427924262256	-2.923704013370
C	-2.405365050831	2.389172280141	0.823119694088
H	-2.762710640133	1.482920197329	1.319015366141
C	-3.062668698665	3.612349139620	1.025373827752
H	-3.933086524467	3.658016388947	1.678407099159
C	-2.560217736614	4.753416660764	0.386025482970
H	-3.029046603329	5.726464259378	0.537342179697
C	-1.473236525669	4.629181729924	-0.451060490805
H	-1.080448975070	5.500695983794	-0.971571017598

C	-0.878310120958	3.338769928149	-0.655537167460
C	0.131662984696	3.115402521217	-1.583869934681
C	0.662264503689	4.153617883614	-2.497493575311
H	0.646588321748	5.203861578850	-2.209296145080
C	1.826310282052	-2.129387300296	-1.972267020200
H	2.503739797960	-2.423606676271	-1.158585108422
C	0.486322954928	-2.835610054273	-1.819270179651
H	-0.214377393555	-2.487298301857	-2.591160787415
C	0.327736192130	-3.381764278879	0.582608462134
H	1.414872406471	-3.249819163437	0.704981767567
C	-0.328544986924	-2.960561758293	1.874117743468
C	-0.777873763792	-3.890788479436	2.808528919558
H	-0.702360817498	-4.958731077459	2.603559759781
C	-1.316527672575	-3.425957574478	4.002298858589
H	-1.682684697247	-4.126161170593	4.753948175857
C	-1.365362723771	-2.056889338949	4.237611350948
H	-1.750264581920	-1.682697495146	5.184290810683
C	-0.891775978676	-1.188102102727	3.254368659078
C	-0.784912165504	0.284923448896	3.467666055657
C	-1.306323409612	0.926071901799	4.592432865648
H	-1.904327039220	0.381309784120	5.320793058258
C	-1.046671480886	2.279447659683	4.782252607559
H	-1.445654741355	2.794990290739	5.656777105990
C	-0.257320781778	2.954300561733	3.856729962693
H	-0.000183847642	4.005141559710	3.984111723542
C	0.195308922899	2.252067815807	2.747006176448
H	0.814038916432	2.728165154143	1.983218562120
H	0.622123803683	-3.922436790790	-1.958811782457
N	-2.564226992277	-0.418155304355	-1.095578401656
O	-1.512309656192	-0.313922961788	-1.809156987401
O	-2.348512022653	-0.560240384983	0.158292015892
O	-3.667656926290	-0.384924090228	-1.559105753182
N	2.792396509353	0.241335846379	1.136379606334
O	2.214083080944	-0.887738828043	0.982346932852
O	2.182602055438	1.229609428178	0.601558613740
O	3.825333419584	0.362323872091	1.728285299121
H	0.397235565326	-0.489185639441	-3.551128245283
H	0.134932861737	-4.449882805909	0.383415204782
H	-1.136135820845	-2.643521943058	-0.602058600445
H	2.539407803245	-0.264465132525	-1.559262956395

MEX between T1 and S0

Electronic energy = -1853.015683205275 (hartree)

Eu	0.154510451359	0.033383162109	0.198649053253
N	-1.251451779861	2.300046657337	-0.114824246630
N	1.037221338122	1.831806296238	-1.484877913482
N	1.575676907175	-0.679643309354	-1.928394266860
N	-0.132647351168	-2.486229212063	-0.456862867847
N	-0.310152874630	-1.647488387056	2.166643191186
N	-0.333352469663	0.994970236882	2.577552733246
C	1.001690129926	3.847787815537	-3.550798811623
H	1.258444535330	4.500208346431	-4.388262918641
C	0.638994860001	2.502998737756	-3.785172674121
H	0.440323899633	2.140120576297	-4.795338722149
C	0.898463933162	1.498816015209	-2.718944975976

