

Electronic Supplementary Information

to the paper: “Selectivity of bis-triazinyl bipyridine ligands for americium(III) in Am/Eu separation by solvent extraction. Part 1. Quantum mechanical study on the structures of BTBP complexes and on the energy of the separation”, by J. Narbutt and W. P. Oziminski

1. Structures

Table S1. NPA charges and Cartesian coordinates in the optimized structure of $[\text{Am}(\text{C2-BTBP})(\text{NO}_3)_3]$

Atom number	Number in the Figure	Atom type	NPA charge	X	Y	Z
1		Am	1.37263	0.003758	-0.23696	-0.00433
2	O2	O	-0.50856	-1.01371	0.178656	-2.28895
3	N3	N	0.76715	0.086954	0.241702	-2.94579
4		O	-0.3695	0.12116	0.418172	-4.14822
5	O2	O	-0.51548	1.151957	0.116305	-2.23809
6	N1	N	-0.43982	1.379101	2.056399	-0.01954
7		C	0.20707	0.747549	3.24221	-0.08718
8		C	-0.2271	1.460806	4.433676	-0.29175
9		H	0.24506	0.946289	5.381131	-0.39112
10		C	-0.17962	2.846335	4.389389	-0.39101
11		H	0.25395	3.41291	5.301928	-0.55033
12		C	-0.21284	3.495355	3.164717	-0.29012
13		H	0.27186	4.571996	3.074783	-0.35539
14		C	0.20229	2.720655	2.014391	-0.11436
15		C	0.41509	3.389487	0.685681	-0.02872
16		N	-0.45709	4.733366	0.658791	-0.04391
17		C	0.27092	5.313779	-0.52968	0.035172
18		C	0.20274	4.508396	-1.70308	0.136819
19		N	-0.1737	3.184034	-1.59947	0.141626
20	N2	N	-0.25595	2.621896	-0.39822	0.054845
21		C	-0.49307	5.099658	-3.0883	0.237204
22		H	0.25261	5.738822	-3.25193	-0.6433
23		H	0.25148	5.786471	-3.10694	1.096342
24		C	-0.67906	4.07549	-4.21932	0.359105
25		H	0.24936	3.455229	-4.10088	1.251683
26		H	0.23571	4.597299	-5.17966	0.423203
27		H	0.25192	3.40338	-4.24521	-0.50261
28		C	-0.49906	6.821006	-0.6073	0.01633
29		H	0.2594	7.116832	-1.2727	-0.80769
30		H	0.2592	7.145978	-1.12848	0.928632
31		C	-0.67698	7.537468	0.737382	-0.10712
32		H	0.23946	7.260335	1.251267	-1.03235
33		H	0.23993	8.620897	0.581707	-0.11132

34		H	0.23973	7.287777	1.3985	0.727934
35	O1	O	-0.51298	-0.2274	-2.47739	1.081641
36		N	0.77386	-0.16529	-3.16916	0.000447
37		O	-0.37698	-0.29395	-4.37896	-0.0045
38	O2	O	-0.5109	1.044428	0.114648	2.275917
39	N3	N	0.76734	-0.04864	0.251614	2.936
40		O	-0.36947	-0.06667	0.430456	4.13843
41	O2	O	-0.51334	-1.12073	0.197461	2.23176
42	N1	N	-0.43759	-1.37094	2.05571	0.001379
43		C	0.20685	-0.74078	3.242374	0.057666
44		C	-0.22699	-1.45483	4.435044	0.252396
45		H	0.24479	-0.94125	5.383999	0.341965
46		C	-0.17994	-2.84013	4.390169	0.355036
47		H	0.25384	-3.40739	5.303518	0.507105
48		C	-0.21241	-3.48782	3.163806	0.267211
49		H	0.27182	-4.56416	3.072836	0.336542
50		C	0.20294	-2.71215	2.013017	0.099541
51		C	0.41504	-3.37838	0.682435	0.026107
52		N	-0.45741	-4.72178	0.649005	0.059239
53		C	0.27129	-5.29701	-0.54279	-0.01092
54		C	0.20343	-4.48748	-1.71227	-0.12814
55		N	-0.17261	-3.16422	-1.60153	-0.14942
56	N2	N	-0.25831	-2.60711	-0.39793	-0.06554
57		C	-0.49327	-5.07058	-3.10136	-0.22352
58		H	0.2533	-5.66017	-3.28634	0.687242
59		H	0.25001	-5.80242	-3.11157	-1.04452
60		C	-0.67992	-4.04385	-4.21984	-0.42093
61		H	0.24881	-3.47516	-4.07995	-1.34434
62		H	0.23494	-4.56091	-5.18347	-0.47476
63		H	0.25529	-3.32207	-4.25714	0.398628
64		C	-0.49908	-6.80315	-0.62869	0.034005
65		H	0.25958	-7.08034	-1.30604	0.85466
66		H	0.25929	-7.14174	-1.14034	-0.8788
67		C	-0.67697	-7.52435	0.710453	0.186609
68		H	0.23952	-7.2317	1.215631	1.111895
69		H	0.2398	-8.60664	0.548655	0.210444
70		H	0.23953	-7.29484	1.382214	-0.64572
71	O1	O	-0.51288	0.038486	-2.4963	-1.07549

