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Supporting Information

Energetic Ionic Liquids based on Anionic Rare-Earth Nitrate Complexes

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TABLE S1. Calculated (B3LYP/6-31+G**//MP2/6-311++G**) Total Energy (E_0), Zero-Point Energy (ZPE), Values of Thermal Correction (H_T), and Heats of Formation (HOF) of the cations.

Name	E_0 (au)	ZPE (au)	H_T (kJ/mol)	HOF (kJ/mol)
guanidinium cation	-205.2570379	0.088421	16. 4	575.9
4-amino-1*H*-1,2,4-triazolium cation	-297.2005028	0.089612	15.5	910.7
4-amino-1-methyl-1,2,4-triazolium cation	-336.4026071	0.116980	18.1	866.6
4-amino-1-ethyl-1,2,4-triazolium cation	-375.6060696	0.145786	23.2	828.2
4-amino-1-butyl-1,2,4-triazolium cation	-453.9995324	0.202675	30.4	782.6
1,5-diamino-4-methyl-tetrazolium cation	-407.63759	0.121200	23.7	974.3
1,5-diamino-4*H*-tetrazolium cation	-368.4345101	0.093584	18.9	1018.0
1,2,4-triazolium cation	-242.00879	0.07324	12.0	835.0[1]
1,2,3,4-tetrazolium cation	-257.98206	0.06029	11.8	1016.5
CH_4	-40.3796224	0.044793	10.0	-74.6[2]
CH_3NH_2	-95.59384	0.06403	11.5	-23.0[2]
NH_2NH_2	-111.5836915	0.05331	11.0	95.4[2]
NH_3	-56.4154647	0.034384	10.0	-45.9[2]
CH_3CH_3	-79.571631	0.07461	11.6	-84.0[2]
$CH_3CH_2CH_3$	-118.76734	0.10328	14.4	-103.8[2]

Geometry Coordinates

B3LYP/6-31+G(d,p) optimized geometries (Å)

guanidinium cation

N	-1.321565	-0.205759	-0.001103
H	-1.712671	-1.117729	-0.190869
H	-1.970964	0.542506	0.196530
N	0.482509	1.247196	-0.000648
H	-0.111583	2.041503	-0.192387
H	1.455076	1.435319	0.197728
C	-0.000067	-0.000207	0.000163
N	0.839274	-1.041242	0.000175
H	0.515935	-1.978052	0.195878
H	1.823085	-0.923670	-0.196822

4-amino-1*H*-1,2,4-triazolium cation

C	-0.172838	-1.076494	0.000083
N	0.646548	-0.011281	0.000012

H	0.138613	-2.111769	0.000087
N	-1.420322	0.777774	0.000105
C	-0.158532	1.114920	-0.000022
H	0.217205	2.128611	-0.000051
N	2.040327	-0.142025	-0.000050
H	2.429365	0.280973	-0.840035
H	2.429399	0.280570	0.840123
N	-1.401764	-0.583657	-0.000104
H	-2.279887	-1.094613	-0.000224

4-amino-1-methyl-1,2,4-triazolium cation

C	0.006248	-0.892372	0.000023
N	1.094927	-0.099125	0.000000
H	0.023968	-1.972845	0.000022
N	-0.672815	1.221604	-0.000062
C	0.633882	1.200485	0.000071
H	1.273413	2.071788	0.000093
N	2.397847	-0.610898	-0.000041
H	2.889464	-0.311583	-0.839054
H	2.889422	-0.311798	0.839074
N	-1.048666	-0.091165	0.000002
C	-2.477522	-0.450248	0.000000
H	-2.708511	-1.025521	-0.897763
H	-2.708536	-1.025431	0.897815
H	-3.033921	0.485286	-0.000055

4-amino-1-ethyl-1,2,4-triazolium cation

C	-0.453418	-0.887568	-0.137908
N	-1.533490	-0.103428	0.053323
H	-0.465042	-1.967675	-0.154799
N	0.204983	1.230107	-0.213824
C	-1.083823	1.199207	-0.001677
H	-1.720357	2.065219	0.113005
N	-2.816937	-0.624592	0.253783
H	-3.169571	-0.342863	1.165488
H	-3.438629	-0.317566	-0.490684
N	0.581950	-0.079408	-0.297782
C	2.006363	-0.427326	-0.524049
H	2.025570	-1.498340	-0.738854
H	2.307146	0.113529	-1.424300
C	2.877284	-0.063878	0.674751
H	2.578027	-0.615324	1.570632
H	3.913068	-0.326452	0.443355
H	2.835814	1.008113	0.880951

4-amino-1-butyl-1,2,4-triazolium cation

C	-1.468585	-0.855263	-0.221426
N	-2.546990	-0.156485	0.187768
H	-1.423537	-1.930526	-0.314183
N	-0.947058	1.301181	-0.244621
C	-2.183445	1.173298	0.158119
H	-2.840937	1.987160	0.429243

N	-3.754124	-0.770754	0.540764
H	-3.976720	-0.569096	1.512693
H	-4.498727	-0.457806	-0.077781
N	-0.516687	0.026648	-0.479700
C	0.875809	-0.214898	-0.925207
H	0.902993	-1.239757	-1.304759
H	1.045223	0.469640	-1.759876
C	1.890069	0.004538	0.201158
H	1.668208	-0.680790	1.029579
H	1.784042	1.025836	0.584477
C	3.327571	-0.223032	-0.294010
H	3.420364	-1.241373	-0.694116
H	3.535969	0.460086	-1.127533
C	4.364487	-0.010810	0.814701
H	4.204225	-0.702692	1.648806
H	5.376146	-0.177806	0.434653
H	4.321326	1.010001	1.209300