C	1.133687159147	0.064911415602	-3.100933930198
H	1.848564750788	0.022284540187	-3.945314293469
H	2.025181515811	-2.411702707743	-3.109527534155
C	-2.454329853486	2.456537467790	0.445430733228
H	-2.859361759167	1.571960508589	0.942089512745
C	-3.177076652686	3.646737309974	0.415601758750
H	-4.155482830734	3.700869870058	0.890986186322
C	-2.605159678010	4.755735993595	-0.215712881525
H	-3.132949716451	5.709755208455	-0.249202354647
C	-1.355629107642	4.629969223338	-0.792385484375
H	-0.871130145990	5.481509030813	-1.270717884135
C	-0.699211488459	3.373451843352	-0.763421701189
C	0.602571789493	3.197610969200	-1.293561929323
C	1.230027815784	4.179443887760	-2.234043645705
H	1.895728368740	4.984426615015	-1.916099146858
C	1.671591788359	-2.135751319466	-2.100835818803
H	2.428245294687	-2.485591859644	-1.384484909193
C	0.333954612835	-2.804040124848	-1.816321636156
H	-0.426654770112	-2.425981630840	-2.513149345258
C	0.421627189258	-3.343846868560	0.595297609443
H	1.509070029259	-3.177276110317	0.651786455097
C	-0.176118020311	-2.960020252917	1.926775494004
C	-0.560674880253	-3.924794884947	2.853852070197
H	-0.437559414778	-4.984057640102	2.628576322949
C	-1.104656506363	-3.507659260510	4.062061714974
H	-1.424180589858	-4.236133768213	4.807603134006
C	-1.229152538093	-2.147313242636	4.314881342403
H	-1.651076380857	-1.810148805656	5.259166314721
C	-0.810724087568	-1.236929239733	3.344368159305
C	-0.808726507098	0.237246598126	3.580566310167
C	-1.199443471662	0.803762723732	4.795205130961
H	-1.597601670009	0.189999320386	5.600335745038
C	-1.056810958963	2.174059086390	4.984045935187
H	-1.351338710556	2.630396118901	5.929579844746
C	-0.506328542263	2.943161424203	3.964890027199
H	-0.344405191097	4.014268693598	4.078718061035
C	-0.164629207678	2.306571066906	2.780352959959
H	0.275915412071	2.865442513621	1.953392458939
H	0.428192546740	-3.892692320367	-1.974796776373
N	-2.471504222685	-0.331045196319	-1.048515835639
O	-1.411490941707	-0.190406118452	-1.743835289014
O	-2.271752609435	-0.520378853561	0.199737467754
O	-3.568753399832	-0.271386530125	-1.523932353366
N	2.866185475370	0.060409031505	1.296465750296
O	2.316584399756	-0.994161462715	0.808296313821
O	2.180524951298	1.119595945016	1.173514731428
O	3.941771554888	0.031832805381	1.820532418113
H	0.173734232063	-0.338702258476	-3.460018683369
H	0.244722797364	-4.414431741643	0.395372458294
H	-1.147760263979	-2.594588269722	-0.434963132210
H	2.491428114657	-0.327433149292	-1.647023526620

MEX between T1 and ⁵D₀

Electronic energy = -1853.034855434425 (hartree)