Table S2. NPA charges and Cartesian coordinates in the optimized structure of [Eu(C2-BTBP)(NO₃)₃]

Atom number	Number in the Figure	Atom type	NPA charge	X	Y	Z
1		Eu	1.79921	0.000453	-0.00177	0.012319
2	O2	O	-0.53918	2.497072	-0.00612	-0.24041
3	N3	N	0.75579	2.645562	1.26284	-0.34127
4		O	-0.38505	3.740749	1.781907	-0.46466

5	O2	O	-0.54068	1.563183	1.94761	-0.31376
6	N1	N	-0.46475	-0.44276	1.284266	-2.26684
7		C	0.20688	-0.07725	0.761134	-3.44972
8		C	-0.2302	-0.17802	1.505517	-4.63548
9		H	0.24381	0.149732	1.095306	-5.58228
10		C	-0.18139	-0.68945	2.796937	-4.58667
11		H	0.25332	-0.77365	3.386554	-5.49461
12		C	-0.21679	-1.08505	3.324788	-3.36351
13		H	0.27137	-1.49133	4.323676	-3.26931
14		C	0.20202	-0.93643	2.534558	-2.21995
15		C	0.41401	-1.33138	3.080049	-0.89192
16		N	-0.46081	-1.86439	4.313312	-0.84828
17		C	0.26875	-2.20834	4.779014	0.344342
18		C	0.19782	-2.01469	3.967675	1.50154
19		N	-0.17236	-1.48114	2.757324	1.379941
20	N2	N	-0.288	-1.13131	2.314741	0.177913
21		C	-0.49419	-2.3843	4.422404	2.892759
22		H	0.25261	-1.81682	5.338961	3.11424
23		H	0.24994	-3.4391	4.73421	2.886064
24		C	-0.68118	-2.1497	3.380668	3.990391
25		H	0.24944	-2.74342	2.478998	3.816998
26		H	0.23459	-2.43346	3.801681	4.960376
27		H	0.25614	-1.10275	3.0707	4.036784
28		C	-0.49917	-2.80057	6.163784	0.443197
29		H	0.25918	-2.19102	6.744131	1.150895
30		H	0.25889	-3.7855	6.078877	0.925203
31		C	-0.6769	-2.92523	6.9112	-0.88441
32		H	0.23955	-1.9483	7.042702	-1.35898
33		H	0.23949	-3.36127	7.90068	-0.7143
34		H	0.23946	-3.56513	6.369015	-1.58674
35	O1	O	-0.5463	-1.03151	-0.61016	2.156701
36		N	0.75658	-0.18241	0.010465	2.893108
37		O	-0.38744	-0.27476	0.038244	4.107034
38	O2	O	-0.53795	-2.4515	0.00696	-0.53377
39	N3	N	0.75573	-2.584	-1.26052	-0.66518
40		O	-0.3851	-3.6553	-1.77985	-0.92351
41	O2	O	-0.54187	-1.51063	-1.9447	-0.5164
42	N1	N	-0.46633	0.684792	-1.20565	-2.25128
43		C	0.20726	0.445365	-0.63971	-3.44692
44		C	-0.23023	0.672656	-1.34142	-4.64116
45		H	0.24394	0.44571	-0.89708	-5.60196
46		C	-0.18116	1.179178	-2.63442	-4.58474
47		H	0.25337	1.360285	-3.19129	-5.49918
48		C	-0.217	1.444672	-3.20626	-3.34631
49		H	0.27143	1.841416	-4.20831	-3.2456
50		C	0.20194	1.17391	-2.4575	-2.19722
51		C	0.41406	1.427838	-3.05191	-0.85566
52		N	-0.46067	1.959892	-4.28522	-0.80292
53		C	0.26859	2.177223	-4.79671	0.400543

