Electronic Supplementary Information

to the paper "On the selectivity of diglycolamide (TODGA) and bis-triazine-bipyridine (BTBP) ligands in actinide/lanthanide complexation and solvent extraction separation – a theoretical approach" by Jerzy Narbutt, Artur Wodyński and Magdalena Pecul

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Table S1. Cartesian coordinates and charges (Mulliken, QTAIM and NPA methods) of atoms in the EuL_3^{3+} complex (L = *N,N,N′,N′*-tetraethyl-diglycolamide, TEDGA)

Nr	attribution	at.	x	y	z	Mulliken	QTAIM	NPA
1		H	3.137321	0.446286	-7.937151	-0.14900	0.01490	0.22628
2		H	1.958040	1.495653	-8.715333	-0.14280	0.00640	0.21359
3		C	2.103381	0.795118	-7.890160	0.51090	0.06230	-0.60653
4		H	1.962994	1.330086	-6.948561	-0.13740	-0.00300	0.20748
5		H	-2.16842	-1.456963	-9.478486	-0.14520	-0.01250	0.20045
6		H	-0.56703	-1.671770	-10.199841	-0.14000	0.01270	0.21796
7		H	4.372287	-1.860191	-4.915519	-0.14610	-0.01380	0.19903
8		C	-1.37343	-0.954686	-10.035402	0.51920	0.06030	-0.60797
9		H	4.364496	0.831402	-0.552699	-0.13650	0.00860	0.21544
10		H	-1.77111	-0.676443	-11.013423	-0.13300	0.03210	0.23652
11		C	5.052056	-1.502364	-4.138156	0.51670	0.05890	-0.60771
12		C	1.153708	-0.398117	-7.986051	0.38140	0.31880	-0.21934
13		H	5.869495	-2.220595	-4.048708	-0.13200	0.03260	0.23690
14		C	3.670337	1.449716	-1.125775	0.51290	0.06190	-0.60538
15		H	4.001848	2.486069	-1.030864	-0.14920	0.01520	0.22619
16		H	1.326398	-0.957805	-8.906320	-0.09950	0.02710	0.21857
17		H	5.480868	-0.554650	-4.469037	-0.13990	0.01220	0.21741
18		H	1.300163	-1.078162	-7.148615	-0.08330	0.03120	0.21902
19		H	2.677792	1.361914	-0.678258	-0.14860	-0.01180	0.20110
20		C	-0.87548	0.296439	-9.311415	0.36650	0.31770	-0.22261
21	amide(L2)	N	-0.27069	0.007735	-7.989773	-0.28990	-0.97380	-0.31592
22		H	3.956802	-2.320691	-2.450247	-0.10500	0.01010	0.20490
23		C	4.347029	-1.360726	-2.789131	0.36640	0.31810	-0.22269
24		H	4.622852	1.178769	-3.055232	-0.10240	0.02740	0.21868
25		C	3.639111	1.052774	-2.600996	0.38360	0.31830	-0.22054
26		H	-1.67998	1.022159	-9.189236	-0.10870	0.00690	0.20380
27		H	-0.10716	0.797345	-9.902931	-0.08380	0.03860	0.22816
28	amide(L1)	N	3.251355	-0.362846	-2.800891	-0.28880	-0.97370	-0.31399
29		H	-1.53329	5.427357	-6.841934	-0.15120	0.01790	0.22755
30		H	-2.13709	6.150136	-5.355226	-0.13860	0.00850	0.21630
31		H	5.054069	-1.037652	-2.023094	-0.08300	0.04100	0.22854
32		H	0.328766	5.574172	-5.195337	-0.10410	0.02660	0.21918
33		C	-1.72927	5.232942	-5.785208	0.51560	0.06320	-0.60521
34	amide(L2)	C	-0.93239	0.089994	-6.840892	0.53050	1.27020	0.66221
35		H	2.933695	1.669158	-3.155631	-0.07710	0.03900	0.22426
36	amide(L2)	O	-0.41294	-0.179969	-5.732139	-0.64980	-1.14570	-0.71906
37	amide(L1)	C	1.973179	-0.673171	-2.980580	0.52720	1.26600	0.66324
38	CH_2 eth. L1	H	2.143734	-2.577814	-4.012527	-0.11150	0.04230	0.21013
39		C	-0.43676	4.803762	-5.092257	0.38660	0.32460	-0.22093
40		H	1.436318	5.217126	-1.815903	-0.14580	-0.01410	0.19892
41	amide(L1)	O	1.057555	0.184639	-2.990269	-0.64860	-1.14460	-0.72089