Eu	0.067590507953	0.017028933104	0.090842309402
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N	-1.346523115348	2.235461139962	0.043681136311
N	0.541005880099	1.776873309704	-1.768381972747
N	1.657048454818	-0.668401716476	-1.878803106627
N	-0.127222217693	-2.524573900710	-0.518004479258
N	-0.413660062206	-1.641665446850	2.086242755104
N	-0.090335463616	0.960717523996	2.536066468663
C	1.142183938043	3.760558113159	-3.712950966683
H	1.495482390230	4.493111199201	-4.439171315933
C	1.221205828264	2.376087350605	-4.005964305721
H	1.581189587928	2.019518400399	-4.970829492974
C	0.993838824684	1.431235965517	-2.933616696205
C	1.312551772315	-0.025552866104	-3.146392059236
H	2.105809007776	-0.140015090276	-3.906428850995
H	2.302352388318	-2.428294836356	-2.920246977055
C	-2.409139346317	2.390485715513	0.817921919837
H	-2.768813384816	1.484174146159	1.312018731739
C	-3.063364050332	3.614980537890	1.022711189547
H	-3.933817181442	3.661588068680	1.675621664498
C	-2.557431496438	4.756276122114	0.386412576256
H	-3.023231421906	5.730369828076	0.540310725325
C	-1.470773836749	4.631048616226	-0.450876273762
H	-1.075253072796	5.502761896369	-0.968967894558
C	-0.879245928835	3.339436639686	-0.658344946567
C	0.129764619084	3.114911549594	-1.587354926029
C	0.661960264204	4.152592030243	-2.500239461415
H	0.643538486041	5.203146705591	-2.213451908123
C	1.826542176167	-2.129284818194	-1.970048438427
H	2.502434473332	-2.422554752565	-1.154705927728
C	0.486614398775	-2.836045427111	-1.819278249573
H	-0.213025630521	-2.488132329456	-2.592292472757
C	0.326413702116	-3.381351583968	0.582096494231
H	1.413423051118	-3.248515190423	0.704700065162
C	-0.330146818344	-2.960448788020	1.873466152194
C	-0.779346741144	-3.891214654900	2.807360241389
H	-0.704066082881	-4.959019513651	2.601590427452
C	-1.317772427493	-3.427047484847	4.001464599274
H	-1.684055657919	-4.127620742984	4.752709234954
C	-1.365606870150	-2.058176125057	4.237821711145
H	-1.750377226967	-1.684754713779	5.184818904406
C	-0.891557072389	-1.188758460242	3.255274463899
C	-0.783891670450	0.284025958961	3.470062472519
C	-1.294223863122	0.922103295408	4.601679336845
H	-1.883841124909	0.375100237823	5.335124240462
C	-1.034190613254	2.275245745608	4.792162035901
H	-1.424658100463	2.788115805982	5.672083807826
C	-0.255160158423	2.953149936720	3.860201059829
H	0.002003938420	4.004011401636	3.987308555165
C	0.187749077716	2.253663175174	2.744894391062
H	0.798924470303	2.732369957696	1.976727189736
H	0.623115234551	-3.922834973103	-1.958449979806
N	-2.566206555018	-0.424350410905	-1.102020563964
O	-1.513172289629	-0.316914226040	-1.813507116145
O	-2.352719561359	-0.561995634802	0.152728912119
O	-3.668609146895	-0.398082297576	-1.568390711487

N	2.783958268078	0.252035509357	1.139955255019
O	2.210339457156	-0.879295237274	0.985091019217
O	2.173405699714	1.237247801104	0.600293247642
O	3.813389657644	0.377844292162	1.736959687348
H	0.397631477169	-0.490818721905	-3.551139000642
H	0.134612512148	-4.449724899258	0.383278786641
H	-1.137573878589	-2.645767805712	-0.603943792882
H	2.538289784235	-0.263811730885	-1.557827970824

MEX between T1 and ⁵D₁

Electronic energy = -1853.034304418815 (hartree)