54		C	0.19738	1.854339	-4.03232	1.560674
55		N	-0.17231	1.330405	-2.81851	1.43005
56	N2	N	-0.28724	1.110895	-2.32873	0.215401
57		C	-0.49409	2.074939	-4.54264	2.964135
58		H	0.25239	1.506375	-5.47745	3.081344
59		H	0.25054	3.130467	-4.83594	3.063492
60		C	-0.68079	1.696499	-3.55524	4.071503
61		H	0.24963	2.285729	-2.63665	4.0042
62		H	0.23496	1.878558	-4.01383	5.048794
63		H	0.25467	0.643675	-3.26777	4.011263
64		C	-0.49916	2.765399	-6.18258	0.508338
65		H	0.25911	2.085357	-6.79374	1.119314
66		H	0.25884	3.689886	-6.11468	1.100172
67		C	-0.67691	3.042615	-6.87409	-0.82645
68		H	0.23956	2.125435	-6.98968	-1.41152
69		H	0.23955	3.46538	-7.86807	-0.64924
70		H	0.23953	3.75187	-6.30098	-1.43078
71	O1	O	-0.54609	0.769495	0.600867	2.266084

Table S3. NPA charges and Cartesian coordinates in the optimized structure of $[\text{Am}(\text{C2-BTBP})_2]^{3+}$

Atom number	Number in the Figure	Atom type	NPA charge	X	Y	Z
1		H	0.26417	-0.00696	0.001811	-0.0007
2		C	-0.21083	-0.00442	0.000579	1.081215
3		C	0.18582	0.022321	-0.00646	3.80935
4		C	0.2234	0.461571	-1.10808	1.805391
5		C	-0.15037	-0.47074	1.121663	1.758743
6		C	-0.19682	-0.45816	1.125722	3.150568
7	N1	N	-0.51694	0.465541	-1.10342	3.155996
8		H	0.28286	-0.83532	1.982657	1.20725
9		H	0.29208	-0.80373	1.974082	3.728101
10		C	0.22345	0.971427	-2.3301	1.122604
11		C	-0.19682	1.925544	-4.63758	-0.06508
12		C	-0.2108	0.991063	-2.4385	-0.27689
13	N1	N	-0.51686	1.415816	-3.33854	1.903425
14		C	0.18582	1.874036	-4.46763	1.318803
15		C	-0.15043	1.47519	-3.59758	-0.87311
16		H	0.26417	0.633455	-1.63413	-0.90591
17		H	0.28286	1.496606	-3.68941	-1.95454
18		H	0.29206	2.306603	-5.56409	-0.47625
19		C	0.4197	0.072345	-0.03208	5.29398
20		C	0.2248	0.216039	-0.15205	7.938003
21	N2	N	-0.36281	0.5764	-1.12108	5.876832
22		N	-0.44148	-0.38166	1.040522	5.958582
23		C	0.31319	-0.3234	1.013742	7.282335
24		N	-0.20141	0.646438	-1.18006	7.218831

