Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Molecules mimicking atoms: Monomers and dimers of alkali metal solvated electron precursors

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Table S1. CCSD(T)/aug-cc-pVTZ optimal geometries for $M(NH_3)_4^{0,\pm}$. Cartesian coordinates are given in Å.

$Li(NH_3)_4$

Li	0.000000	0.000000	0.000000
N	1.696888	0.000000	1.199881
N	-1.696888	0.000000	1.199881
N	0.000000	1.696888	-1.199881
N	0.000000	-1.696888	-1.199881
H	-2.562769	0.000000	0.660935
H	-1.748736	0.814033	1.812151
H	-1.748736	-0.814033	1.812151
H	0.814033	1.748736	-1.812151
H	0.000000	2.562769	-0.660935
H	-0.814033	1.748736	-1.812151
H	0.814033	-1.748736	-1.812151
H	0.000000	-2.562769	-0.660935
H	-0.814033	-1.748736	-1.812151
H	1.748736	0.814033	1.812151
H	1.748736	-0.814033	1.812151
H	2.562769	0.000000	0.660935

$Na(NH_3)_4$

Na	0.000000	0.000000	0.000000
N	2.022555	0.000000	1.430162
N	-2.022555	0.000000	1.430162
N	0.000000	2.022555	-1.430162
N	0.000000	-2.022555	-1.430162
H	-2.888065	0.000000	0.891951
H	-2.074737	0.813328	2.042170
H	-2.074737	-0.813328	2.042170
H	0.813328	2.074737	-2.042170
H	0.000000	2.888065	-0.891951
H	-0.813328	2.074737	-2.042170
H	0.813328	-2.074737	-2.042170
H	0.000000	-2.888065	-0.891951
H	-0.813328	-2.074737	-2.042170
H	2.074737	0.813328	2.042170
H	2.074737	-0.813328	2.042170
H	2.888065	0.000000	0.891951

$Li(NH_3)_4^+$

Li	0.000000	0.000000	0.000000
N	1.722061	0.000000	1.217681
N	-1.722061	0.000000	1.217681
N	0.000000	1.722061	-1.217681
N	0.000000	-1.722061	-1.217681
H	-2.592646	0.000000	0.691192
H	-1.785070	0.807577	1.833278
H	-1.785070	-0.807577	1.833278
H	0.807577	1.785070	-1.833278
H	0.000000	2.592646	-0.691192
H	-0.807577	1.785070	-1.833278
H	0.807577	-1.785070	-1.833278
H	0.000000	-2.592646	-0.691192
H	-0.807577	-1.785070	-1.833278
H	1.785070	0.807577	1.833278
H	1.785070	-0.807577	1.833278
H	2.592646	0.000000	0.691192

$Na(NH_3)_4^+$

Na	0.000000	0.000000	0.000000
N	2.044102	0.000000	1.445399
N	-2.044102	0.000000	1.445399
N	0.000000	2.044102	-1.445399
N	0.000000	-2.044102	-1.445399
H	-2.914607	0.000000	0.919270
H	-2.107325	0.807282	2.060938
H	-2.107325	-0.807282	2.060938
H	0.807282	2.107325	-2.060938
H	0.000000	2.914607	-0.919270
H	-0.807282	2.107325	-2.060938
H	0.807282	-2.107325	-2.060938
H	0.000000	-2.914607	-0.919270
H	-0.807282	-2.107325	-2.060938
H	2.107325	0.807282	2.060938
H	2.107325	-0.807282	2.060938
H	2.914607	0.000000	0.919270

$Li(NH_3)_4^-$

Li	0.000000	0.000000	0.000000
N	1.697093	0.000000	1.200026
N	-1.697093	0.000000	1.200026
N	0.000000	1.697093	-1.200026
N	0.000000	-1.697093	-1.200026
H	-2.562989	0.000000	0.660576
H	-1.748592	0.814397	1.812307
H	-1.748592	-0.814397	1.812307
H	0.814397	1.748592	-1.812307
H	0.000000	2.562989	-0.660576
H	-0.814397	1.748592	-1.812307
H	0.814397	-1.748592	-1.812307
H	0.000000	-2.562989	-0.660576
H	-0.814397	-1.748592	-1.812307
H	1.748592	0.814397	1.812307
H	1.748592	-0.814397	1.812307
H	2.562989	0.000000	0.660576

