Aufbau principle for diffuse electrons of double–shell metal ammonia complexes: the case of $M(NH_3)_4@12NH_3$, M=Li, Be^+, B^{2+}

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Electron propagator results for $Li(NH_3)_4@(NH_3)_{12}$

Table S1. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $Li(NH_3)_4@(NH_3)_{12}^+$, at neutral geometry (optimized at CAM-B3LYP/aug-cc-pVTZ level), from diagonal electron propagator methods[a] using the cc-pVDZ basis for Li, N and 12 inner H atoms, and d-aug-cc-pVDZ basis for 36 outer H atoms. All valence electrons correlated.

Neutral Final State	KT[b]	D2[c]	OVGF[d]	P3[e]	P3+[f]
^{2}A	-1.432	-1.675 (0.991)	-1.692 (0.989)	-1.692 (0.989)	-1.691 (0.989)
^{2}T	-1.270	-1.453 (0.993)	-1.467 (0.991)	-1.468 (0.991)	-1.467 (0.991)
^{2}E	-1.028	-1.135 (0.996)	-1.145 (0.995)	-1.145 (0.995)	-1.144 (0.995)
^{2}T	-1.013	-1.129 (0.995)	-1.137 (0.994)	-1.140 (0.994)	-1.139 (0.994)
^{2}T	-0.739	-0.803 (0.997)	-0.809 (0.997)	-0.810 (0.997)	-0.810 (0.997)
^{2}A	-0.733	-0.816 (0.997)	-0.822 (0.996)	-0.825 (0.996)	-0.824 (0.996)
^{2}T	-0.733	-0.801 (0.997)	-0.807 (0.997)	-0.809 (0.996)	-0.809 (0.996)
^{2}T	-0.488	-0.593 (0.996)	-0.600 (0.995)	-0.601 (0.995)	-0.601 (0.995)
^{2}A	-0.476	-0.710 (0.992)	-0.726 (0.990)	-0.723 (0.989)	-0.722 (0.990)
^{2}T	-0.440	-0.476 (0.999)	-0.480 (0.998)	-0.481 (0.998)	-0.481 (0.998)
^{2}E	-0.437	-0.474 (0.999)	-0.478 (0.998)	-0.479 (0.998)	-0.479 (0.998)
^{2}A	-0.373	-0.415 (0.998)	-0.419 (0.998)	-0.420 (0.998)	-0.420 (0.998)
^{2}T	-0.314	-0.467 (0.994)	-0.479 (0.993)	-0.478 (0.993)	-0.477 (0.993)
^{2}E	-0.282	-0.386 (0.996)	-0.394 (0.995)	-0.394 (0.995)	-0.393 (0.995)
^{2}T	-0.263	-0.379 (0.996)	-0.385 (0.995)	-0.388 (0.994)	-0.387 (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 S2*.** Excitation energies (eV) of $Li(NH_3)_4@(NH_3)_{12}$ inferred from electron attachment energies in Table S1.

Neutral Final State	KT	D2	OVGF	P3	P3+
^2A	0.000	0.000	0.000	0.000	0.000
^2T	0.162	0.222	0.225	0.224	0.224
^2E	0.404	0.540	0.547	0.547	0.547
^2T	0.419	0.546	0.555	0.552	0.552
^2T	0.693	0.872	0.883	0.882	0.881
^2A	0.699	0.859	0.870	0.867	0.867
^2T	0.699	0.874	0.885	0.883	0.882
^2T	0.944	1.082	1.092	1.091	1.090
^2A	0.956	0.965	0.966	0.969	0.969
^2T	0.992	1.199	1.212	1.211	1.210
^2E	0.995	1.201	1.214	1.213	1.212
^2A	1.059	1.260	1.273	1.272	1.271
^2T	1.118	1.208	1.213	1.214	1.214
^2E	1.150	1.289	1.298	1.298	1.298
^2T	1.169	1.296	1.307	1.304	1.304

Table S3. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $Li(NH_3)_4@(NH_3)_{12}^+$, at neutral geometry (optimized at CAM-B3LYP/aug-cc-pVTZ level), from Koopmans's theorem and the diagonal second-order electron propagator method using the cc-pVTZ basis for Li, N and 12 inner H atoms, and d-aug-cc-pVTZ basis for 36 outer H atoms. All valence electrons correlated.

Neutral Final State	KT	D2
^{2}A	-1.43295	-1.700 (0.991)
^{2}T	-1.27213	-1.472 (0.993)
^{2}E	-1.03349	-1.146 (0.996)
^{2}T	-1.01852	-1.141 (0.995)
^{2}T	-0.754844	-0.817 (0.998)
^{2}A	-0.754028	-0.839 (0.997)
^{2}T	-0.747769	-0.817 (0.997)
^{2}A	-0.5728	-0.802 (0.992)
^{2}T	-0.546949	-0.679 (0.995)
^{2}T	-0.47375	-0.507 (0.999)
^{2}E	-0.471301	-0.506 (0.999)
^{2}A	-0.428035	-0.465 (0.999)
^{2}T	-0.382048	-0.507 (0.996)
^{2}E	-0.368987	-0.475 (0.996)
^{2}T	-0.355653	-0.478 (0.996)

***Table S4*.** Excitation energies (eV) of $Li(NH_3)_4@(NH_3)_{12}$ inferred from electron attachment energies in Table S3.