25		C	0.4197	2.324246	-5.56344	2.21528
26		C	0.22483	3.085646	-7.47553	3.885676
27		N	-0.44146	2.801176	-6.68309	1.652083
28	N2	N	-0.36291	2.2173	-5.36907	3.530763
29		N	-0.20138	2.605976	-6.34039	4.376207
30		C	0.31319	3.190185	-7.65975	2.4591
31		H	0.28286	-0.82281	-6.71756	9.436582
32		C	-0.15042	-0.45881	-6.11651	8.609168
33		C	-0.19682	-1.28263	-5.833	7.523678
34		C	-0.21079	0.841411	-5.62387	8.618575
35		C	0.18583	-0.76378	-5.05727	6.486512
36		H	0.29206	-2.30092	-6.19627	7.461917
37		C	0.22343	1.299778	-4.84506	7.544315
38		H	0.26416	1.483553	-5.85194	9.458927
39	N1	N	-0.51687	0.495181	-4.56585	6.496097
40		C	0.41972	-1.6046	-4.75142	5.300459
41		C	0.2234	2.684699	-4.29704	7.510434
42		N	-0.44146	-2.863	-5.21447	5.283405
43	N2	N	-0.36291	-1.05096	-4.03977	4.317236
44		C	-0.21082	3.589719	-4.5156	8.561085
45	N1	N	-0.51691	3.041075	-3.57536	6.425848
46		C	0.31319	-3.60259	-4.94604	4.216907
47		N	-0.20139	-1.77641	-3.74868	3.222578
48		Am	1.64104	1.354159	-3.14666	4.494941
49		H	0.26417	3.30735	-5.09087	9.432806
50		C	-0.15038	4.872951	-3.98509	8.488899
51		C	0.18581	4.28567	-3.05183	6.366445
52		C	0.22482	-3.02872	-4.17776	3.139701
53	N2	N	-0.36288	3.672564	-2.059	4.25416
54		C	-0.19682	5.2342	-3.23564	7.373018
55		H	0.28286	5.580408	-4.15101	9.295337
56		C	0.4197	4.625708	-2.23945	5.169946
57		N	-0.20139	3.938383	-1.32381	3.159552
58		H	0.29207	6.217609	-2.79452	7.268102
59		N	-0.44146	5.862954	-1.72923	5.085153
60		C	0.2248	5.142962	-0.78833	3.012965
61		C	0.3132	6.15458	-0.99737	4.019405
62		C	-0.5038	3.511737	-8.55245	4.849974
63		C	-0.67668	3.349021	-8.2224	6.333592
64		H	0.27513	4.560073	-8.80385	4.634787
65		H	0.27559	2.950665	-9.46581	4.605876
66		H	0.26417	3.687837	-9.07233	6.932205
67		H	0.23131	3.943056	-7.34767	6.615824
68		H	0.23209	2.303335	-8.02203	6.586366
69		C	-0.513	3.72907	-8.92978	1.864356
70		C	-0.68321	3.777262	-8.97573	0.337047
71		H	0.27903	3.127129	-9.76426	2.255266
72		H	0.27877	4.731899	-9.09771	2.285891
73		H	0.2673	4.184247	-9.938	0.016175