$Na(NH_3)_4^-$

Na	0.000000	0.000000	0.000000
N	2.019459	0.000000	1.427973
N	-2.019459	0.000000	1.427973
N	0.000000	2.019459	-1.427973
N	0.000000	-2.019459	-1.427973
H	-2.884840	0.000000	0.888838
H	-2.070923	0.813917	2.039890
H	-2.070923	-0.813917	2.039890
H	0.813917	2.070923	-2.039890
H	0.000000	2.884840	-0.888838
H	-0.813917	2.070923	-2.039890
H	0.813917	-2.070923	-2.039890
H	0.000000	-2.884840	-0.888838
H	-0.813917	-2.070923	-2.039890
H	2.070923	0.813917	2.039890
H	2.070923	-0.813917	2.039890
H	2.884840	0.000000	0.888838

Table S2. B3LYP/aug-cc-pVTZ harmonic vibrational frequencies (cm^{-1}) for $M(NH_3)_4^{0,\pm}$.

$Li(NH_3)_4$	$Li(NH_3)_4^+$	$Li(NH_3)_4^-$	$Na(NH_3)_4$	$Na(NH_3)_4^+$	$Na(NH_3)_4^-$
81.1	76.8	82.4	47.3	46.1	48.5
81.1	80.6	82.4	47.3	46.1	48.5
104.0	80.6	108.5	51.4	60.7	51.7
104.0	98.7	108.5	51.4	64.6	51.7
104.0	98.7	108.5	51.4	64.6	51.7
107.8	98.7	127.4	94.1	64.6	109.2
116.3	120.4	135.7	98.1	72.4	112.2
116.3	120.4	135.7	98.1	72.4	112.2
116.3	120.4	135.7	98.1	72.4	112.2
232.4	221.7	233.0	187.9	185.6	188.8
333.6	340.0	340.2	237.7	229.6	239.1
333.6	340.0	340.2	237.7	229.6	239.1
333.6	340.0	340.2	237.7	229.6	239.1
334.6	349.0	343.9	298.4	328.3	302.7
334.6	349.0	343.9	298.4	328.3	302.7
334.6	349.0	343.9	298.4	328.3	302.7
417.5	437.5	422.5	305.0	382.6	331.3
417.5	437.5	422.5	305.0	382.6	331.3
494.8	554.2	509.8	305.0	421.9	331.3
494.8	554.2	509.8	339.5	421.9	342.8
494.8	554.2	509.8	339.5	421.9	342.8
1160.0	1225.3	1147.4	1134.1	1198.5	1118.7
1160.0	1225.3	1147.4	1134.1	1198.5	1118.7
1160.0	1225.3	1147.4	1134.1	1198.5	1118.7
1167.3	1237.3	1155.7	1136.4	1205.7	1121.1
1634.7	1668.1	1628.8	1640.4	1669.8	1633.0
1634.7	1668.1	1628.8	1640.4	1669.8	1633.0
1642.1	1668.1	1637.9	1644.7	1669.8	1638.0
1642.1	1672.7	1637.9	1644.7	1672.5	1638.0
1642.1	1672.7	1637.9	1644.7	1672.5	1638.0
1643.1	1679.9	1638.8	1645.5	1675.9	1639.7
1643.1	1679.9	1638.8	1645.5	1675.9	1639.7
1643.1	1679.9	1638.8	1645.5	1675.9	1639.7
3363.4	3455.0	3349.1	3374.1	3458.7	3358.0
3363.4	3455.0	3349.1	3374.1	3458.7	3358.0
3363.4	3455.0	3349.1	3374.1	3458.7	3358.0
3381.1	3456.1	3356.2	3390.9	3459.3	3365.2
3478.3	3549.9	3462.1	3494.9	3556.5	3477.2
3478.3	3549.9	3462.1	3494.9	3556.5	3477.2
3478.3	3550.1	3462.1	3494.9	3556.5	3477.2
3481.1	3550.1	3463.4	3496.2	3556.5	3477.8
3481.1	3550.1	3463.4	3496.2	3556.5	3477.8
3486.0	3550.8	3469.4	3498.6	3556.9	3480.8
3486.0	3550.8	3469.4	3498.6	3556.9	3480.8
3486.0	3550.8	3469.4	3498.6	3556.9	3480.8

Table S3. DFT/B3LYP optimal geometries for $[M(NH_3)_4]_2$. The cc-pVTZ/$_{Li,Na,N}$ aug-cc-pVTZ/$_H$ basis set was employed. Cartesian coordinates are given in Å.