Neutral Final State	KT	D2
^2A	0.000	0.000
^2T	0.161	0.228
^2E	0.399	0.554
^2T	0.414	0.559
^2T	0.678	0.883
^2A	0.679	0.861
^2T	0.685	0.883
^2A	0.860	0.898
^2T	0.886	1.021
^2T	0.959	1.193
^2E	0.962	1.194
^2A	1.005	1.235
^2T	1.051	1.193
^2E	1.064	1.225
^2T	1.077	1.222

Electron propagator results for $Be(NH_3)_4@(NH_3)_{12}^+$

Table S5. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $Be(NH_3)_4@(NH_3)_{12}^{2+}$, at cation geometry (optimized at CAM-B3LYP/aug-cc-pVTZ level), from diagonal electron propagator methods using the cc-pVDZ basis for Be, N and 12 inner H atoms, and d-aug-cc-pVDZ basis for 36 outer H atoms. All valence electrons correlated.

Cation Final State	KT	D2	OVGF	P3	P3+
^2A	-3.687	-4.199 (0.982)	-4.211 (0.980)	-4.218 (0.979)	-4.217 (0.979)
^2T	-3.382	-3.792 (0.985)	-3.806 (0.983)	-3.813 (0.982)	-3.811 (0.982)
^2E	-2.969	-3.240 (0.990)	-3.254 (0.988)	-3.258 (0.987)	-3.257 (0.988)
^2T	-2.918	-3.214 (0.989)	-3.227 (0.987)	-3.233 (0.986)	-3.232 (0.986)
^2T	-2.487	-2.672 (0.993)	-2.683 (0.993)	-2.688 (0.991)	-2.687 (0.991)
^2A	-2.454	-2.636 (0.993)	-2.645 (0.994)	-2.652 (0.991)	-2.651 (0.991)
^2T	-2.424	-2.622 (0.992)	-2.635 (0.990)	-2.639 (0.990)	-2.638 (0.990)
^2A	-2.303	-2.554 (0.991)	-2.555 (0.990)	-2.560 (0.989)	-2.559 (0.989)
^2T	-2.125	-2.351 (0.992)	-2.354 (0.991)	-2.358 (0.990)	-2.357 (0.990)
^2A	-1.983	-2.153 (0.994)	-2.164 (0.992)	-2.167 (0.992)	-2.166 (0.992)
^2T	-1.962	-2.074 (0.996)	-2.081 (0.995)	-2.085 (0.994)	-2.084 (0.994)
^2T	-1.951	-2.075 (0.995)	-2.083 (0.994)	-2.088 (0.994)	-2.087 (0.994)
^2E	-1.947	-2.072 (0.995)	-2.079 (0.995)	-2.082 (0.994)	-2.082 (0.994)
^2E	-1.857	-2.006 (0.994)	-2.013 (0.994)	-2.015 (0.993)	-2.014 (0.993)
^2T	-1.822	-2.016 (0.993)	-2.021 (0.992)	-2.025 (0.991)	-2.024 (0.991)

Table S6. Excitation energies (eV) of $Be(NH_3)_4@(NH_3)_{12}^+$ inferred from electron attachment energies in Table S5.

Cation Final State	KT	D2	OVGF	P3	P3+
^2A	0.000	0.000	0.000	0.000	0.000
^2T	0.305	0.407	0.405	0.405	0.406
^2E	0.718	0.959	0.957	0.960	0.960
^2T	0.769	0.985	0.984	0.985	0.985
^2T	1.200	1.527	1.528	1.530	1.530
^2A	1.233	1.563	1.566	1.566	1.566
^2T	1.263	1.577	1.576	1.579	1.579
^2A	1.384	1.645	1.656	1.658	1.658
^2T	1.562	1.848	1.857	1.860	1.860
^2A	1.704	2.046	2.047	2.051	2.051
^2T	1.725	2.125	2.130	2.133	2.133
^2T	1.736	2.124	2.128	2.130	2.130
^2E	1.740	2.127	2.132	2.136	2.135
^2E	1.830	2.193	2.198	2.203	2.203
^2T	1.865	2.183	2.190	2.193	2.193

Table S7. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $Be(NH_3)_4@(NH_3)_{12}^{2+}$, at cation geometry (optimized at CAM-B3LYP/aug-cc-pVTZ level), from Koopmans's theorem and the diagonal second-order electron propagator method using the cc-pVTZ basis for Be, N and 12 inner H atoms, and d-aug-cc-pVTZ basis for 36 outer H atoms. All valence electrons correlated.