42	ether(L1)	C	1.588611	-2.138190	-3.177006	0.53600	0.47630	-0.15674
43		H	-2.48922	4.451361	-5.712812	-0.15290	-0.01730	0.19788
44	ether(L2)	C	-2.39271	0.538573	-6.862841	0.53240	0.47570	-0.15662
45		H	-0.04636	3.885700	-5.527806	-0.07480	0.03720	0.22374
46	CH_2 eth. L2	H	-2.46688	1.571062	-7.224891	-0.11980	0.04000	0.20924
47	CH_2 eth. L1	H	1.812533	-2.714249	-2.270952	-0.11810	0.04050	0.21039
48		C	0.988810	6.038554	-2.381115	0.51830	0.05830	-0.60819
49	amide(L3)	N	-0.61844	4.568848	-3.641313	-0.29430	-0.97680	-0.31609
50	amide(L3)	O	-1.03393	2.360137	-3.966073	-0.65580	-1.14910	-0.72423
51	CH_2 eth. L2	H	-2.98787	-0.103338	-7.520946	-0.10840	0.04170	0.21028
52	amide(L3)	C	-0.90301	3.347558	-3.203696	0.53480	1.27110	0.66282
53		C	-0.46464	5.745785	-2.753440	0.37270	0.31710	-0.22277
54		H	1.602094	6.217856	-3.266157	-0.13840	0.01300	0.21785
55	ether(L1)	O	0.192643	-2.163179	-3.440884	-0.57710	-1.01390	-0.52551
56		H	-1.07672	5.607374	-1.861807	-0.10870	0.00930	0.20486
57	ether (L2)	O	-2.86821	0.454346	-5.525943	-0.57940	-1.01330	-0.52515
58		Eu	-1.28646	0.001523	-3.482049	2.03060	2.32330	2.15000
59		H	1.032902	6.936977	-1.762271	-0.13450	0.03330	0.23689
60	CH_2 eth. L3	H	-0.68453	1.730969	0.500933	-0.10820	0.04300	0.21043
61	CH_2 eth. L3	H	-0.24688	3.521511	-1.135394	-0.10450	0.04450	0.21002
62	ether(L3)	C	-1.09568	3.128742	-1.703997	0.53140	0.47080	-0.15712
63		H	-1.32789	-2.565544	2.039477	-0.09910	0.02770	0.21865
64	ether(L1)	C	-0.32486	-3.464340	-3.683976	0.53460	0.46810	-0.15739
65		H	-2.20216	0.936136	2.178061	-0.10860	0.00770	0.20392
66	ether(L3)	C	-1.47642	1.357921	-0.157077	0.53240	0.46680	-0.15671
67	amide(L3)	O	-1.44574	-0.789792	-1.205818	-0.64970	-1.14370	-0.72002
68	ether(L2)	C	-4.23379	0.817527	-5.377299	0.53440	0.46930	-0.15639
69	amide(L3)	C	-1.54068	-0.168000	-0.120733	0.52970	1.26580	0.66199
70	CH_2 eth. L1	H	0.150249	-3.899972	-4.571317	-0.11790	0.04170	0.21035
71		H	0.294398	0.586369	2.513571	-0.14510	-0.01280	0.20038
72		H	-0.89862	6.594741	-3.284405	-0.08680	0.04020	0.22869
73	CH_2 eth. L2	H	-4.39996	1.835383	-5.752233	-0.12280	0.03990	0.20925
74	ether(L3)	O	-1.21497	1.726378	-1.505066	-0.58030	-1.01180	-0.52558
75	CH_2 eth. L1	H	-0.12776	-4.119657	-2.828922	-0.11200	0.04200	0.20960
76	amide(L3)	N	-1.69813	-0.774922	1.049949	-0.28920	-0.97060	-0.31502
77		H	-3.84992	-2.353260	1.817118	-0.14250	0.00540	0.21366
78		C	-1.78974	-2.252370	1.102129	0.38070	0.32250	-0.21939
79		C	-1.78650	-0.058103	2.343996	0.36680	0.31600	-0.22270
80		C	-0.45030	0.024014	3.082431	0.51890	0.06150	-0.60794
81	CH_2 eth. L2	H	-4.87300	0.131916	-5.942526	-0.10530	0.04360	0.21020
82	amide(L2)	O	-3.59453	0.571894	-3.087276	-0.65300	-1.15030	-0.72287
83		C	-3.23007	-2.754660	1.012474	0.51070	0.06160	-0.60660
84	CH_2 eth. L3	H	-2.00599	3.639562	-1.365580	-0.12170	0.03790	0.20949
85	CH_2 eth. L3	H	-2.43129	1.785211	0.172131	-0.11930	0.04120	0.20968
86	amide(L2)	C	-4.54676	0.756699	-3.883504	0.53560	1.27440	0.66351

87		H	-0.59325	0.527656	4.040543	-0.13280	0.03160	0.23666
88	amide(L1)	O	-2.30080	-2.144692	-3.940952	-0.65170	-1.14770	-0.72158
89	amide(L1)	C	-1.82703	-3.305060	-3.912416	0.52700	1.27410	0.66280
90		H	-3.24528	-3.843118	1.101561	-0.14860	0.01600	0.22652
91		H	-1.18955	-2.648312	0.284733	-0.08340	0.03130	0.21920
92		H	-2.52176	-0.593628	2.947030	-0.08340	0.03910	0.22837
93		H	-7.60479	1.848933	-3.920151	-0.08800	0.04100	0.22876
94		H	-0.04374	-0.967697	3.289185	-0.13990	0.01310	0.21801
95		H	-2.56703	-6.338291	-4.807129	-0.08270	0.04050	0.22830
96		H	-3.67951	-2.481421	0.055485	-0.13740	-0.00420	0.20766
97	amide(L2)	N	-5.80345	0.913155	-3.484516	-0.29430	-0.97950	-0.31514
98		H	-0.98539	-5.759276	-4.365225	-0.10560	0.00940	0.20463
99		C	-6.93843	1.137774	-4.411231	0.37400	0.31960	-0.22270
100	amide(L1)	N	-2.56902	-4.394184	-4.078791	-0.29010	-0.97510	-0.31593
101		C	-2.02754	-5.773083	-4.045118	0.36610	0.31440	-0.22269
102		H	-6.57682	1.639108	-5.309380	-0.10830	0.00950	0.20508
103		H	-5.40427	0.204764	-1.563147	-0.07520	0.03820	0.22380
104		C	-6.12555	0.866379	-2.039559	0.38630	0.32420	-0.22084
105		C	-4.02529	-4.257084	-4.310704	0.38450	0.32020	-0.22059
106		H	-7.11093	0.406959	-1.949238	-0.10370	0.02900	0.21923
107		H	-4.36048	-3.365462	-3.783597	-0.07720	0.03920	0.22401
108		C	-7.69481	-0.142789	-4.764543	0.51830	0.05980	-0.60816
109		C	-2.17148	-6.448111	-2.680998	0.51690	0.06130	-0.60773
110		H	-4.50313	-5.120302	-3.845454	-0.10270	0.02650	0.21852
111		H	-1.79051	-7.469756	-2.737534	-0.13240	0.03170	0.23660
112		H	-8.53761	0.099271	-5.415062	-0.13480	0.03210	0.23702
113		H	-8.09555	-0.631477	-3.874512	-0.13860	0.01220	0.21781
114		C	-6.11450	2.249009	-1.389039	0.51570	0.06100	-0.60524
115		H	-5.12153	2.700769	-1.448494	-0.15290	-0.01680	0.19821
116		H	-3.21571	-6.502713	-2.367705	-0.14000	0.01130	0.21740
117		H	-1.60920	-5.920922	-1.906161	-0.14610	-0.01470	0.19891
118		H	-7.05751	-0.858494	-5.289987	-0.14500	-0.01510	0.19891
119		C	-4.37792	-4.179598	-5.795488	0.51270	0.06370	-0.60533
120		H	-6.39202	2.162409	-0.336270	-0.15080	0.01700	0.22772
121		H	-6.82958	2.926754	-1.859920	-0.13840	0.00910	0.21626
122		H	-3.93300	-3.294098	-6.255005	-0.14910	-0.01320	0.20059
123		H	-4.03596	-5.061486	-6.341318	-0.13650	0.00790	0.21549
124		H	-5.46226	-4.122951	-5.913841	-0.14990	0.01480	0.22571