74	H	0.2438	2.780015	-8.86689	-0.09889
75	H	0.24387	4.415499	-8.18517	-0.06794
76	C	-0.513	-0.82104	2.198273	8.06102
77	C	-0.68321	-1.36184	3.35851	7.225254
78	H	0.27899	-0.00043	2.541313	8.709414
79	H	0.2788	-1.58927	1.838989	8.762663
80	H	0.2673	-1.69431	4.159824	7.890029
81	H	0.24378	-0.59434	3.765587	6.56071
82	H	0.24389	-2.21432	3.049078	6.613793
83	C	-0.50379	0.306846	-0.23691	9.43992
84	C	-0.67668	0.89669	-1.53073	10.00083
85	H	0.27515	-0.70056	-0.0758	9.849414
86	H	0.27557	0.891665	0.624733	9.792273
87	H	0.26416	0.912833	-1.47701	11.09279
88	H	0.23134	0.299692	-2.40081	9.710632
89	H	0.23202	1.921861	-1.68716	9.651452
90	C	-0.51301	7.530233	-0.40734	3.890758
91	C	-0.68321	8.491454	-0.71574	5.038823
92	H	0.279	7.417596	0.680357	3.76532
93	H	0.2788	7.95277	-0.74864	2.933392
94	H	0.2673	9.455833	-0.24078	4.84147
95	H	0.24379	8.113703	-0.33346	5.99148
96	H	0.24389	8.658124	-1.7916	5.144166
97	C	-0.5038	5.419042	0.034394	1.780863
98	C	-0.67668	4.258341	0.171186	0.795679
99	H	0.27514	6.29235	-0.39926	1.273118
100	H	0.27558	5.752501	1.029894	2.107011
101	H	0.26416	4.574179	0.785523	-0.05188
102	H	0.23133	3.943089	-0.80395	0.411753
103	H	0.23204	3.392671	0.651646	1.261816
104	C	-0.50379	-3.8229	-3.84359	1.903235
105	C	-0.67668	-3.09149	-3.02115	0.842516
106	H	0.27515	-4.73655	-3.32017	2.219152
107	H	0.27558	-4.17962	-4.78684	1.465492
108	H	0.26416	-3.76255	-2.84145	-0.00182
109	H	0.23131	-2.77318	-2.05166	1.238046
110	H	0.23207	-2.20654	-3.54587	0.469652
111	C	-0.513	-5.01701	-5.44947	4.161537
112	C	-0.68321	-5.48167	-6.24959	5.378499
113	H	0.27902	-5.12353	-6.04832	3.244183
114	H	0.27878	-5.67484	-4.58233	3.997493
115	H	0.2673	-6.51842	-6.56294	5.231802
116	H	0.2438	-4.87347	-7.14695	5.524217
117	H	0.24388	-5.43385	-5.65198	6.293333

Table S4. NPA charges and Cartesian coordinates in the optimized structure of [Eu(C2-BTBP)₂]³⁺

Atom number	Number in the Figure	Atom type	NPA charge	X	Y	Z
1		H	0.26446	-0.01023	0.008113	-0.0024
2		C	-0.21549	-0.00741	0.007046	1.079664
3		C	0.18189	0.015547	0.00808	3.808256
4		C	0.21998	0.921943	0.769646	1.804129
5		C	-0.15147	-0.94357	-0.76574	1.758448
6		C	-0.20033	-0.93643	-0.77169	3.150519
7	N1	N	-0.54002	0.921468	0.766517	3.154158
8		H	0.28275	-1.66774	-1.35782	1.207659
9		H	0.29185	-1.63926	-1.35858	3.728765
10		C	0.22	1.946595	1.611285	1.126961
11		C	-0.20034	3.876558	3.210235	-0.03949
12		C	-0.2155	2.039219	1.684387	-0.27169
13	N1	N	-0.54005	2.790532	2.309049	1.916578
14		C	0.18189	3.728526	3.093264	1.34301
15		C	-0.15147	3.012592	2.487021	-0.85707
16		H	0.26447	1.364872	1.125781	-0.90739
17		H	0.28275	3.093866	2.549197	-1.93775
18		H	0.29185	4.648832	3.853806	-0.4422
19		C	0.41819	0.068332	0.020792	5.292013
20		C	0.21746	0.243682	0.087602	7.935094
21	N2	N	-0.38951	1.011042	0.767984	5.870164
22		N	-0.44497	-0.82636	-0.72038	5.961154
23		C	0.31129	-0.76665	-0.70973	7.285204
24		N	-0.20895	1.096869	0.799945	7.211091
25		C	0.41816	4.61915	3.857706	2.252383
26		C	0.21746	6.153232	5.199599	3.945618
27		N	-0.44499	5.560592	4.638566	1.703239
28	N2	N	-0.38946	4.422689	3.724242	3.56572
29		N	-0.20894	5.20307	4.405894	4.421803
30		C	0.31128	6.345491	5.32425	2.522111
31		Eu	2.00474	2.619926	2.16605	4.471866
32		H	0.28275	2.266425	6.35048	9.352635
33		C	-0.15148	2.326808	5.646279	8.528743
34		C	-0.20034	1.483018	5.770103	7.428467
35		C	-0.21549	3.252982	4.609151	8.558669
36		C	0.18189	1.602633	4.837401	6.397607
37		H	0.29185	0.747455	6.561167	7.351433
38		C	0.21998	3.319012	3.704277	7.487698
39		H	0.26447	3.912136	4.516002	9.411729
40	N1	N	-0.54003	2.494492	3.823684	6.425391
41		C	0.41817	0.732482	4.939924	5.198939
42		C	0.21998	4.293661	2.578894	7.468198