$[Li(NH_3)_4]_2$				$[Na(NH_3)_4]_2$			
Li	0.000000	0.000000	3.162713	Na	-3.216300	-0.000553	-0.000584
Li	-0.000000	-0.000000	-3.162713	Na	3.216061	0.000588	0.000615
N	0.000000	1.921827	2.369803	N	-2.254286	-1.653683	1.528333
N	-1.664351	-0.960913	2.369803	N	2.253988	-2.150408	-0.664788
N	1.664351	-0.960913	2.369803	N	2.248077	0.501228	2.192575
N	1.664351	0.960913	-2.369803	N	-5.694533	0.002619	-0.000316
N	-1.664351	0.960913	-2.369803	N	5.694118	-0.002528	0.001186
N	0.000000	0.000000	5.252932	N	-2.249701	-0.502750	-2.192458
N	-0.000000	-0.000000	-5.252932	N	-2.252045	2.150219	0.661065
H	0.000000	1.770152	1.356827	N	2.254587	1.655164	-1.525591
H	-1.532997	-0.885076	1.356827	H	-2.403478	-2.642107	1.332516
H	1.532997	-0.885076	1.356827	H	-2.401828	-1.530643	2.528944
H	1.532997	0.885076	-1.356827	H	2.403325	-2.955716	-0.059365
H	-1.532997	0.885076	-1.356827	H	-1.258411	-1.483302	1.368526
H	-0.816514	2.499548	2.564777	H	2.392596	-0.164249	2.950394
H	0.816514	2.499548	2.564777	H	1.257748	-1.927641	-0.595635
H	-1.756415	-1.956896	2.564777	H	2.402693	-2.472857	-1.619633
H	-2.572929	-0.542652	2.564777	H	-6.078745	-0.690046	0.636168
H	2.572929	-0.542652	2.564777	H	1.252101	0.451793	1.963042
H	1.756415	-1.956896	2.564777	H	-6.077043	-0.201600	-0.919247
H	2.572929	0.542652	-2.564777	H	6.076661	0.200966	0.920243
H	1.756415	1.956896	-2.564777	H	2.397980	1.428482	2.587241
H	-1.756415	1.956896	-2.564777	H	-2.398196	-1.430423	-2.586501
H	-2.572929	0.542652	-2.564777	H	6.075115	-0.901088	-0.281537
H	0.000000	-0.941915	5.635517	H	-1.253732	-0.451859	-1.963616
H	0.815723	0.470958	5.635517	H	-6.076254	0.901125	0.281950
H	-0.815723	0.470958	5.635517	H	6.078781	0.690018	-0.635160
H	-0.815723	-0.470958	-5.635517	H	-2.398746	2.474139	1.615762
H	0.000000	0.941915	-5.635517	H	-1.255923	1.926889	0.590505
H	0.815723	-0.470958	-5.635517	H	-2.396279	0.162225	-2.950321
N	-0.000000	-1.921827	-2.369803	H	1.258943	1.485472	-1.363513
H	-0.000000	-1.770152	-1.356827	H	-2.400935	2.955528	0.055121
H	-0.816514	-2.499548	-2.564777	H	2.400339	1.531721	-2.526233
H	0.816514	-2.499548	-2.564777	H	2.404481	2.643756	-1.330040

Table S4. DFT/B3LYP harmonic vibrational frequencies (cm^{-1}) for $[M(NH_3)_4]_2$. The cc-pVTZ/$_{Li,Na,N}$ aug-cc-pVTZ/$_H$ basis set was employed.