Eu	0.066872862981	0.018525131405	0.089030545482
N	-1.342405711237	2.242539767312	0.048058822137
N	0.525824468497	1.780867644132	-1.776517435150
N	1.656842407345	-0.667146836194	-1.879018118996
N	-0.127238230494	-2.523609909712	-0.518144002763
N	-0.414143836591	-1.640637835380	2.084906462241
N	-0.090474154105	0.961031907106	2.535046962909
C	1.151110662830	3.752998837197	-3.710417144239
H	1.492364781259	4.489750980537	-4.438406792809
C	1.237473576874	2.374022179555	-4.002631753063
H	1.589044200302	2.019121438678	-4.970965352688
C	0.998801636469	1.432978055791	-2.939347551737
C	1.311789601562	-0.025910227113	-3.147855425935
H	2.105334857668	-0.143104442875	-3.907006922751
H	2.302656794602	-2.427147634403	-2.920183431194
C	-2.409196416239	2.393041640554	0.821820597547
H	-2.770020988286	1.483909647359	1.309616342399
C	-3.062921509950	3.615316388991	1.026436282152
H	-3.936060058696	3.661498665656	1.675608550028
C	-2.557071417928	4.755165749784	0.391437398575
H	-3.025973382813	5.728676347724	0.539551088384
C	-1.466566391230	4.629561069142	-0.444539339068
H	-1.076159633307	5.499432120210	-0.969799750906
C	-0.876638024711	3.343920151686	-0.645945025495
C	0.134800501933	3.113999614982	-1.590957995836
C	0.658918706394	4.143834622200	-2.496389094497
H	0.624718469373	5.196540066026	-2.217345013462
C	1.826182061869	-2.128472651354	-1.970190760633
H	2.502471239076	-2.421504377427	-1.154990522641
C	0.486418484955	-2.835476793571	-1.819411373560
H	-0.212688853596	-2.487731101163	-2.592896279261
C	0.326717125608	-3.380397680654	0.581725477338
H	1.413634933838	-3.247487268923	0.704475509959
C	-0.330092969543	-2.959520824896	1.872789262970
C	-0.779228926006	-3.890471675973	2.806701277191
H	-0.703692384840	-4.958312408166	2.601067264348
C	-1.317408044610	-3.426546466315	4.000963784354
H	-1.683736706630	-4.127142541809	4.752231426319
C	-1.365581785655	-2.057640659659	4.236986325995
H	-1.750077947106	-1.684224789199	5.184123555054
C	-0.891515140325	-1.188204109546	3.254356868079
C	-0.784403196984	0.284514281608	3.468956788850
C	-1.294294949497	0.922281451675	4.600997887498
H	-1.884012484999	0.375152774704	5.334312044631

C	-1.034410831300	2.275393834317	4.791767680752
H	-1.424922933992	2.788135495884	5.671749122167
C	-0.254788590212	2.953052583037	3.860135514836
H	0.002403244290	4.003895876982	3.987349096101
C	0.187935816269	2.253802809790	2.744612901751
H	0.799658785907	2.732408239600	1.976885263166
H	0.623634987197	-3.922268640388	-1.958190058308
N	-2.567314854418	-0.424134356059	-1.101859266194
O	-1.514765497971	-0.317316786627	-1.813861443832
O	-2.353241898956	-0.560235278332	0.153172055569
O	-3.670004075524	-0.397872079588	-1.567466497136
N	2.783017885945	0.252360245045	1.139322403881
O	2.209014950064	-0.878622874073	0.984393757310
O	2.173346692488	1.237588862518	0.598085649402
O	3.812893248872	0.377758988365	1.735549385232
H	0.396839979575	-0.492160295213	-3.550555982360
H	0.134603802121	-4.448753192569	0.382736672501
H	-1.137557310513	-2.645250213061	-0.603536329266
H	2.538639632091	-0.263520989320	-1.558479453351

MEX between T1 and ⁵D₂

Electronic energy = -1853.032585668572 (hartree)

Eu	0.047839662224	0.016492050805	0.072302325074
N	-1.351822945876	2.240205612790	0.057140079787
N	0.456728204368	1.773885493264	-1.826692809334
N	1.655946332373	-0.669637029952	-1.879607880971
N	-0.133525165499	-2.526871685084	-0.523734786014
N	-0.418026266628	-1.640544952995	2.077789021172
N	-0.082127968777	0.959086150031	2.530022229520
C	1.192315063899	3.742980411125	-3.708403084844
H	1.532856264417	4.491369257549	-4.424064810379
C	1.403410861621	2.375575721413	-3.957308842769
H	1.886876009624	2.033873534921	-4.871442235041
C	1.042180900693	1.435005539507	-2.948547230558
C	1.310358767799	-0.034027042993	-3.151972617841
H	2.086829959858	-0.185769399813	-3.921761109410
H	2.309317177114	-2.431170659106	-2.911329961224
C	-2.405004274370	2.394352538270	0.844974938396
H	-2.762146421956	1.487484527149	1.339781793984
C	-3.054827847121	3.619713251639	1.058510818920
H	-3.928224645571	3.665019310583	1.707703329666
C	-2.537956263071	4.762364516004	0.435847586057
H	-2.990882099649	5.740211604650	0.603762291017
C	-1.456784937511	4.633620707376	-0.409193274799
H	-1.055730690168	5.510066566464	-0.913788102807
C	-0.890827138091	3.340185212447	-0.645938729791
C	0.075099898591	3.099807106180	-1.641043838275
C	0.552681208724	4.121050078339	-2.557336670783
H	0.376528896192	5.174142120330	-2.349342144127
C	1.827089333090	-2.130307109750	-1.965040906336
H	2.497332227585	-2.420734044812	-1.144119683553
C	0.487003618802	-2.837810341465	-1.821984673485
H	-0.209083050817	-2.490953882702	-2.598657408737
C	0.322910492445	-3.380688446868	0.577299135927
H	1.409608299534	-3.244637102398	0.699128725098