1,5-diamino-4-methyl-tetrazolium cation

C	0.015400	0.608371	-0.000002
N	1.070948	-0.235973	-0.000003
N	0.625821	-1.539709	0.000001
N	-0.637344	-1.512320	0.000018
N	-1.057975	-0.198681	-0.000015
N	0.084884	1.933576	0.000021
H	1.000085	2.369554	0.000013
H	-0.739521	2.516578	-0.000035
N	2.388355	0.176842	-0.000005
H	2.860771	-0.162415	0.836451
H	2.860759	-0.162380	-0.836482
C	-2.483670	0.137308	-0.000003
H	-2.734056	0.702498	0.900845
H	-2.733930	0.703009	-0.900565
H	-3.027312	-0.807060	-0.000310

1,5-diamino-4*H*-tetrazolium cation

C	-0.169518	0.731015	0.000001
N	-0.332230	-0.611344	0.000001
N	0.900190	-1.238153	-0.000001
N	1.789356	-0.344684	0.000000
N	1.165458	0.884456	0.000001
N	-1.144434	1.625521	-0.000005
H	-2.102518	1.291838	-0.000001
H	-0.969528	2.620728	0.000020
N	-1.564057	-1.232884	0.000000
H	-1.669006	-1.803784	-0.837399
H	-1.669015	-1.803770	0.837407
H	1.727190	1.728519	-0.000002

TABLE S2. Calculated (MP2/SBKJC+d[3]) Total Energy (E_0), Scaled Zero-Point Energy (ZPE),[4] Values of Thermal Correction (H_T), and Heats of Formation (HOF*)* of $[M(NO_3)_6]^{3-}$, $[M(L)_4]^-$, $[NO_3]^-$, and $[L]^-$ anions (M = La,Ce; L = F,Cl).

Name	E_0 (au)	ZPE (au)	H_T (kJ/mol)	HOF (kJ/mol)
$[La(NO_3)_6]^{3-}$	-375.386523	0.094049	75.3	-1924.5
$[Ce(NO_3)_6]^{3-}$	-382.505659	0.094215	74.9	-1911.6
$[LaF_4]^-$	-127.762092	0.005142	22.2	-1996.9[5]
$[LaCl_4]^-$	-90.962002	0.003179	25.5	-1254.2[5]
$[CeF_4]^-$	-134.899719	0.005168	22.2	-1998.2[5]
$[NO_3]^-$	-57.334849	0.013808	10.9	-306.2[6]
$[F]^-$	-24.018946	0	0	-265.1[6]
$[Cl]^-$	-14.871336	0	0	-233.8[6]

Geometry Coordinates

MP2/SBKJC+(d) optimized geometries (Å)

$[La(NO_3)_6]^{3-}$ anion

La	.000000	.000000	.000000
O	-1.610453	-.929796	1.926717
O	1.610453	-.929796	1.926717
O	.000000	-1.859591	-1.926717
O	1.610453	.929796	-1.926717
O	-1.610453	.929796	-1.926717
O	.000000	1.859591	1.926717
N	-2.534764	-1.463447	1.187168
N	2.534764	-1.463447	1.187168
N	.000000	-2.926893	-1.187168
N	2.534764	1.463447	-1.187168
N	-2.534764	1.463447	-1.187168
N	.000000	2.926893	1.187168
O	-2.397008	-1.383913	-.090771
O	2.397008	-1.383913	-.090771
O	.000000	-2.767826	.090771
O	2.397008	1.383913	.090771
O	-2.397008	1.383913	.090771
O	.000000	2.767826	-.090771
O	-3.539128	-2.043317	1.716065
O	3.539128	-2.043317	1.716065
O	.000000	-4.086633	-1.716065
O	3.539128	2.043317	-1.716065
O	-3.539128	2.043317	-1.716065
O	.000000	4.086633	1.716065

$[Ce(NO_3)_6]^{3-}$ anion

Ce	.000000	.000000	.000000
O	-1.555958	-.898333	1.902795
O	1.555958	-.898333	1.902795
O	.000000	-1.796666	-1.902795
O	1.555958	.898333	-1.902795
O	-1.555958	.898333	-1.902795
O	.000000	1.796666	1.902795
N	-2.488875	-1.436953	1.177648
N	2.488875	-1.436953	1.177648
N	.000000	-2.873905	-1.177648
N	2.488875	1.436953	-1.177648

N	-2.488875	1.436953	-1.177648
N	.000000	2.873905	1.177648
O	-2.363399	-1.364509	-.101132
O	2.363399	-1.364509	-.101132
O	.000000	-2.729018	.101132
O	2.363399	1.364509	.101132
O	-2.363399	1.364509	.101132
O	.000000	2.729018	-.101132
O	-3.487490	-2.013503	1.721882
O	3.487490	-2.013503	1.721882
O	.000000	-4.027006	-1.721882
O	3.487490	2.013503	-1.721882
O	-3.487490	2.013503	-1.721882
O	.000000	4.027006	1.721882

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