Table S2: Cartesian coordinates and charges (Mulliken, QTAIM and NPA methods) of the atoms in the AmL_3^{3+} complex (L = *N,N,N′,N′*-tetraethyl-diglycolamide, TEDGA)

Nr	attribution	at.	x	y	z	Mulliken	QTAIM	NPA
1		H	3.568489	0.319992	-6.531660	-0.14980	0.01440	0.22590
2		H	2.411815	1.392119	-7.312568	-0.14230	0.00560	0.21359
3		C	2.545970	0.700223	-6.478272	0.51050	0.06500	-0.60646
4		H	2.432891	1.254097	-5.543987	-0.13620	-0.00280	0.20746
5		H	-1.809518	-1.433503	-7.996540	-0.14520	-0.01350	0.20004
6		H	-0.222380	-1.706044	-8.729137	-0.14000	0.01170	0.21800
7		H	4.779053	-1.881643	-3.514140	-0.14660	-0.01580	0.19852
8		C	-1.003686	-0.961734	-8.564512	0.51890	0.06020	-0.60794
9		H	4.938143	0.879383	0.792222	-0.13850	0.00880	0.21484
10		H	-1.400672	-0.679301	-9.541619	-0.13310	0.03170	0.23632
11		C	5.483478	-1.513236	-2.764132	0.51820	0.05890	-0.60756
12		C	1.560469	-0.465733	-6.544713	0.38530	0.31970	-0.21939
13		H	6.299731	-2.234118	-2.685686	-0.13290	0.03230	0.23639
14		C	4.224098	1.493058	0.238920	0.51310	0.06400	-0.60565
15		H	4.563348	2.529052	0.306621	-0.14950	0.01400	0.22595
16		H	1.705272	-1.043422	-7.458748	-0.10040	0.02590	0.21806
17		H	5.906715	-0.574128	-3.125347	-0.14020	0.01240	0.21719
18		H	1.697462	-1.137907	-5.699469	-0.08510	0.03050	0.21873
19		H	3.250273	1.415857	0.727544	-0.14880	-0.01210	0.20188
20		C	-0.458822	0.278709	-7.855916	0.36820	0.31880	-0.22245
21	amide(L2)	N	0.148701	-0.018222	-6.537412	-0.29290	-0.97230	-0.31572
22		H	4.435509	-2.293729	-1.028935	-0.10860	0.00880	0.20439
23		C	4.819740	-1.342371	-1.397537	0.37070	0.32000	-0.22241
24		H	5.099011	1.191552	-1.722190	-0.10040	0.02650	0.21778
25		C	4.132811	1.077205	-1.228662	0.38600	0.31930	-0.22083
26		H	-1.237723	1.031855	-7.733773	-0.11080	0.00810	0.20350
27		H	0.319843	0.749012	-8.458833	-0.08360	0.03830	0.22835
28	amide(L1)	N	3.729873	-0.338392	-1.395163	-0.29560	-0.97320	-0.31535
29		H	-0.903326	5.577026	-5.192426	-0.15000	0.01700	0.22782
30		H	-1.560785	6.264428	-3.711581	-0.13960	0.00800	0.21569
31		H	5.551440	-1.009354	-0.659470	-0.08480	0.04010	0.22828
32		H	0.892855	5.664339	-3.471236	-0.10260	0.02780	0.21868
33		C	-1.142847	5.355834	-4.150070	0.51530	0.06680	-0.60528
34	amide(L2)	C	-0.500090	0.090312	-5.382469	0.52190	1.27090	0.66322
35		H	3.409808	1.690636	-1.763345	-0.07710	0.03760	0.22410
36	amide(L2)	O	0.021309	-0.187247	-4.276940	-0.63670	-1.14190	-0.69588
37	amide(L1)	C	2.444429	-0.642922	-1.535205	0.51820	1.26700	0.66531
38	CH_2 eth. L1	H	2.585063	-2.565902	-2.537443	-0.11600	0.04090	0.20868
39		C	0.118474	4.897647	-3.419329	0.38930	0.31810	-0.22092
40		H	1.864760	5.216306	-0.064624	-0.14530	-0.01580	0.19908
41	amide(L1)	O	1.535790	0.222022	-1.532889	-0.63590	-1.14110	-0.69903