$[Li(NH_3)_4]_2$				$[Na(NH_3)_4]_2$			
15.7	230.9	1144.3	3315.9	5.1	185.8	1123.0	3330.9
21.5	231.2	1144.4	3315.9	10.2	186.1	1123.4	3332.1
21.6	319.7	1165.7	3319.8	13.5	237.7	1139.9	3333.2
26.9	319.7	1165.7	3319.8	16.8	237.8	1141.6	3334.4
26.9	320.0	1169.2	3327.6	19.1	238.0	1142.3	3341.0
34.3	320.0	1169.2	3329.5	20.9	238.0	1144.1	3342.3
34.6	325.9	1169.2	3414.3	24.6	240.0	1144.6	3423.4
42.9	326.0	1177.0	3415.2	29.4	240.2	1146.9	3424.5
71.1	343.5	1627.3	3433.9	29.9	291.0	1631.0	3446.3
71.1	344.3	1627.3	3435.6	31.9	291.5	1631.2	3448.5
71.9	344.3	1632.5	3442.0	35.3	294.6	1635.6	3451.0
71.9	347.0	1632.5	3442.0	37.7	295.2	1635.7	3451.7
85.1	347.0	1637.1	3442.6	40.8	296.0	1635.8	3452.3
85.1	356.0	1637.2	3442.6	41.8	296.5	1638.0	3453.0
87.6	415.7	1637.2	3490.8	44.5	330.8	1638.1	3498.2
89.1	415.7	1637.4	3490.8	44.6	332.1	1638.2	3498.5
91.9	417.2	1637.4	3491.0	53.4	333.3	1638.5	3498.8
91.9	417.2	1638.4	3491.0	56.6	343.6	1639.6	3499.4
103.7	509.2	1639.3	3495.8	60.7	345.0	1641.3	3501.3
103.8	509.3	1641.1	3495.9	61.5	353.4	1641.3	3502.1
106.9	516.2	1652.4	3531.6	62.4	353.6	1656.1	3541.0
106.9	518.8	1652.4	3531.6	63.2	354.3	1656.2	3541.6
114.9	519.0	1652.7	3531.6	64.0	355.2	1656.6	3541.9
119.2	538.4	1652.7	3531.6	67.1	375.3	1656.7	3542.2

* The optimal structure for $[Na(NH_3)_4]_2$ was found to have seven imaginary frequencies related to internal rotations of ammonia ligands. Our attempts to re-optimize the structure after performing manually these rotations led to the same structure. We suspect that it is a rather artificial technical issue.

Table S5. CASPT2 optimal geometry for $[Li(NH_3)_4]_2$. The cc-pVTZ/$_{Li,Na,N}$ aug-cc-pVTZ/$_H$ basis set was employed. Cartesian coordinates are given in Å.

$[Li(NH_3)_4]_2$
Li 0.000000 0.000000 3.182534
Li 0.000000 0.000000 -3.182534
N -1.901969 0.000000 2.332416
N 0.950984 -1.647153 2.332416
N 0.950984 1.647153 2.332416
N -0.950984 1.647153 -2.332416
N -0.950984 -1.647153 -2.332416
N 0.000000 0.000000 5.285950
N 0.000000 0.000000 -5.285950
H -1.648673 0.000000 1.339441
H 0.824336 -1.427792 1.339441
H 0.824336 1.427792 1.339441
H -0.824336 1.427792 -1.339441
H -0.824336 -1.427792 -1.339441
H -2.501704 -0.813493 2.450891
H -2.501704 0.813493 2.450891
H 1.955358 -1.759793 2.450891
H 0.546346 -2.573286 2.450891
H 0.546346 2.573286 2.450891
H 1.955358 1.759793 2.450891
H -0.546346 2.573286 -2.450891
H -1.955358 1.759793 -2.450891
H -1.955358 -1.759793 -2.450891
H -0.546346 -2.573286 -2.450891
H 0.938175 0.000000 5.669731
H -0.469088 0.812483 5.669731
H -0.469088 -0.812483 5.669731
H 0.469088 -0.812483 -5.669731
H -0.938175 0.000000 -5.669731
H 0.469088 0.812483 -5.669731
N 1.901969 0.000000 -2.332416
H 1.648673 0.000000 -1.339441
H 2.501704 -0.813493 -2.450891
H 2.501704 0.813493 -2.450891

Table S6. Electron attachment energies (eV) and pole strengths (in parentheses) of $Li(NH_3)_4^+$ from diagonal electron propagator methods[a] calculated at the geometry of $Li(NH_3)_4$ using the cc-pVTZ/$_{Li}$ cc-pVTZ/$_N$ d-aug-cc-pVTZ/$_H$ basis sets. 1s orbitals of Li and N were frozen.