Cation Final State	KT	D2
^2A	-3.68442	-4.255 (0.981)
^2T	-3.37993	-3.839 (0.984)
^2E	-2.96659	-3.270 (0.989)
^2T	-2.91679	-3.248 (0.988)
^2T	-2.48304	-2.692 (0.992)
^2A	-2.44848	-2.654 (0.992)
^2T	-2.42209	-2.646 (0.992)
^2A	-2.31923	-2.587 (0.991)
^2T	-2.13909	-2.378 (0.992)
^2A	-1.99133	-2.178 (0.993)
^2T	-1.95541	-2.080 (0.995)
^2E	-1.95024	-2.097 (0.995)
^2T	-1.94534	-2.084 (0.995)
^2E	-1.86915	-2.016 (0.995)
^2T	-1.85119	-2.047 (0.993)

Table S8. Excitation energies (eV) of $Be(NH_3)_4@(NH_3)_{12}^+$ inferred from electron attachment energies in Table S7.

Cation Final State	KT	D2
^2A	0.000	0.000
^2T	0.304	0.416
^2E	0.718	0.985
^2T	0.768	1.007
^2T	1.201	1.563
^2A	1.236	1.601
^2T	1.262	1.609
^2A	1.365	1.668
^2T	1.545	1.877
^2A	1.693	2.077
^2T	1.729	2.175
^2E	1.734	2.158
^2T	1.739	2.171
^2E	1.815	2.239
^2T	1.833	2.208

Electron propagator results for $B(NH_3)_4@(NH_3)_{12}^{2+}$

Table S9. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $B(NH_3)_4@(NH_3)_{12}^{3+}$, at dication geometry (optimized at CAM-B3LYP/aug-cc-pVTZ level), from diagonal electron propagator methods using the cc-pVDZ basis for B, N and 12 inner H atoms, and d-aug-cc-pVDZ basis for 36 outer H atoms. All valence electrons correlated.

Dication Final State	KT	D2	OVGF	P3	P3+
^{2}A	-6.351	-7.113 (0.974)	-7.094 (0.972)	-7.120 (0.970)	-7.120 (0.970)
^{2}T	-5.903	-6.535 (0.978)	-6.530 (0.976)	-6.551 (0.974)	-6.550 (0.974)
^{2}E	-5.339	-5.800 (0.983)	-5.803 (0.982)	-5.818 (0.980)	-5.816 (0.980)
^{2}T	-5.241	-5.745 (0.982)	-5.750 (0.980)	-5.765 (0.978)	-5.763 (0.979)
^{2}T	-4.691	-5.050 (0.987)	-5.058 (0.985)	-5.070 (0.984)	-5.068 (0.984)
^{2}A	-4.590	-4.931 (0.987)	-4.938 (0.985)	-4.950 (0.984)	-4.948 (0.984)
^{2}T	-4.542	-4.920 (0.986)	-4.932 (0.984)	-4.943 (0.983)	-4.941 (0.983)
^{2}A	-4.391	-4.848 (0.983)	-4.821 (0.982)	-4.844 (0.980)	-4.844 (0.981)
^{2}A	-4.134	-4.570 (0.985)	-4.560 (0.983)	-4.578 (0.982)	-4.577 (0.982)
^{2}T	-4.034	-4.399 (0.987)	-4.384 (0.986)	-4.399 (0.985)	-4.399 (0.985)
^{2}T	-3.930	-4.223 (0.989)	-4.233 (0.987)	-4.243 (0.986)	-4.242 (0.987)
^{2}T	-3.906	-4.156 (0.991)	-4.166 (0.989)	-4.175 (0.988)	-4.174 (0.988)
^{2}E	-3.860	-4.143 (0.990)	-4.147 (0.988)	-4.156 (0.987)	-4.155 (0.987)
^{2}E	-3.670	-3.971 (0.989)	-3.970 (0.988)	-3.980 (0.987)	-3.979 (0.987)
^{2}T	-3.574	-3.896 (0.988)	-3.888 (0.988)	-3.901 (0.986)	-3.900 (0.987)

Table S10 Excitation energies (eV) of $B(NH_3)_4@(NH_3)_{12}^{2+}$ inferred from electron attachment energies in Table S9.

Dication Final State	KT	D2	OVGF	P3	P3+
^2A	0.000	0.000	0.000	0.000	0.000
^2T	0.448	0.578	0.564	0.569	0.570
^2E	1.012	1.313	1.291	1.302	1.304
^2T	1.110	1.368	1.344	1.355	1.357
^2T	1.660	2.063	2.036	2.050	2.052
^2A	1.761	2.182	2.156	2.170	2.172
^2T	1.809	2.193	2.162	2.177	2.179
^2A	1.960	2.265	2.273	2.276	2.276
^2A	2.217	2.543	2.534	2.542	2.543
^2T	2.317	2.714	2.710	2.721	2.721
^2T	2.421	2.890	2.861	2.877	2.878
^2T	2.445	2.957	2.928	2.945	2.946
^2E	2.491	2.970	2.947	2.964	2.965
^2E	2.681	3.142	3.124	3.140	3.141
^2T	2.777	3.217	3.206	3.219	3.220

Table S11. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $B(NH_3)_4@(NH_3)_{12}^{3+}$, at dication geometry (optimized at CAM-B3LYP/aug-cc-pVTZ level), from Koopmans's theorem and the diagonal second-order electron propagator method using the cc-pVTZ basis for B, N and 12 inner H atoms, and d-aug-cc-pVTZ basis for 36 outer H atoms. All valence electrons correlated.