42	ether(L1)	C	2.051551	-2.110815	-1.696157	0.54960	0.47600	-0.15689
43		H	-1.910422	4.578741	-4.129974	-0.15300	-0.01660	0.19859
44	ether(L2)	C	-1.947077	0.582368	-5.401580	0.54530	0.46870	-0.15768
45		H	0.518820	3.988381	-3.864051	-0.07420	0.03880	0.22437
46	CH_2 eth. L2	H	-1.992243	1.614788	-5.768215	-0.12130	0.03910	0.20886
47	CH_2 eth. L1	H	2.300095	-2.669894	-0.785822	-0.12310	0.03980	0.20867
48		C	1.442549	6.054387	-0.624783	0.51820	0.06080	-0.60824
49	amide(L3)	N	-0.121330	4.625983	-1.982760	-0.29730	-0.97250	-0.31457
50	amide(L3)	O	-0.532719	2.430030	-2.383480	-0.64160	-1.14400	-0.70003
51	CH_2 eth. L2	H	-2.561667	-0.044766	-6.055743	-0.11470	0.04280	0.20939
52	amide(L3)	C	-0.428090	3.395888	-1.588413	0.52590	1.26970	0.66486
53		C	0.003073	5.779325	-1.059758	0.37390	0.31890	-0.22244
54		H	2.089854	6.253313	-1.480895	-0.13890	0.01240	0.21782
55	ether(L1)	O	0.648955	-2.145970	-1.922953	-0.57080	-1.01430	-0.51444
56		H	-0.643502	5.621935	-0.196090	-0.10980	0.00810	0.20450
57	ether (L2)	O	-2.431083	0.518858	-4.064187	-0.57740	-1.00910	-0.51567
58		Eu	-0.868522	0.036711	-1.974559	1.97700	2.30380	1.99298
59		H	1.466730	6.936270	0.018462	-0.13410	0.03280	0.23675
60	CH_2 eth. L3	H	-0.295920	1.727194	2.068433	-0.11490	0.04280	0.20934
61	CH_2 eth. L3	H	0.151358	3.508847	0.505185	-0.10820	0.04340	0.20951
62	ether(L3)	C	-0.680884	3.141219	-0.103386	0.54290	0.46530	-0.15735
63		H	-0.857535	-2.574368	3.596899	-0.10030	0.02620	0.21805
64	ether(L1)	C	0.131546	-3.455400	-2.116992	0.54960	0.47130	-0.15687
65		H	-1.797636	0.910206	3.741671	-0.11090	0.00700	0.20354
66	ether(L3)	C	-1.082246	1.346156	1.408582	0.54530	0.46270	-0.15770
67	amide(L3)	O	-1.018908	-0.801742	0.353064	-0.63700	-1.13800	-0.69601
68	ether(L2)	C	-3.802666	0.876593	-3.938833	0.54300	0.46530	-0.15735
69	amide(L3)	C	-1.120797	-0.181578	1.437575	0.52190	1.26690	0.66325
70	CH_2 eth. L1	H	0.591317	-3.914889	-3.000438	-0.12310	0.03960	0.20867
71		H	0.707773	0.607918	4.065311	-0.14520	-0.01420	0.20002
72		H	-0.406255	6.643625	-1.585444	-0.08780	0.03930	0.22884
73	CH_2 eth. L2	H	-3.960440	1.903354	-4.292075	-0.12480	0.03980	0.20864
74	ether(L3)	O	-0.825408	1.735405	0.063408	-0.57740	-1.00540	-0.51574
75	CH_2 eth. L1	H	0.350182	-4.084360	-1.247411	-0.11590	0.04130	0.20869
76	amide(L3)	N	-1.265845	-0.790606	2.610024	-0.29290	-0.96920	-0.31568
77		H	-3.384221	-2.403668	3.399345	-0.14230	0.00550	0.21361
78		C	-1.333148	-2.269087	2.663749	0.38520	0.32330	-0.21940
79		C	-1.361652	-0.075822	3.904491	0.36840	0.31680	-0.22247
80		C	-0.023999	0.031705	4.637164	0.51890	0.05980	-0.60793
81	CH_2 eth. L2	H	-4.423224	0.205072	-4.540513	-0.10820	0.04380	0.20949
82	amide(L2)	O	-3.237338	0.566162	-1.634397	-0.64170	-1.14170	-0.70017
83		C	-2.765998	-2.794741	2.588384	0.51040	0.06300	-0.60648
84	CH_2 eth. L3	H	-1.595982	3.656648	0.214076	-0.12470	0.04060	0.20864
85	CH_2 eth. L3	H	-2.043195	1.756623	1.740964	-0.12100	0.04120	0.20894
86	amide(L2)	C	-4.162009	0.775037	-2.457405	0.52590	1.27050	0.66486

87		H	-0.172083	0.532321	5.596098	-0.13300	0.03180	0.23634
88	amide(L1)	O	-1.870075	-2.165472	-2.371974	-0.63590	-1.13820	-0.69888
89	amide(L1)	C	-1.376624	-3.317715	-2.320693	0.51820	1.26840	0.66531
90		H	-2.762621	-3.883338	2.677389	-0.14970	0.01480	0.22592
91		H	-0.734191	-2.656135	1.841281	-0.08510	0.03070	0.21865
92		H	-2.083591	-0.625373	4.510960	-0.08360	0.03910	0.22837
93		H	-7.217074	1.872639	-2.564331	-0.08780	0.04000	0.22888
94		H	0.402237	-0.952179	4.841674	-0.14000	0.01340	0.21799
95		H	-2.094433	-6.384014	-3.118812	-0.08480	0.03870	0.22825
96		H	-3.230072	-2.528599	1.636420	-0.13630	-0.00410	0.20751
97	amide(L2)	N	-5.430820	0.923987	-2.095933	-0.29740	-0.97690	-0.31461
98		H	-0.511692	-5.773959	-2.726029	-0.10850	0.00790	0.20437
99		C	-6.535088	1.174584	-3.052685	0.37410	0.31910	-0.22247
100	amide(L1)	N	-2.106823	-4.420578	-2.444562	-0.29560	-0.97350	-0.31532
101		C	-1.546788	-5.791159	-2.384206	0.37060	0.32140	-0.22237
102		H	-6.144891	1.699848	-3.924821	-0.10990	0.00780	0.20451
103		H	-5.094852	0.166499	-0.180552	-0.07420	0.03890	0.22437
104		C	-5.800729	0.839584	-0.663763	0.38910	0.32360	-0.22094
105		C	-3.569165	-4.310420	-2.652919	0.38620	0.32140	-0.22082
106		H	-6.787953	0.377439	-0.618796	-0.10250	0.02750	0.21865
107		H	-3.905339	-3.402418	-2.155488	-0.07700	0.03660	0.22409
108		C	-7.279393	-0.095612	-3.464512	0.51810	0.06110	-0.60825
109		C	-1.654590	-6.429631	-0.999250	0.51840	0.05940	-0.60755
110		H	-4.026476	-5.160076	-2.143902	-0.10060	0.02500	0.21780
111		H	-1.261228	-7.447507	-1.035217	-0.13300	0.03260	0.23638
112		H	-8.100333	0.164373	-4.135730	-0.13420	0.03200	0.23675
113		H	-7.709153	-0.607162	-2.601294	-0.13880	0.01270	0.21783
114		C	-5.813621	2.204965	0.022125	0.51530	0.05960	-0.60530
115		H	-4.819859	2.658527	0.009240	-0.15300	-0.01560	0.19870
116		H	-2.691622	-6.488769	-0.663693	-0.14020	0.01090	0.21721
117		H	-1.084225	-5.873850	-0.250778	-0.14660	-0.01530	0.19854
118		H	-6.625430	-0.798108	-3.987301	-0.14520	-0.01620	0.19899
119		C	-3.952086	-4.297769	-4.132187	0.51310	0.06530	-0.60565
120		H	-6.126855	2.090354	1.062100	-0.14990	0.01820	0.22783
121		H	-6.513234	2.894371	-0.455076	-0.13960	0.00910	0.21567
122		H	-3.526846	-3.427924	-4.637746	-0.14890	-0.01050	0.20184
123		H	-3.612074	-5.198067	-4.648361	-0.13850	0.00700	0.21487
124		H	-5.039171	-4.256864	-4.229838	-0.14950	0.01360	0.22592