Final State	KT[b]	D2[c]	OVGF[d]	P3[e]	P3+[f]
$^2A_1$	-2.440	-2.829 (0.987)	-2.817 (0.986)	-2.837 (0.985)	-2.837 (0.985)
$^2T_2$	-1.891	-2.110 (0.992)	-2.108 (0.991)	-2.119 (0.991)	-2.118 (0.991)
$^2T_2$	-1.324	-1.430 (0.996)	-1.431 (0.996)	-1.437 (0.995)	-1.436 (0.995)
^2E	-1.315	-1.402 (0.997)	-1.404 (0.997)	-1.408 (0.996)	-1.408 (0.996)
$^2A_1$	-1.093	-1.275 (0.994)	-1.266 (0.993)	-1.276 (0.993)	-1.276 (0.993)
$^2T_1$	-0.810	-0.845 (0.999)	-0.846 (0.998)	-0.849 (0.998)	-0.848 (0.998)
$^2T_2$	-0.783	-0.955 (0.994)	-0.949 (0.994)	-0.958 (0.993)	-0.958 (0.993)
^2E	-0.392	-0.507 (0.996)	-0.507 (0.995)	-0.513 (0.995)	-0.512 (0.995)
$^2T_2$	-0.392	-0.570 (0.994)	-0.566 (0.993)	-0.576 (0.993)	-0.575 (0.993)
$^2T_2$	-0.139	-0.269 (0.995)	-0.273 (0.996)	-0.279 (0.994)	-0.278 (0.994)

[a] Accuracy of the methods increases from left to right. For a brief introduction to and numerical comparison of propagator methods, see, for example, Dolgounitcheva, O.; Díaz-Tinoco, M.; Zakrzewski, V. G.; Richard, R. M.; Marom, N.; Sherill, C. D.; Ortiz J. V. *J. Chem. Theory Comput.* **2016**, *12*, 627-637.

[b] Koopmans's theorem

[c] Diagonal second-order approximation

[d] Outer valence Green function method

[e] Partial third-order quasiparticle method

[f] Renormalized partial third-order quasiparticle method

Table S7. Excitation energies (eV) of $Li(NH_3)_4$ inferred from electron attachment energies in Table S6.

Final State	KT	D2	OVGF	P3	P3+
$^2A_1$	0.000	0.000	0.000	0.000	0.000
$^2T_2$	0.549	0.719	0.709	0.718	0.719
$^2T_2$	1.116	1.399	1.386	1.400	1.401
^2E	1.125	1.427	1.413	1.429	1.429
$^2A_1$	1.347	1.554	1.551	1.561	1.561
$^2T_1$	1.630	1.984	1.971	1.988	1.989
$^2T_2$	1.657	1.874	1.868	1.879	1.879
^2E	2.048	2.322	2.310	2.324	2.325
$^2T_2$	2.048	2.259	2.251	2.261	2.262
$^2T_2$	2.301	2.560	2.544	2.558	2.559

Table S8. Electron attachment energies (eV) and pole strengths (in parentheses) of $Na(NH_3)_4^+$ from diagonal electron propagator methods calculated at the geometry of $Na(NH_3)_4$ using the cc-pVTZ/$_{Na}$ cc-pVTZ/$_N$ d-aug-cc-pVTZ/$_H$ basis sets. 1s, 2s and 2p orbitals of Na and 1s of N were frozen.