C	-0.333567974146	-2.959562912669	1.867755695791
C	-0.778957846814	-3.889861240556	2.804118813296
H	-0.701605804814	-4.957747559680	2.599781752552
C	-1.316119977979	-3.424476732395	3.998205974516
H	-1.680957169121	-4.124303436381	4.750963253264
C	-1.364514951886	-2.055329562177	4.232593359391
H	-1.746525651161	-1.680535036842	5.180149463465
C	-0.893274727849	-1.186953318008	3.247571496287
C	-0.780670447476	0.284926469603	3.462192944569
C	-1.294438891063	0.924604333305	4.591495416242
H	-1.889177126032	0.379167356304	5.322010911316
C	-1.029714331713	2.276427577284	4.783770431835
H	-1.422916474178	2.790826836382	5.661633641101
C	-0.243143391414	2.951080075853	3.855645638112
H	0.017959524482	4.000761670439	3.984407021605
C	0.201596118928	2.250431026710	2.741537201833
H	0.818276608542	2.726035753441	1.975736500321
H	0.624487924516	-3.924497248601	-1.960152543413
N	-2.596180330356	-0.429907990980	-1.086902330282
O	-1.550217959927	-0.342753009275	-1.810779001235
O	-2.370140440601	-0.556602566643	0.167255923377
O	-3.703539902761	-0.396134349058	-1.540787706689
N	2.763914785982	0.276586068382	1.110268088721
O	2.193454046049	-0.858228096926	0.979666545615
O	2.149567131544	1.250473132686	0.551580060607
O	3.792860611978	0.418277677643	1.704455869291
H	0.373627118373	-0.476957567023	-3.530026616398
H	0.134297181808	-4.449724588030	0.379460946378
H	-1.142970072979	-2.653848448535	-0.613175812540
H	2.538006216211	-0.263261397160	-1.563332502468

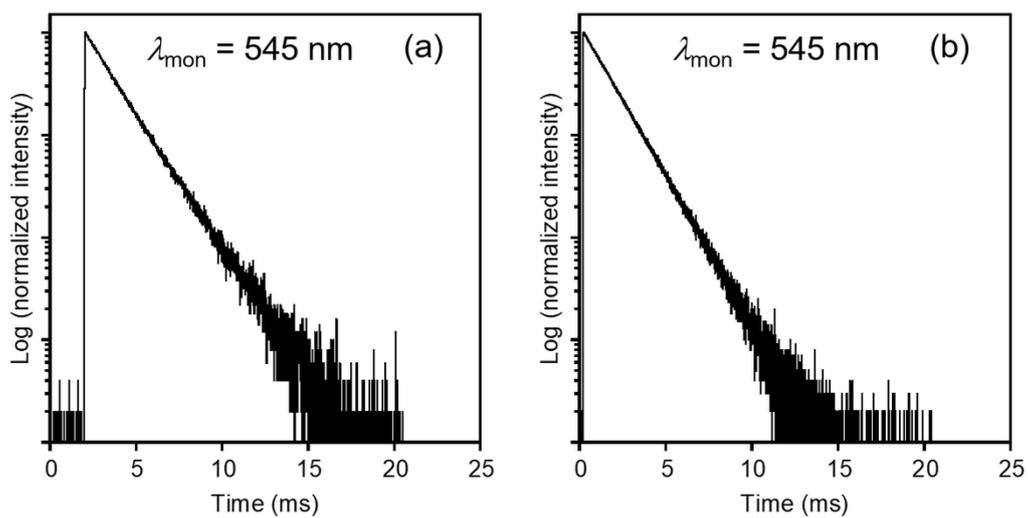


Fig. S8 Luminescence decay curves of TbLH in acetonitrile (a) and TbLC₁₈ (b) in chloroform. $\lambda_{\text{ex}} = 280 \text{ nm}$.