Table S3: Distances (Ĺ) between the donor oxygen atoms in the first coordination sphere of the $M(TEDGA)_3^{3+}$ complexes. O_{am} and O_{eth} denote the side (amide) and central (etheral), respectively, oxygen atoms in the coordinated TEDGA ligands (L1 – L3).

$Eu(TEDGA)_3^{3+}$			.....	$Am(TEDGA)_3^{3+}$		
$O_{am1}L2$	$O_{am1}L1$	3.13		$O_{am1}L2$	$O_{am1}L1$	3.16
$O_{am1}L2$	$O_{am2}L1$	3.26		$O_{am1}L2$	$O_{am2}L1$	3.33
$O_{am1}L2$	$O_{am1}L3$	3.16		$O_{am1}L2$	$O_{am1}L3$	3.28
$O_{am1}L2$	$O_{am2}L3$	4.68		$O_{am1}L2$	$O_{am2}L3$	4.79
$O_{am2}L2$	$O_{am1}L1$	4.67		$O_{am2}L2$	$O_{am1}L1$	4.79
$O_{am2}L2$	$O_{am2}L1$	3.13		$O_{am2}L2$	$O_{am2}L1$	3.14
$O_{am2}L2$	$O_{am1}L3$	3.24		$O_{am2}L2$	$O_{am1}L3$	3.37
$O_{am2}L2$	$O_{am2}L3$	3.16		$O_{am2}L2$	$O_{am2}L3$	3.28
$O_{am1}L1$	$O_{am1}L3$	3.17		$O_{am1}L1$	$O_{am1}L3$	3.14
$O_{am1}L1$	$O_{am2}L3$	3.22		$O_{am1}L1$	$O_{am2}L3$	3.34
$O_{am2}L1$	$O_{am1}L3$	4.68		$O_{am2}L1$	$O_{am1}L3$	4.79
$O_{am2}L1$	$O_{am2}L3$	3.17		$O_{am2}L1$	$O_{am2}L3$	3.17
$O_{am1}L2$	$O_{am2}L2$	4.20		$O_{am1}L2$	$O_{am2}L2$	4.13
$O_{am1}L1$	$O_{am2}L1$	4.20		$O_{am1}L1$	$O_{am2}L1$	4.24
$O_{am1}L3$	$O_{am2}L3$	4.20		$O_{am1}L3$	$O_{am2}L3$	4.26
$O_{am1}L2$	$O_{eth}L2$	2.55		$O_{am1}L2$	$O_{eth}L2$	2.56
$O_{am2}L2$	$O_{eth}L2$	2.55		$O_{am2}L2$	$O_{eth}L2$	2.56
$O_{am1}L1$	$O_{eth}L1$	2.54		$O_{am1}L1$	$O_{eth}L1$	2.56
$O_{am2}L1$	$O_{eth}L1$	2.54		$O_{am2}L1$	$O_{eth}L1$	2.56
$O_{am1}L3$	$O_{eth}L3$	2.55		$O_{am1}L3$	$O_{eth}L3$	2.56
$O_{am2}L3$	$O_{eth}L3$	2.54		O(s2)L3	O(c)L3	2.56

Table S4: Cartesian coordinates and charges (Mulliken, QTAIM and NPA) of the atoms in the free *N,N,N′,N′*-tetraethyl-diglycolamide (TEDGA) molecule