Final State	KT	D2	OVGF	P3	P3+
$^2A_1$	-2.344	-2.701 (0.988)	-2.696 (0.987)	-2.712 (0.986)	-2.711 (0.986)
$^2T_2$	-1.835	-2.046 (0.993)	-2.046 (0.992)	-2.056 (0.991)	-2.055 (0.991)
$^2T_2$	-1.286	-1.384 (0.996)	-1.386 (0.996)	-1.391 (0.995)	-1.391 (0.995)
^2E	-1.282	-1.362 (0.997)	-1.365 (0.997)	-1.368 (0.996)	-1.368 (0.996)
$^2A_1$	-1.060	-1.229 (0.994)	-1.224 (0.993)	-1.232 (0.993)	-1.232 (0.993)
$^2T_2$	-0.847	-0.979 (0.995)	-0.977 (0.995)	-0.983 (0.994)	-0.982 (0.995)
$^2T_1$	-0.805	-0.842 (0.999)	-0.843 (0.998)	-0.845 (0.998)	-0.845 (0.998)
$^2T_2$	-0.373	-0.523 (0.995)	-0.523 (0.994)	-0.530 (0.993)	-0.529 (0.994)
^2E	-0.360	-0.471 (0.996)	-0.473 (0.995)	-0.478 (0.995)	-0.477 (0.995)
$^2T_2$	-0.044	-0.202 (0.994)	-0.206 (0.993)	-0.214 (0.993)	-0.213 (0.993)

Table S9. Excitation energies (eV) of $Na(NH_3)_4$ inferred from electron attachment energies in Table S8.

Final State	KT	D2	OVGF	P3	P3+
$^2A_1$	0.000	0.000	0.000	0.000	0.000
$^2T_2$	0.509	0.655	0.650	0.656	0.656
$^2T_2$	1.058	1.317	1.310	1.321	1.320
^2E	1.062	1.339	1.331	1.344	1.343
$^2A_1$	1.284	1.472	1.472	1.480	1.479
$^2T_2$	1.497	1.722	1.719	1.729	1.729
$^2T_1$	1.539	1.859	1.853	1.867	1.866
$^2T_2$	1.971	2.178	2.173	2.182	2.182
^2E	1.984	2.230	2.223	2.234	2.234
$^2T_2$	2.300	2.499	2.490	2.498	2.498

Importance of diffuse functions

We repeated several calculations to study the effect of diffuse functions in the basis set. In agreement with our previous work on Be-SEPs we found that they are important for the calculation of accurate geometries, excitation energies and the stabilization of the anionic systems over the neutral ones. In Tables S10-S12 and Figure S2 we report our results using a plain cc-pVTZ basis set on all atoms.

Figure S2. CCSD(T)/cc-pVTZ PECs for the dissociation of one or four ammonia ligands from $M(NH_3)_4$, M = Li, Na.

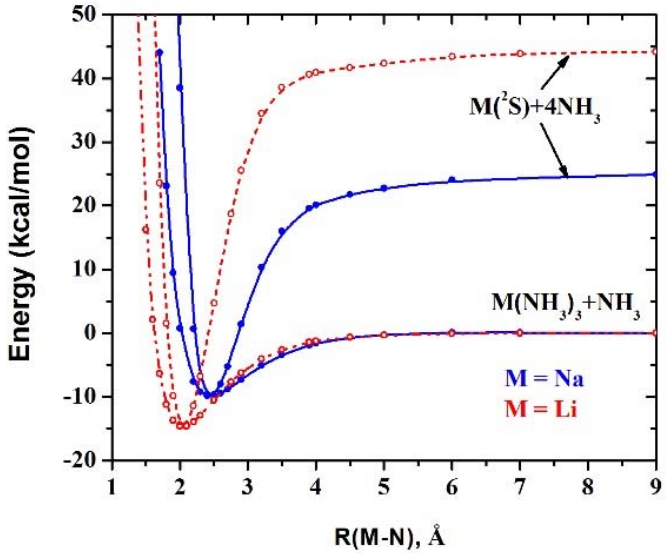

Table S10. CCSD(T)/cc-pVTZ optimized M-N and N-H bond distances (Å), M-N-H angles (degrees), and relative energies ΔE (eV) for M = Li and Na.