Dication Final State	KT	D2
^{2}A	-6.34352	-7.194 (0.973)
^{2}T	-5.89834	-6.605 (0.977)
^{2}E	-5.33479	-5.853 (0.982)
^{2}T	-5.24037	-5.805 (0.981)
^{2}T	-4.69043	-5.101 (0.985)
^{2}A	-4.58947	-4.969 (0.986)
^{2}T	-4.54267	-4.970 (0.985)
^{2}A	-4.40144	-4.979 (0.980)
^{2}A	-4.13314	-4.642 (0.983)
^{2}T	-4.03246	-4.462 (0.985)
^{2}T	-3.93041	-4.268 (0.988)
^{2}T	-3.90565	-4.192 (0.990)
^{2}E	-3.85776	-4.195 (0.988)
^{2}E	-3.66293	-4.028 (0.988)
^{2}T	-3.57231	-3.956 (0.987)

Table S12. Excitation energies (eV) of $B(NH_3)_4@(NH_3)_{12}^{2+}$ inferred from electron attachment energies in Table S11.

Dication Final State	KT	D2
^2A	0.000	0.000
^2T	0.445	0.589
^2E	1.009	1.341
^2T	1.103	1.389
^2T	1.653	2.093
^2A	1.754	2.225
^2T	1.801	2.224
^2A	1.942	2.215
^2A	2.210	2.552
^2T	2.311	2.732
^2T	2.413	2.926
^2T	2.438	3.002
^2E	2.486	2.999
^2E	2.681	3.166
^2T	2.771	3.238

Lowest vertical electron attachment and detachment energies for the studied species

Table S13. The lowest vertical electron detachment (VEDE) and the negative of the lowest vertical attachment (-VEAE) energies (eV) calculated with D2 and P3+ in two basis sets: da*x*z denotes that cc-pV*X*Z is used on all inner atoms, whereas d-aug-cc-pV*X*Z is used on 36 external H atoms, where *X* = D, T. cP3+/datz labels a composite P3+ result, where the difference between P3+/dadz and D2/dadz is added to the D2/datz result. The VEAE and VEDE values reported in this table have pole strengths high above 0.85.

Species	D2 / dadz	P3+ / dadz	D2 / datz	cP3+ / datz
$Li(NH_3)_4@12NH_3^+$ (-VEAE)	1.68	1.69	1.70	1.71
$Li(NH_3)_4@12NH_3^-$ (VEDE)	0.30[a]	0.29	0.33	0.32
$Be(NH_3)_4@12NH_3^{2+}$ (-VEAE)	4.20	4.22	4.26	4.28
$Be(NH_3)_4@12NH_3$ (VEDE)	2.37	2.36	2.41	2.40
$B(NH_3)_4@12NH_3^{3+}$ (-VEAE)	7.11	7.12	7.19	7.20
$B(NH_3)_4@12NH_3^+$ (VEDE)	4.94	4.92	5.00	4.98

[a] The D2 result in the tadz basis (cc-pVDZ on all inner atoms and t-aug-cc-pVDZ on 36 external H atoms) is 0.33 eV.

Cartesian coordinates for the studied species

Table S14. Cartesian coordinates (in Å) of all the studied $Li(NH_3)_4@12NH_3^q$ species at CAM-B3LYP/aug-cc-pVTZ.