Nr	attribution	at.	x	y	z	Mulliken	QTAIM	NPA
1		H	6,62696586	-0,07483	1,03982902	-0,18	-0,0191	0,20334
2		H	5,41142586	1,00431405	0,34169202	-0,1743	-0,0309	0,19119
3		C	5,59092686	0,26488305	1,12788202	0,5147	0,0499	-0,60508
4		H	5,47223486	0,75174005	2,09729002	-0,1227	0,0189	0,22
5		H	1,23801586	-1,996441	-0,247357	-0,1404	-0,0136	0,20236
6		H	2,77748386	-2,201904	-1,087004	-0,1603	-0,0117	0,20444
7		C	1,97942386	-1,48818	-0,868629	0,5213	0,0569	-0,60602
8		H	1,50403886	-1,215658	-1,815487	-0,1834	-0,0233	0,20409
9		C	4,63010986	-0,921021	1,01593902	0,3754	0,3646	-0,22013
10		H	4,77909886	-1,449599	0,07012402	-0,125	-0,0199	0,18778
11		H	4,81864986	-1,625011	1,82628402	-0,0807	0,0358	0,23031
12		C	2,52839086	-0,240462	-0,166326	0,3672	0,3661	-0,21966
13	amide(1)	N	3,21879986	-0,523949	1,09111802	-0,3321	-0,9733	-0,39406
14		H	1,72269586	0,47341505	0,01046202	-0,1212	-0,0079	0,19811
15		H	3,23598486	0,27161805	-0,826266	-0,1131	-0,0044	0,20077
16	amide(1)	C	2,64907786	-0,440034	2,34043802	0,5183	1,2983	0,64609
17	amide(1)	O	3,26907586	-0,682003	3,35602602	-0,5533	-1,0899	-0,59189
18	ether (1)	C	1,17471686	-0,006951	2,38322002	0,559	0,5145	-0,1599
19	CH2(1) ether	H	1,09120186	1,02695105	2,00709402	-0,1692	-0,0131	0,17013
20	CH2(1) ether	H	0,57510686	-0,64344	1,71347802	-0,1581	-0,0053	0,16664
21	ether	O	0,71271186	-0,093827	3,70424002	-0,4837	-0,9625	-0,4569
22	ether(2)	C	-0,6309901	0,29125005	3,81394602	0,5579	0,4881	-0,15997
23	CH2(2) ether	H	-0,7735431	1,32605505	3,45771302	-0,171	-0,013	0,17013
24	CH2(2) ether	H	-1,2754211	-0,354081	3,19687402	-0,1566	0,0003	0,16643
25	amide(2)	O	-0,2452841	-0,000733	6,17062402	-0,554	-1,1069	-0,59202
26	amide(2)	C	-1,0538861	0,21163405	5,29007202	0,5195	1,3164	0,64622
27		H	-4,1072901	1,41193805	4,95092102	-0,1125	-0,0049	0,20095
28	amide(2)	N	-2,3902821	0,41082705	5,54761902	-0,3326	-0,9975	-0,394
29		C	-3,4087331	0,67982505	4,53324802	0,3669	0,3611	-0,21995
30		H	-2,9504191	1,17018105	3,67322402	-0,1218	-0,0032	0,19813
31		H	-2,1938011	-0,361213	7,46473202	-0,0798	0,0377	0,231
32		C	-2,8256861	0,36124905	6,94870802	0,3769	0,3535	-0,22022
33		H	-3,8521781	-0,01595	6,96717102	-0,1256	-0,0139	0,1877
34		C	-4,1785351	-0,566527	4,08076702	0,5201	0,0584	-0,60614
35		H	-4,9522201	-0,295986	3,35624102	-0,1831	-0,0214	0,20411
36		H	-4,6665081	-1,05647	4,92669602	-0,1596	-0,0039	0,20459
37		C	-2,7382911	1,71859005	7,65039002	0,514	0,0642	-0,60507
38		H	-1,7021271	2,06022505	7,67777402	-0,1234	0,013	0,21947
39		H	-3,5112851	-1,294608	3,61310602	-0,1394	-0,013	0,20254
40		H	-3,0993341	1,63870205	8,67986502	-0,1799	-0,0178	0,2035
41		H	-3,3416931	2,47547905	7,14042302	-0,1746	-0,0273	0,19098

Table S5: Cartesian coordinates and charges (Mulliken, QTAIM and NPA) of atoms in the hydrated ion $Eu(H_2O)_9^{3+}$

Nr	atom	x	y	z	Mulliken	QTAIM	NPA
1	Eu	-0,00022	0,00008	0,00000	2,4926	2,3679	2,13999
2	O	0,00755	-0,01072	2,49681	-0,6064	-1,1308	-0,99841
3	H	0,77509	-0,00691	3,08662	0,3261	0,6024	0,54776
4	H	-0,77267	-0,09636	3,06338	0,3342	0,6011	0,54962
5	O	2,40304	-0,18385	0,70271	-0,6122	-1,1331	-1,00075
6	H	3,00601	0,56063	0,84100	0,334	0,6016	0,54855
7	H	2,90110	-0,97997	0,93725	0,3251	0,6001	0,5466
8	O	0,30824	-2,37534	0,70013	-0,6076	-1,1289	-0,99822
9	H	0,57306	-3,09752	0,11248	0,3338	0,6024	0,54904
10	H	0,26363	-2,75250	1,59043	0,3253	0,5982	0,54755
11	O	-2,18394	-0,89123	0,88774	-0,615	-1,1288	-1,00046
12	H	-2,99804	-0,38402	1,01696	0,3432	0,5997	0,54745
13	H	-2,38428	-1,80012	1,15354	0,341	0,5991	0,54735
14	O	0,81476	2,21439	0,88696	-0,6152	-1,1261	-1,00051
15	H	0,81639	2,49255	1,81396	0,3434	0,5983	0,54742
16	H	1,19849	2,94595	0,38254	0,341	0,5981	0,54733
17	O	0,62906	1,46761	-1,91807	-0,6076	-1,1286	-0,99822
18	H	1,31882	1,26798	-2,56721	0,3339	0,6018	0,54903
19	H	0,21205	2,29090	-2,20990	0,3253	0,5989	0,54754
20	O	-1,48091	-0,70480	-1,90060	-0,612	-1,131	-1,0007
21	H	-1,44470	-0,42306	-2,82590	0,3251	0,5988	0,5466
22	H	-2,24859	-1,28986	-1,82773	0,3339	0,6014	0,54856
23	O	-1,78742	1,73347	-0,18463	-0,6064	-1,1333	-0,99838
24	H	-1,79708	2,58451	0,27656	0,3342	0,6029	0,54961
25	H	-2,55661	1,73172	-0,77228	0,326	0,6031	0,54779
26	O	1,33954	-1,29686	-1,73816	-0,6248	-1,1328	-1,0033
27	H	2,29805	-1,42909	-1,75384	0,3445	0,5991	0,54556
28	H	0,99266	-1,75599	-2,51622	0,3445	0,5987	0,54557

Table S6: Cartesian coordinates and charges (Mulliken, QTAIM and NPA) of atoms in the hydrated ion $Am(H_2O)_9^{3+}$