Species	M-N	N-H	M-N-H	ΔE	ΔE
$Li(NH_3)_4^+$	2.111	1.017	113.6	-233.321634	2.65
$Li(NH_3)_4$	2.050	1.019	112.2	-233.419113	0.0
$Li(NH_3)_4^-$	2.008	1.019	110.9	-233.406380	0.35
$Na(NH_3)_4^+$	2.503	1.016	113.7	-387.711798	2.57
$Na(NH_3)_4$	2.453	1.018	112.5	-387.806107	0.0
$Na(NH_3)_4^-$	2.412	1.019	111.6	-387.797282	0.24

Table S11. CASSCF/cc-pVTZ, CASPT2/cc-pVTZ and P3+/cc-pVTZ excitation energies (eV) of $Li(NH_3)_4$ and $Na(NH_3)_4$. States in red denote unbound states with respect to the ionization limit.

E.C.[a]	$Li(NH_3)_4$			$Na(NH_3)_4$		
	CASSCF	CASPT2	P3+	CASSCF	CASPT2	P3+
$1s^1$	0.00	0.00	0.00	0.00	0.00	0.00
$1p^1$	0.37	0.63	0.63	0.30	0.53	0.54
	0.37	0.63	0.63	0.30	0.53	0.54
	0.37	0.64	0.63	0.30	0.53	0.54
?	3.55	3.35	3.36	2.75	2.81	2.80
?	3.55	3.35	3.36	2.75	2.81	2.80
?	3.55	3.36	3.36	2.75	2.81	2.80
?	4.14	3.98	4.03	3.57	3.33	3.35
?	4.14	3.98	4.05	3.57	3.33	3.35
?	4.14	3.99	4.05	3.57	3.33	3.35

[a] Electronic configuration.

Table S12. Optimized CCSD(T)/cc-pVTZ Cartesian coordinates (in Å) for $Li(NH_3)_4^{0,\pm}$

$\underline{Li(NH_3)_4}$

Li	0.0000000000	0.0000000000	-0.0000000087
N	1.6736870189	0.0000000000	1.1834754458
N	-1.6736870189	0.0000000000	1.1834754458
N	0.0000000000	1.6736870320	-1.1834754447
N	0.0000000000	-1.6736870320	-1.1834754447
H	-2.5332000287	0.0000000000	0.6358393724
H	-1.7162063344	0.8169936879	1.7912429217
H	-1.7162063344	-0.8169936879	1.7912429217
H	0.8169936879	1.7162063542	-1.7912429201
H	0.0000000000	2.5332000358	-0.6358393617
H	-0.8169936879	1.7162063542	-1.7912429201
H	0.8169936879	-1.7162063542	-1.7912429201
H	0.0000000000	-2.5332000358	-0.6358393617
H	-0.8169936879	-1.7162063542	-1.7912429201
H	1.7162063344	0.8169936879	1.7912429217
H	1.7162063344	-0.8169936879	1.7912429217
H	2.5332000287	0.0000000000	0.6358393724

$Li(NH_3)_4^+$

Li	0.0000000000	0.0000000000	-0.0000000090
N	1.7232599709	0.0000000000	1.2185288166
N	-1.7232599709	0.0000000000	1.2185288166
N	0.0000000000	1.7232599844	-1.2185288154
N	0.0000000000	-1.7232599844	-1.2185288154
H	-2.5937167179	0.0000000000	0.6935378754
H	-1.7872636816	0.8064530300	1.8340346834
H	-1.7872636816	-0.8064530300	1.8340346834
H	0.8064530300	1.7872637019	-1.8340346815
H	0.0000000000	2.5937167256	-0.6935378646
H	-0.8064530300	1.7872637019	-1.8340346815
H	0.8064530300	-1.7872637019	-1.8340346815
H	0.0000000000	-2.5937167256	-0.6935378646
H	-0.8064530300	-1.7872637019	-1.8340346815
H	1.7872636816	0.8064530300	1.8340346834
H	1.7872636816	-0.8064530300	1.8340346834
H	2.5937167179	0.0000000000	0.6935378754