43		N	-0.44499	-0.16386	5.936002	5.153884
44	N2	N	-0.38948	0.90134	4.033836	4.233673
45		C	-0.21548	5.197469	2.362817	8.520139
46	N1	N	-0.54006	4.274147	1.765567	6.390818
47	N2	N	-0.38949	4.144995	0.139187	4.217209
48		C	0.31129	-0.9307	6.025127	4.076484
49		N	-0.20894	0.138182	4.097078	3.129096
50		H	0.26447	5.215762	3.012923	9.384953
51		C	-0.15147	6.087359	1.295889	8.456225
52		C	0.18189	5.134811	0.72623	6.337592
53		C	0.41818	5.060914	-0.15253	5.143076
54		N	-0.20895	4.040932	-0.63721	3.125033
55		C	0.21746	-0.76781	5.059572	3.018141
56		C	-0.20034	6.059749	0.455658	7.346642
57		H	0.28275	6.791565	1.12103	9.263603
58		N	-0.44499	5.910825	-1.18671	5.067679
59		C	0.21746	4.849722	-1.67963	2.987958
60		H	0.29185	6.726576	-0.39189	7.247777
61		C	0.31128	5.832021	-1.97127	4.002286
62		C	-0.5053	-1.60997	5.113003	1.769523
63		C	-0.67752	-1.32996	4.027243	0.730726
64		H	0.27523	-1.48157	6.106617	1.316966
65		H	0.275	-2.66644	5.079401	2.071649
66		H	0.2638	-1.99467	4.165909	-0.12616
67		H	0.23254	-0.29692	4.073962	0.372943
68		H	0.23162	-1.50516	3.028007	1.140927
69		C	-0.51331	-1.94621	7.128882	3.989816
70		C	-0.6832	-1.99968	8.073085	5.190926
71		H	0.27885	-2.93029	6.665869	3.820341
72		H	0.27901	-1.74919	7.693126	3.065516
73		H	0.26731	-2.76827	8.831526	5.021828
74		H	0.24385	-2.24836	7.537192	6.111411
75		H	0.24383	-1.04492	8.585159	5.341057
76		C	-0.50529	4.712414	-2.53842	1.757155
77		C	-0.67752	3.630198	-2.11221	0.765418
78		H	0.27525	4.534427	-3.57273	2.084426
79		H	0.27499	5.689847	-2.56987	1.25499
80		H	0.2638	3.621494	-2.80457	-0.08068
81		H	0.23253	2.638262	-2.12443	1.227225
82		H	0.23161	3.816099	-1.10482	0.380629
83		C	-0.51331	6.768031	-3.14039	3.883253
84		C	-0.68319	7.752679	-3.31842	5.039037
85		H	0.27885	7.308365	-3.04093	2.929481
86		H	0.27902	6.156915	-4.04688	3.755515
87		H	0.26731	8.380837	-4.19235	4.848719
88		H	0.24384	8.405966	-2.44785	5.146844
89		H	0.24383	7.232435	-3.47479	5.988362
90		C	-0.5053	7.01365	5.957153	4.923878
91		C	-0.67752	6.698798	5.730095	6.402288