Nr	atom	x	y	z	Mulliken	QTAIM	NPA
1	Am	0,016015	0,006667	-0,006129	2,2158	2,3552	2,01613
2	O	-0,025389	-0,005419	2,535689	-0,5632	-1,1266	-0,98287
3	H	0,718701	0,005485	3,154589	0,3222	0,6002	0,54811
4	H	-0,823629	-0,090084	3,076620	0,3253	0,6	0,54922
5	O	2,415079	-0,295392	0,777413	-0,5585	-1,1278	-0,98863
6	H	3,050319	0,418316	0,932479	0,3221	0,5994	0,54908
7	H	2,853915	-1,114729	1,047756	0,3207	0,5993	0,54794
8	O	0,267285	-2,462016	0,647278	-0,5591	-1,1275	-0,98624
9	H	0,523913	-3,176899	0,047230	0,3243	0,6013	0,54815
10	H	0,184061	-2,867872	1,522098	0,3164	0,5966	0,54636
11	O	-2,230307	-0,932609	0,893886	-0,5603	-1,1259	-0,98723
12	H	-3,040421	-0,434570	1,073114	0,3269	0,5974	0,54609
13	H	-2,428455	-1,852601	1,119289	0,3268	0,5978	0,54609
14	O	0,994456	2,222068	0,812759	-0,5516	-1,1273	-0,98668
15	H	1,049254	2,550912	1,721545	0,3211	0,6012	0,54812
16	H	1,363721	2,917716	0,250221	0,326	0,5985	0,54854
17	O	0,545987	1,536170	-1,965863	-0,5577	-1,1275	-0,98617
18	H	1,215671	1,370694	-2,644912	0,3232	0,6014	0,54954
19	H	0,086222	2,346674	-2,227900	0,321	0,5987	0,54808
20	O	-1,535282	-0,653760	-1,907961	-0,5645	-1,1258	-0,98684
21	H	-1,530392	-0,351422	-2,827412	0,3214	0,5977	0,54753
22	H	-2,310216	-1,226698	-1,817556	0,3244	0,5992	0,54871
23	O	-1,798241	1,822121	-0,034325	-0,559	-1,1276	-0,98448
24	H	-1,757881	2,660966	0,447020	0,3243	0,5996	0,5484
25	H	-2,619877	1,849651	-0,545330	0,3173	0,6011	0,54697
26	O	1,398407	-1,220469	-1,771574	-0,5513	-1,1269	-0,98933
27	H	2,355744	-1,359612	-1,742191	0,3256	0,5995	0,54798
28	H	1,085501	-1,658014	-2,576343	0,3205	0,5986	0,54742

Table S7. Energies, E_i, and Gibbs free energies, G_i, of formation (from spherical spin-restricted atoms) of the Am and Eu species studied (L = TEDGA) in various media (med.), and the differences in the complex formation energies, $\Delta(\Delta E_{cf})_{Am/Eu}$, Gibbs free energies, $\Delta(\Delta G_{cf})_{Am/Eu}$, and in Gibbs free energies of complex partition ($H_2O \rightarrow$TCE; TCE = CH_2Cl-$CHCl_2$), $\Delta(\Delta G_p)_{Am/Eu}$, [kJ/mol], calculated using one-component ZORA method, using two different functionals. Solvent effects evaluated using COSMO method.

functional		B3LYP			PBE						
species, i	med.	E_i(Eu)	E_i(Am)	$\Delta(\Delta E_{cf})$	E_i(Eu)	E_i(Am)	$\Delta(\Delta E_{cf})$	G_i(Eu)	G_i(Am)	$\Delta(\Delta G_{cf})$	$\Delta(\Delta G_p)$
M^{3+}	gas	+2604.0	+2923.8	–	+3352.6	+3438.2	–	–	–	–	–
$[M(H_2O)_9]^{3+}$	H_2O	-16086.3	-15598.9	–	-12702.5	-12519.3	–	-2939.1	-2896.3	–	–
$[M(L)_3]^{3+}$	gas	-77268.1	-76785.0	+163.4	-66955.8	-66766.1	+104.1	–	–	–	–
	H_2O	-78191.9	-77706.6	-2.1	-67878.7	-67686.2	+9.4	-15618.5	-15573.1	+2.1	–
	TCE	-78063.5	-77576.6	–	-67750.8	-67556.7	–	-15586.6	-15542.0	–	-0.8

Table S8. Electron density shifts on the central metal(III) ion from H_2O ligands in nonahydrates of Eu^{III} and Am^{III}. The shift values per one H_2O ligand have been calculated using the formula $\Delta q(H_2O)_M = [3 - q(M^{III})]/9$, where $q(M^{III})$ denotes the partial charge on the central metal(III) ion in the nonahydrate, calculated using Mulliken, QTAIM and NPA methods (Tables S5 and S6).

	Mulliken	QTAIM	NPA
$q(Am^{III})$	2.216	2.355	2.016
$q(Eu^{III})$	2.493	2.368	2.140
$\Delta q(H_2O)_{Am}$	0.087	0.072	0.109
$\Delta q(H_2O)_{Eu}$	0.056	0.070	0.096

Table S9. Ionization energies (ionization potentials, IP), electron affinities (EA) and hardness (η) values, [eV], of some ligands (S9-A) and metal ions studied (S9-B).
According to the definition, $EA(M^{3+}) = IP_3(M^{3+})$.

S9-A	TEDGA	C2-BTBP	H_2O	H_2O	ether[x]	ketone[y]	amide[z]
source	this work			Ref.*			Ref.[#]
IP	7.92	7.27	12.73	12.6	10.0	9.7	-
EA	–0.94	0.56	–1.49	–6.4	–6.0	–1.5	-
η	4.43	3.36	7.11	9.5	8.0	5.6	2.72

[x] CH_3-O-CH_3; [y] CH_3-(C=O)-CH_3; [z] $CH_3(C=O)N(CH_3)_2$

* R. G. Pearson, *Inorg. Chem.*, 1988, **77**, 734-740.

[#] S. Chasviseda, W. Rakraia, N. Morakota and B. Wanno, *Int. Trans. J. Eng. Manag. Appl. Sci. Technol*. (eISSN: 1906-9642), 2011, 73-82 (http://TuEngr.com/V02/073-082.pdf).

S9-B	one-component ZORA		two-component ZORA		Literature data			
	Am	Eu	Am	Eu	Am	Eu	Am	Eu
IP_1	5.911	5.629	5.923	5.629	5.99[v]	5.670[v]	-	-
IP_2	12.091	11.478	13.907	11.477	-	11.245[v]	-	-
IP_3	25.176	27.785	21.020	25.108	-	24.915[v]	-	-
IP_4	39.100	45.571	37.067	43.120	34.2[q]	42.700[v]	-	-
$\eta(M^{3+})$	6.96	8.89	8.02	9.01	-	8.89	7.35[p]	10.75[p]

[v] http://en.wikipedia.org/wiki/Molar_ionization_energies_of_the_elements; http://www.webelements.com/europium/atoms.html

[q] S. Siekierski and J. Burgess, Concise Chemistry of the Elements, Horwood Chemical Science, 2002, Fig. 18.8, p. 180.