$[Li(NH_3)_4@12NH_3]$				$[Li(NH_3)_4@12NH_3]^+$				$[Li(NH_3)_4@12NH_3]^-$			
Li	0.000000	0.000000	0.000000	Li	0.000000	0.000000	0.000000	Li	0.000000	0.000000	0.000000
N	-1.204833	-1.204833	1.204833	N	1.208834	-1.208834	1.208834	N	-1.203870	-1.203870	1.203870
N	1.204833	1.204833	1.204833	N	-1.208834	1.208834	1.208834	N	1.203870	1.203870	1.203870
N	1.204833	-1.204833	-1.204833	N	1.208834	1.208834	-1.208834	N	1.203870	-1.203870	-1.203870
N	-1.204833	1.204833	-1.204833	N	-1.208834	-1.208834	-1.208834	N	-1.203870	1.203870	-1.203870
H	1.814879	1.814879	0.665697	H	-1.821253	1.821253	0.674700	H	1.813810	1.813810	0.664557
H	1.814879	0.665697	1.814879	H	-0.674700	1.821253	1.821253	H	1.813810	0.664557	1.813810
H	0.665697	1.814879	1.814879	H	-1.821253	0.674700	1.821253	H	0.664557	1.813810	1.813810
H	0.665697	-1.814879	-1.814879	H	1.821253	0.674700	-1.821253	H	0.664557	-1.813810	-1.813810
H	1.814879	-1.814879	-0.665697	H	1.821253	1.821253	-0.674700	H	1.813810	-1.813810	-0.664557
H	1.814879	-0.665697	-1.814879	H	0.674700	1.821253	-1.821253	H	1.813810	-0.664557	-1.813810
H	-1.814879	0.665697	-1.814879	H	-0.674700	-1.821253	-1.821253	H	-1.813810	0.664557	-1.813810
H	-1.814879	1.814879	-0.665697	H	-1.821253	-1.821253	-0.674700	H	-1.813810	1.813810	-0.664557
H	-0.665697	1.814879	-1.814879	H	-1.821253	-0.674700	-1.821253	H	-0.664557	1.813810	-1.813810
H	-0.665697	-1.814879	1.814879	H	1.821253	-0.674700	1.821253	H	-0.664557	-1.813810	1.813810
H	-1.814879	-0.665697	1.814879	H	0.674700	-1.821253	1.821253	H	-1.813810	-0.664557	1.813810
H	-1.814879	-1.814879	0.665697	H	1.821253	-1.821253	0.674700	H	-1.813810	-1.813810	0.664557
N	3.340287	3.340287	-0.306021	N	-3.390161	3.390161	-0.231404	N	3.334335	3.334335	-0.309916
N	3.340287	-0.306021	3.340287	N	0.231404	3.390161	3.390161	N	3.334335	-0.309916	3.334335
N	-0.306021	3.340287	3.340287	N	-3.390161	-0.231404	3.390161	N	-0.309916	3.334335	3.334335
N	-0.306021	-3.340287	-3.340287	N	3.390161	-0.231404	-3.390161	N	-0.309916	-3.334335	-3.334335
N	3.340287	-3.340287	0.306021	N	3.390161	3.390161	0.231404	N	3.334335	-3.334335	0.309916
N	3.340287	0.306021	-3.340287	N	-0.231404	3.390161	-3.390161	N	3.334335	0.309916	-3.334335

N	-3.340287	-0.306021	-3.340287	N	0.231404	-3.390161	-3.390161	N	-3.334335	-0.309916	-3.334335
N	-3.340287	3.340287	0.306021	N	-3.390161	-3.390161	0.231404	N	-3.334335	3.334335	0.309916
N	0.306021	3.340287	-3.340287	N	-3.390161	0.231404	-3.390161	N	0.309916	3.334335	-3.334335
N	0.306021	-3.340287	3.340287	N	3.390161	0.231404	3.390161	N	0.309916	-3.334335	3.334335
N	-3.340287	0.306021	3.340287	N	-0.231404	-3.390161	3.390161	N	-3.334335	0.309916	3.334335
N	-3.340287	-3.340287	-0.306021	N	3.390161	-3.390161	-0.231404	N	-3.334335	-3.334335	-0.309916
H	2.983317	3.640508	-1.204474	H	-3.721974	3.046538	-1.123204	H	2.979319	3.626550	-1.212039
H	3.640508	-1.204474	2.983317	H	1.123204	3.721974	3.046538	H	3.626550	-1.212039	2.979319
H	-1.204474	2.983317	3.640508	H	-3.046538	-1.123204	3.721974	H	-1.212039	2.979319	3.626550
H	-1.204474	-2.983317	-3.640508	H	3.046538	-1.123204	-3.721974	H	-1.212039	-2.979319	-3.626550
H	2.983317	-3.640508	1.204474	H	3.721974	3.046538	1.123204	H	2.979319	-3.626550	1.212039
H	3.640508	1.204474	-2.983317	H	-1.123204	3.721974	-3.046538	H	3.626550	1.212039	-2.979319
H	-3.640508	-1.204474	-2.983317	H	1.123204	-3.721974	-3.046538	H	-3.626550	-1.212039	-2.979319
H	-2.983317	3.640508	1.204474	H	-3.721974	-3.046538	1.123204	H	-2.979319	3.626550	1.212039
H	1.204474	2.983317	-3.640508	H	-3.046538	1.123204	-3.721974	H	1.212039	2.979319	-3.626550
H	1.204474	-2.983317	3.640508	H	3.046538	1.123204	3.721974	H	1.212039	-2.979319	3.626550
H	-3.640508	1.204474	2.983317	H	-1.123204	-3.721974	3.046538	H	-3.626550	1.212039	2.979319
H	-2.983317	-3.640508	-1.204474	H	3.721974	-3.046538	-1.123204	H	-2.979319	-3.626550	-1.212039
H	3.488636	4.168793	0.256430	H	-4.201206	3.542517	0.353812	H	3.475866	4.167396	0.247963
H	4.168793	0.256430	3.488636	H	-0.353812	4.201206	3.542517	H	4.167396	0.247963	3.475866
H	0.256430	3.488636	4.168793	H	-3.542517	0.353812	4.201206	H	0.247963	3.475866	4.167396
H	0.256430	-3.488636	-4.168793	H	3.542517	0.353812	-4.201206	H	0.247963	-3.475866	-4.167396
H	3.488636	-4.168793	-0.256430	H	4.201206	3.542517	-0.353812	H	3.475866	-4.167396	-0.247963
H	4.168793	-0.256430	-3.488636	H	0.353812	4.201206	-3.542517	H	4.167396	-0.247963	-3.475866
H	-4.168793	0.256430	-3.488636	H	-0.353812	-4.201206	-3.542517	H	-4.167396	0.247963	-3.475866
H	-3.488636	4.168793	-0.256430	H	-4.201206	-3.542517	-0.353812	H	-3.475866	4.167396	-0.247963
H	-0.256430	3.488636	-4.168793	H	-3.542517	-0.353812	-4.201206	H	-0.247963	3.475866	-4.167396
H	-0.256430	-3.488636	4.168793	H	3.542517	-0.353812	4.201206	H	-0.247963	-3.475866	4.167396