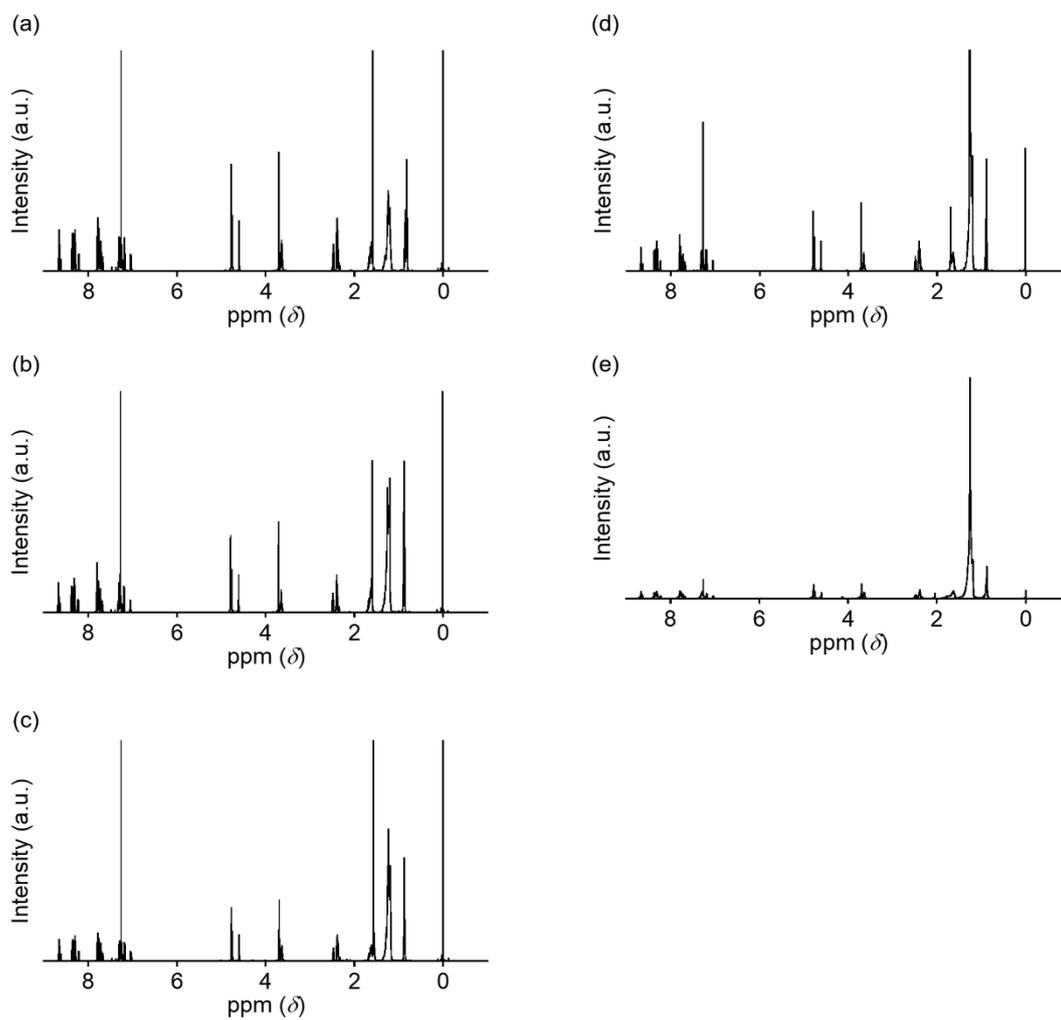


Fig. S9 $^1\text{H-NMR}$ spectra of LC_8 (a), LC_{12} (b), LC_{14} (c), LC_{18} (d), and LC_{22} (e) in CDCl_3-d . In case of LH is already published in our previous report⁷.

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