[p] D. Manna and T. K. Ghanty, *Phys. Chem. Chem. Phys.*, 2012, **14**, 11060-11069.

Table 10. Energy gaps, $E_a - E_d$, and Fock matrix elements, F_{da}. for the bonding M–O orbitals of greatest stabilization energies, $\Delta E(2)$, in the $[Am(TEDGA)_3]^{3+}$ complex. Donor 1-centre NBOs: LP-O_{am} and LP-O_{eth}. Acceptor unfilled 1-centre NBOs of Am^{3+}: LP* NBOs (*d,s,f*) hybrids

		$\Delta E(2)$ kcal/mol	$E_a - E_d$ a.u.	F_{da} a.u.	$\Delta E(2)$ kcal/mol	$E_a - E_d$ a.u.	F_{da} a.u.
		LP(51%s 49%p) O_{am}			LP(11%s 89%p) O_{am}		
Beta	LP* (96%d 4%f) Am	8.8	1.05	0.13	13.0	0.82	0.13
	LP* (s) Am	3.5	1.32	0.09	3.8	1.09	0.08
	LP* (90%d 10%f) Am	6.2	0.80	0.09	2.1	0.58	0.04
	LP* (95%d 5%f) Am	1.3	0.73	0.04	0.2	0.50	0.01
	LP* (f) Am	-	-	-	1.0	0.37	0.03
Alpha	LP* (d) Am	7.9	1.04	0.12	13.4	0.81	0.13
	LP* (s) Am	3.47	1.38	0.09	3.8	1.16	0.08
	LP* (82%d 18%f) Am	5.7	0.74	0.08	2.2	0.51	0.04
	LP* (d) Am	2.07	0.72	0.05	0.6	0.49	0.02
SUM		39.1			40.1		
		LP(~43%s 57% p) O_{eth}			LP(~3%s 97%p) O_{eth}		
Beta	LP* (96%d 4%f) Am	1.5	1.03	0.05	0.1	0.80	0.01
	LP* (96%d 4%f) Am	2.2	1.05	0.06	0.2	0.83	0.02
	LP* (s) Am	3.7	1.29	0.09	0.3	1.07	0.02
	LP* (90%d 10%f) Am	6.8	0.78	0.09	0.04	0.56	0.01
	LP* (89%d 11%f) Am	0.3	0.76	0.02	1.3	0.54	0.03
	LP* (95%d 5%f) Am	5.4	0.70	0.08	1.1	0.48	0.03
Alpha	LP* (98%d 2%f) Am	2.1	1.04	0.06	0.1	0.80	0.01
	LP* (d) Am	1.5	1.02	0.05	0.1	0.78	0.01
	LP* (s) Am	3.9	1.37	0.09	0.2	1.13	0.02
	LP* (d) Am	7.0	0.72	0.09	1.1	0.52	0.03
	LP* (d) Am	4.8	0.70	0.07	1.4	0.47	0.03
SUM		39.1			6.0		

Table 11. Energy gaps, $E_a - E_d$, and Fock matrix elements, F_{da}. for the bonding M–O orbitals of

greatest stabilization energies, $\Delta E(2)$, in the $[Eu(TEDGA)_3]^{3+}$ complex. Donor 1-centre NBOs: LP-O_{am} and LP-O_{eth}. Acceptor unfilled 1-centre NBOs of Eu^{3+}: LP* NBOs (*d,s,f*) hybrids

		$\Delta E(2)$ kcal/mol	$E_a - E_d$ a.u.	F_{da} a.u.	$\Delta E(2)$ kcal/mol	$E_a - E_d$ a.u.	F_{da} a.u.
		LP(56%s 44%p) O_{am}			LP(4%s 96%p) O_{am}		
Beta	LP* (99%d 1%f) Eu	5.8	0.74	0.09	7.2	0.43	0.07
	LP* (99%d 1%f) Eu	1.9	0.74	0.05	0.9	0.43	0.03
	LP* (s) Eu	7.4	3.91	0.22	3.1	3.60	0.13
	LP* (99%d 1%f) Eu	4.4	0.65	0.07	0.5	0.34	0.02
	LP* (98%d 2%f) Eu	1.3	0.65	0.04	0.03	0.34	0.004
	LP* (99%d 1%f) Eu	1.3	0.62	0.04	0.1	0.31	0.01
Alpha	LP* (d) Eu	6.7	0.72	0.09	9.2	0.41	0.08
	LP* (s) Eu	7.4	4.07	0.22	3.6	3.76	0.15
	LP* (99%d 1%f) Eu	5.4	0.63	0.07	0.7	0.33	0.02
	LP* (d) Eu	1.6	0.61	0.04	0.2	0.3	0.01
SUM		43.1			25.5		
		LP(~38%s 62%p) O_{eth}			LP(~8% s 92%p) O_{eth}		
Beta	LP* (99%d 1%f) Eu	2.6	0.65	0.05	0.7	0.47	0.02
	LP* (s) Eu	5.0	3.83	0.18	1.0	3.64	0.08
	LP* (99%d 1%f) Eu	2.3	0.57	0.05	2.7	0.38	0.04
	LP* (98%d 2%f) Eu	1.7	0.57	0.04	0.1	0.38	0.01
	LP* (99%d 1%f) Eu	3.1	0.54	0.05	0.4	0.35	0.01
Alpha	LP* (99%d 1%f) Eu	2.3	0.62	0.05	0.9	0.46	0.03
	LP* (s) Eu	4.9	3.97	0.18	1.4	3.81	0.09
	LP* (99%d 1%f) Eu	2.9	0.54	0.05	2.7	0.37	0.04
	LP* (d) Eu	3.3	0.51	0.05	0.3	0.35	0.01
SUM		28.1			10.1		