92	H	0.27524	6.936292	7.027319	4.684414
93	H	0.27499	8.063397	5.701796	4.720506
94	H	0.2638	7.379911	6.328257	7.013526
95	H	0.23253	5.673512	6.027572	6.642394
96	H	0.23161	6.824157	4.679109	6.680066
97	C	-0.51331	7.411478	6.210616	1.943252
98	C	-0.68319	7.491794	6.236825	0.416842
99	H	0.27884	8.375583	5.899917	2.373926
100	H	0.27903	7.25298	7.225985	2.337498
101	H	0.26731	8.296541	6.908679	0.107723
102	H	0.24384	7.70316	5.244047	0.009367
103	H	0.24384	6.559547	6.597101	-0.02749
104	C	-0.5053	0.36072	0.135926	9.436801
105	C	-0.67753	1.477853	1.020877	9.989297
106	H	0.27524	0.484585	-0.89431	9.799894
107	H	0.275	-0.6088	0.458981	9.842075
108	H	0.2638	1.467714	0.977067	11.08168
109	H	0.23257	2.46038	0.686146	9.642977
110	H	0.23158	1.346097	2.06457	9.687951
111	C	-0.51331	-1.75287	-1.52813	8.069196
112	C	-0.68319	-2.76328	-2.31909	7.238205
113	H	0.27883	-2.27242	-0.85084	8.764066
114	H	0.27904	-1.1817	-2.20317	8.724646
115	H	0.26731	-3.42733	-2.87334	7.906351
116	H	0.24383	-3.37801	-1.6589	6.619682
117	H	0.24385	-2.26618	-3.03813	6.58079

Table S5. Cartesian coordinates in the optimized structure of $[\text{Am}(\text{H}_2\text{O})_9]^{3+}$

Atom type	X	Y	Z
Am	0.007331	0.015589	0.005934
O	0.021842	-0.08944	2.531376
H	0.791499	-0.1157	3.12977
H	-0.76854	-0.15323	3.099111
O	2.43894	-0.25516	0.762534
H	3.072401	0.471198	0.911833
H	2.915142	-1.07517	0.990647
O	0.232425	-2.44239	0.592918
H	0.457315	-3.15345	-0.03525
H	0.175438	-2.86688	1.468941
O	-2.24303	-0.83016	0.956351
H	-3.05031	-0.29831	1.081877
H	-2.47653	-1.73715	1.227405
O	0.920501	2.241351	0.902396
H	0.963022	2.526883	1.834069
H	1.295906	2.97515	0.380909
O	0.555305	1.50411	-1.96259
H	1.247679	1.331522	-2.62737

H	0.110861	2.327452	-2.23772
O	-1.52771	-0.72711	-1.87183
H	-1.52905	-0.44368	-2.80484
H	-2.28925	-1.32803	-1.77318
O	-1.78981	1.835383	-0.12399
H	-1.77888	2.681141	0.361541
H	-2.59476	1.854514	-0.67437
O	1.406491	-1.21853	-1.78309
H	2.36899	-1.37071	-1.75547
H	1.090944	-1.65392	-2.59642

Table S6. Cartesian coordinates in the optimized structure of $[\text{Eu}(\text{H}_2\text{O})_9]^{3+}$

Atom type	X	Y	Z
Eu	0.000098	-0.00023	-0.00042
O	0.001949	-0.00136	2.490242
H	0.769522	-0.00341	3.090451
H	-0.78591	-0.103	3.05446
O	2.399417	-0.17823	0.693931
H	2.998088	0.575757	0.843345
H	2.908761	-0.97494	0.928687
O	0.301582	-2.37181	0.692923
H	0.582598	-3.09121	0.098989
H	0.258578	-2.75954	1.585756
O	-2.17979	-0.88866	0.887217
H	-2.99737	-0.37597	1.020632
H	-2.38726	-1.80399	1.148788
O	0.811549	2.210805	0.885853
H	0.808989	2.490711	1.818984
H	1.205114	2.946448	0.382614
O	0.63524	1.464233	-1.91055
H	1.321163	1.250736	-2.56874
H	0.2213	2.293577	-2.21085
O	-1.47587	-0.71163	-1.89365
H	-1.44457	-0.43531	-2.82742
H	-2.25471	-1.29126	-1.81194
O	-1.78504	1.727443	-0.17368
H	-1.78072	2.588661	0.282006
H	-2.55883	1.735786	-0.7658
O	1.337483	-1.29529	-1.73547
H	2.302967	-1.42285	-1.75682
H	0.988743	-1.76386	-2.51503