H	-4.168793	-0.256430	3.488636	H	0.353812	-4.201206	3.542517	H	-4.167396	-0.247963	3.475866
H	-3.488636	-4.168793	0.256430	H	4.201206	-3.542517	0.353812	H	-3.475866	-4.167396	0.247963
H	4.242931	2.908309	-0.459022	H	-2.960576	4.292344	-0.389540	H	4.239162	2.903961	-0.455920
H	2.908309	-0.459022	4.242931	H	0.389540	2.960576	4.292344	H	2.903961	-0.455920	4.239162
H	-0.459022	4.242931	2.908309	H	-4.292344	-0.389540	2.960576	H	-0.455920	4.239162	2.903961
H	-0.459022	-4.242931	-2.908309	H	4.292344	-0.389540	-2.960576	H	-0.455920	-4.239162	-2.903961
H	4.242931	-2.908309	0.459022	H	2.960576	4.292344	0.389540	H	4.239162	-2.903961	0.455920
H	2.908309	0.459022	-4.242931	H	-0.389540	2.960576	-4.292344	H	2.903961	0.455920	-4.239162
H	-2.908309	-0.459022	-4.242931	H	0.389540	-2.960576	-4.292344	H	-2.903961	-0.455920	-4.239162
H	-4.242931	2.908309	0.459022	H	-2.960576	-4.292344	0.389540	H	-4.239162	2.903961	0.455920
H	0.459022	4.242931	-2.908309	H	-4.292344	0.389540	-2.960576	H	0.455920	4.239162	-2.903961
H	0.459022	-4.242931	2.908309	H	4.292344	0.389540	2.960576	H	0.455920	-4.239162	2.903961
H	-2.908309	0.459022	4.242931	H	-0.389540	-2.960576	4.292344	H	-2.903961	0.455920	4.239162
H	-4.242931	-2.908309	-0.459022	H	2.960576	-4.292344	-0.389540	H	-4.239162	-2.903961	-0.455920

Table S15. Cartesian coordinates (in Å) of all the studied $Be(NH_3)_4@12NH_3^q$ species at CAM-B3LYP/aug-cc-pVTZ.