$Li(NH_3)_4^-$

Li	0.0000000000	0.0000000000	-0.0000000085
N	1.6394666003	0.0000000000	1.1592779557
N	-1.6394666003	0.0000000000	1.1592779557
N	0.0000000000	1.6394666132	-1.1592779546
N	0.0000000000	-1.6394666132	-1.1592779546
H	-2.4858254171	0.0000000000	0.5909410883
H	-1.6607711476	0.8250542631	1.7577440123
H	-1.6607711476	-0.8250542631	1.7577440123
H	0.8250542631	1.6607711670	-1.7577440109
H	0.0000000000	2.4858254237	-0.5909410778
H	-0.8250542631	1.6607711670	-1.7577440109
H	0.8250542631	-1.6607711670	-1.7577440109
H	0.0000000000	-2.4858254237	-0.5909410778
H	-0.8250542631	-1.6607711670	-1.7577440109
H	1.6607711476	0.8250542631	1.7577440123
H	1.6607711476	-0.8250542631	1.7577440123
H	2.4858254171	0.0000000000	0.5909410883

$Na(NH_3)_4$

Na	0.0000000000	0.0000000000	-0.0000000085
N	2.0028971625	0.0000000000	1.4162621737
N	-2.0028971625	0.0000000000	1.4162621737
N	0.0000000000	2.0028971782	-1.4162621686
N	0.0000000000	-2.0028971782	-1.4162621686
H	-2.8643218719	0.0000000000	0.8732510851
H	-2.0496426859	0.8146791796	2.0253814253
H	-2.0496426859	-0.8146791796	2.0253814253
H	0.8146791796	2.0496427083	-2.0253814197
H	0.0000000000	2.8643218816	-0.8732510704
H	-0.8146791796	2.0496427083	-2.0253814197
H	0.8146791796	-2.0496427083	-2.0253814197
H	0.0000000000	-2.8643218816	-0.8732510704
H	-0.8146791796	-2.0496427083	-2.0253814197
H	2.0496426859	0.8146791796	2.0253814253
H	2.0496426859	-0.8146791796	2.0253814253
H	2.8643218719	0.0000000000	0.8732510851

$Na(NH_3)_4^+$

Na	0.0000000000	0.0000000000	-0.0000000087
N	2.0439237674	0.0000000000	1.4452723644
N	-2.0439237674	0.0000000000	1.4452723644
N	0.0000000000	2.0439237834	-1.4452723592
N	0.0000000000	-2.0439237834	-1.4452723592
H	-2.9143505306	0.0000000000	0.9207735885
H	-2.1082604995	0.8060900247	2.0607570295
H	-2.1082604995	-0.8060900247	2.0607570295
H	0.8060900247	2.1082605223	-2.0607570236
H	0.0000000000	2.9143505408	-0.9207735736
H	-0.8060900247	2.1082605223	-2.0607570236
H	0.8060900247	-2.1082605223	-2.0607570236
H	0.0000000000	-2.9143505408	-0.9207735736
H	-0.8060900247	-2.1082605223	-2.0607570236
H	2.1082604995	0.8060900247	2.0607570295
H	2.1082604995	-0.8060900247	2.0607570295
H	2.9143505306	0.0000000000	0.9207735885

$Na(NH_3)_4^-$

Na	0.0000000000	0.0000000000	-0.0000000084
N	1.9696230436	0.0000000000	1.3927338185
N	-1.9696230436	0.0000000000	1.3927338185
N	0.0000000000	1.9696230590	-1.3927338134
N	0.0000000000	-1.9696230590	-1.3927338134
H	-2.8221651776	0.0000000000	0.8352741968
H	-2.0017106237	0.8204545475	1.9955721407
H	-2.0017106237	-0.8204545475	1.9955721407
H	0.8204545475	2.0017106458	-1.9955721353
H	0.0000000000	2.8221651869	-0.8352741823
H	-0.8204545475	2.0017106458	-1.9955721353
H	0.8204545475	-2.0017106458	-1.9955721353
H	0.0000000000	-2.8221651869	-0.8352741823
H	-0.8204545475	-2.0017106458	-1.9955721353
H	2.0017106237	0.8204545475	1.9955721407
H	2.0017106237	-0.8204545475	1.9955721407
H	2.8221651776	0.0000000000	0.8352741968