2. Energies

Table S7. Energies (E) and Gibbs free energies (G), hartree (1 hartree = 2625.5 kJ/mol), of Eu and Am ions and complexes, calculated in the B3LYP/6-31G(d) basis set for the gas phase and the aqueous phase (PCM).

Species	Energies, E		Gibbs free energies, G	
	M = Eu	M = Am	M = Eu	M = Am
gas phase				
M^{3+}	-708.891400	-593.949216	-	-
$[M(OH_2)_9]^{3+}$	-1397.527334	-1282.579310	-1397.359353	-1282.411849
$[M(C2-BTBP)_2]^{3+}$	-3446.378494	-3331.416755	-3445.532339	-3330.572737
$[M(C2-BTBP)(NO_3)_3]$	-2919.850047	-2804.902074	-2919.414180	-2804.466421
PCM, aqueous phase ($\epsilon = 78.4$)				
$[M(OH_2)_9]^{3+}_{aq}$	-1398.082469	-1283.131755	-	-
$[M(C2-BTBP)_2]^{3+}_{aq}$	-3446.729869	-3331.767368	-	-
$[M(C2-BTBP)(NO_3)_3]$	-2919.894928	-2804.949194	-	-

Table S8. Energies (E), hartree (1 hartree = 2625.5 kJ/mol), of Eu and Am ions and complexes, calculated in the B3LYP/6-311G(d,p) basis set for the gas phase and three liquid phases (PCM).

Species	M = Eu	M = Am
gas phase		
$[M(OH_2)_9]^{3+}$	-1397.856818	-1282.894231
$[M(C2-BTBP)_2]^{3+}$	-3447.000941	-3332.034085
$[M(C2-BTBP)(NO_3)_3]$	-2920.409055	-2805.450335
PCM, aqueous phase ($\epsilon = 78.4$)		
$[M(OH_2)_9]^{3+}_{aq}$	-1398.412831	-1283.447719
$[M(C2-BTBP)_2]^{3+}_{aq}$	-3447.34648	-3332.38520
$[M(C2-BTBP)(NO_3)_3]$	-2920.455288	-2805.498061
PCM, organic phase, TCE ($\epsilon = 7.2$)		
$[M(OH_2)_9]^{3+}$	-1398.342841	-1283.381743
$[M(C2-BTBP)_2]^{3+}$	-3447.305824	-3332.334766
$[M(C2-BTBP)(NO_3)_3]$	-2920.443096	-2805.489271
PCM, organic phase, n-octanol ($\epsilon = 10.3$)		
$[M(OH_2)_9]^{3+}$	-1398.363795	-1283.402489
$[M(C2-BTBP)_2]^{3+}$	-3447.319688	-3332.348657
$[M(C2-BTBP)(NO_3)_3]$	-2920.445661	-2805.491895

Table S9. Energies (E), hartree (1 hartree = 2625.5 kJ/mol), of Eu and Am ions and complexes, calculated at the MP2/6-311G(d,p) level of theory for the gas phase and aqueous solution (PCM).

Species	M = Eu	M = Am
gas phase		
$[M(OH_2)_9]^{3+}$	-1395.456691	-1280.274941
$[M(C2-BTBP)(NO_3)_3]$	-2914.193309	-2799.023342
PCM, aqueous phase ($\epsilon = 78.4$)		
$[M(OH_2)_9]^{3+}_{aq}$	-1396.0128	-1280.8284
$[M(C2-BTBP)(NO_3)_3]$	-2914.25016	-2799.08221