$[Be(NH_3)_4@12NH_3]$				$[Be(NH_3)_4@12NH_3]^+$				$[Be(NH_3)_4@12NH_3]^{2+}$				$[Be(NH_3)_4@12NH_3]^-$			
Be	0.000000	0.000000	0.000000	Be	0.000000	0.000000	0.000000	Be	0.000000	0.000000	0.000000	Be	0.000000	0.000000	0.000000
N	0.998138	-0.998138	0.998138	N	0.999577	-0.999577	0.999577	N	1.002132	-1.002132	1.002132	N	0.997220	-0.997220	0.997220
N	-0.998138	0.998138	0.998138	N	-0.999577	0.999577	0.999577	N	-1.002132	1.002132	1.002132	N	-0.997220	0.997220	0.997220
N	0.998138	0.998138	-0.998138	N	0.999577	0.999577	-0.999577	N	1.002132	1.002132	-1.002132	N	0.997220	0.997220	-0.997220
N	-0.998138	-0.998138	-0.998138	N	-0.999577	-0.999577	-0.999577	N	-1.002132	-1.002132	-1.002132	N	-0.997220	-0.997220	-0.997220
H	-1.623416	1.623416	0.476609	H	-1.625303	1.625303	0.478777	H	-1.629354	1.629354	0.484334	H	-1.618262	1.618262	0.466235
H	-0.476609	1.623416	1.623416	H	-0.478777	1.625303	1.625303	H	-0.484334	1.629354	1.629354	H	-0.466235	1.618262	1.618262
H	-1.623416	0.476609	1.623416	H	-1.625303	0.478777	1.625303	H	-1.629354	0.484334	1.629354	H	-1.618262	0.466235	1.618262
H	1.623416	0.476609	-1.623416	H	1.625303	0.478777	-1.625303	H	1.629354	0.484334	-1.629354	H	1.618262	0.466235	-1.618262
H	1.623416	1.623416	-0.476609	H	1.625303	1.625303	-0.478777	H	1.629354	1.629354	-0.484334	H	1.618262	1.618262	-0.466235
H	0.476609	1.623416	-1.623416	H	0.478777	1.625303	-1.625303	H	0.484334	1.629354	-1.629354	H	0.466235	1.618262	-1.618262
H	-0.476609	-1.623416	-1.623416	H	-0.478777	-1.625303	-1.625303	H	-0.484334	-1.629354	-1.629354	H	-0.466235	-1.618262	-1.618262
H	-1.623416	-1.623416	-0.476609	H	-1.625303	-1.625303	-0.478777	H	-1.629354	-1.629354	-0.484334	H	-1.618262	-1.618262	-0.466235
H	-1.623416	-0.476609	-1.623416	H	-1.625303	-0.478777	-1.625303	H	-1.629354	-0.484334	-1.629354	H	-1.618262	-0.466235	-1.618262
H	1.623416	-0.476609	1.623416	H	1.625303	-0.478777	1.625303	H	1.629354	-0.484334	1.629354	H	1.618262	-0.466235	1.618262
H	0.476609	-1.623416	1.623416	H	0.478777	-1.625303	1.625303	H	0.484334	-1.629354	1.629354	H	0.466235	-1.618262	1.618262
H	1.623416	-1.623416	0.476609	H	1.625303	-1.625303	0.478777	H	1.629354	-1.629354	0.484334	H	1.618262	-1.618262	0.466235
N	-3.043206	3.043206	-0.219783	N	-3.056011	3.056011	-0.213679	N	-3.079818	3.079818	-0.192631	N	-3.033080	3.033080	-0.215554
N	0.219783	3.043206	3.043206	N	0.213679	3.056011	3.056011	N	0.192631	3.079818	3.079818	N	0.215554	3.033080	3.033080
N	-3.043206	-0.219783	3.043206	N	-3.056011	-0.213679	3.056011	N	-3.079818	-0.192631	3.079818	N	-3.033080	-0.215554	3.033080
N	3.043206	-0.219783	-3.043206	N	3.056011	-0.213679	-3.056011	N	3.079818	-0.192631	-3.079818	N	3.033080	-0.215554	-3.033080
N	3.043206	3.043206	0.219783	N	3.056011	3.056011	0.213679	N	3.079818	3.079818	0.192631	N	3.033080	3.033080	0.215554
N	-0.219783	3.043206	-3.043206	N	-0.213679	3.056011	-3.056011	N	-0.192631	3.079818	-3.079818	N	-0.215554	3.033080	-3.033080
N	0.219783	-3.043206	-3.043206	N	0.213679	-3.056011	-3.056011	N	0.192631	-3.079818	-3.079818	N	0.215554	-3.033080	-3.033080
N	-3.043206	-3.043206	0.219783	N	-3.056011	-3.056011	0.213679	N	-3.079818	-3.079818	0.192631	N	-3.033080	-3.033080	0.215554
N	-3.043206	0.219783	-3.043206	N	-3.056011	0.213679	-3.056011	N	-3.079818	0.192631	-3.079818	N	-3.033080	0.215554	-3.033080
N	3.043206	0.219783	3.043206	N	3.056011	0.213679	3.056011	N	3.079818	0.192631	3.079818	N	3.033080	0.215554	3.033080
N	-0.219783	-3.043206	3.043206	N	-0.213679	-3.056011	3.056011	N	-0.192631	-3.079818	3.079818	N	-0.215554	-3.033080	3.033080

N	3.043206	-3.043206	-0.219783	N	3.056011	-3.056011	-0.213679	N	3.079818	-3.079818	-0.192631	N	3.033080	-3.033080	-0.215554
H	-3.390925	2.735789	-1.122038	H	-3.407261	2.754250	-1.115798	H	-3.451991	2.782663	-1.086950	H	-3.461174	2.849694	-1.116912
H	1.122038	3.390925	2.735789	H	1.115798	3.407261	2.754250	H	1.086950	3.451991	2.782663	H	1.116912	3.461174	2.849694
H	-2.735789	-1.122038	3.390925	H	-2.754250	-1.115798	3.407261	H	-2.782663	-1.086950	3.451991	H	-2.849694	-1.116912	3.461174
H	2.735789	-1.122038	-3.390925	H	2.754250	-1.115798	-3.407261	H	2.782663	-1.086950	-3.451991	H	2.849694	-1.116912	-3.461174
H	3.390925	2.735789	1.122038	H	3.407261	2.754250	1.115798	H	3.451991	2.782663	1.086950	H	3.461174	2.849694	1.116912
H	-1.122038	3.390925	-2.735789	H	-1.115798	3.407261	-2.754250	H	-1.086950	3.451991	-2.782663	H	-1.116912	3.461174	-2.849694
H	1.122038	-3.390925	-2.735789	H	1.115798	-3.407261	-2.754250	H	1.086950	-3.451991	-2.782663	H	1.116912	-3.461174	-2.849694
H	-3.390925	-2.735789	1.122038	H	-3.407261	-2.754250	1.115798	H	-3.451991	-2.782663	1.086950	H	-3.461174	-2.849694	1.116912
H	-2.735789	1.122038	-3.390925	H	-2.754250	1.115798	-3.407261	H	-2.782663	1.086950	-3.451991	H	-2.849694	1.116912	-3.461174
H	2.735789	1.122038	3.390925	H	2.754250	1.115798	3.407261	H	2.782663	1.086950	3.451991	H	2.849694	1.116912	3.461174
H	-1.122038	-3.390925	2.735789	H	-1.115798	-3.407261	2.754250	H	-1.086950	-3.451991	2.782663	H	-1.116912	-3.461174	2.849694
H	3.390925	-2.735789	-1.122038	H	3.407261	-2.754250	-1.115798	H	3.451991	-2.782663	-1.086950	H	3.461174	-2.849694	-1.116912
H	-3.851731	3.169540	0.380056	H	-3.864178	3.183053	0.385471	H	-3.879134	3.218819	0.414322	H	-3.782251	3.058102	0.468629
H	-0.380056	3.851731	3.169540	H	-0.385471	3.864178	3.183053	H	-0.414322	3.879134	3.218819	H	-0.468629	3.782251	3.058102
H	-3.169540	0.380056	3.851731	H	-3.183053	0.385471	3.864178	H	-3.218819	0.414322	3.879134	H	-3.058102	0.468629	3.782251
H	3.169540	0.380056	-3.851731	H	3.183053	0.385471	-3.864178	H	3.218819	0.414322	-3.879134	H	3.058102	0.468629	-3.782251
H	3.851731	3.169540	-0.380056	H	3.864178	3.183053	-0.385471	H	3.879134	3.218819	-0.414322	H	3.782251	3.058102	-0.468629
H	0.380056	3.851731	-3.169540	H	0.385471	3.864178	-3.183053	H	0.414322	3.879134	-3.218819	H	0.468629	3.782251	-3.058102
H	-0.380056	-3.851731	-3.169540	H	-0.385471	-3.864178	-3.183053	H	-0.414322	-3.879134	-3.218819	H	-0.468629	-3.782251	-3.058102
H	-3.851731	-3.169540	-0.380056	H	-3.864178	-3.183053	-0.385471	H	-3.879134	-3.218819	-0.414322	H	-3.782251	-3.058102	-0.468629
H	-3.169540	-0.380056	-3.851731	H	-3.183053	-0.385471	-3.864178	H	-3.218819	-0.414322	-3.879134	H	-3.058102	-0.468629	-3.782251
H	3.169540	-0.380056	3.851731	H	3.183053	-0.385471	3.864178	H	3.218819	-0.414322	3.879134	H	3.058102	-0.468629	3.782251
H	0.380056	-3.851731	3.169540	H	0.385471	-3.864178	3.183053	H	0.414322	-3.879134	3.218819	H	0.468629	-3.782251	3.058102
H	3.851731	-3.169540	0.380056	H	3.864178	-3.183053	0.385471	H	3.879134	-3.218819	0.414322	H	3.782251	-3.058102	0.468629
H	-2.626192	3.958544	-0.352950	H	-2.643434	3.972996	-0.344724	H	-2.671627	3.996463	-0.333208	H	-2.633428	3.965092	-0.255888
H	0.352950	2.626192	3.958544	H	0.344724	2.643434	3.972996	H	0.333208	2.671627	3.996463	H	0.255888	2.633428	3.965092
H	-3.958544	-0.352950	2.626192	H	-3.972996	-0.344724	2.643434	H	-3.996463	-0.333208	2.671627	H	-3.965092	-0.255888	2.633428
H	3.958544	-0.352950	-2.626192	H	3.972996	-0.344724	-2.643434	H	3.996463	-0.333208	-2.671627	H	3.965092	-0.255888	-2.633428
H	2.626192	3.958544	0.352950	H	2.643434	3.972996	0.344724	H	2.671627	3.996463	0.333208	H	2.633428	3.965092	0.255888
H	-0.352950	2.626192	-3.958544	H	-0.344724	2.643434	-3.972996	H	-0.333208	2.671627	-3.996463	H	-0.255888	2.633428	-3.965092
H	0.352950	-2.626192	-3.958544	H	0.344724	-2.643434	-3.972996	H	0.333208	-2.671627	-3.996463	H	0.255888	-2.633428	-3.965092
H	-2.626192	-3.958544	0.352950	H	-2.643434	-3.972996	0.344724	H	-2.671627	-3.996463	0.333208	H	-2.633428	-3.965092	0.255888
H	-3.958544	0.352950	-2.626192	H	-3.972996	0.344724	-2.643434	H	-3.996463	0.333208	-2.671627	H	-3.965092	0.255888	-2.633428

H	3.958544	0.352950	2.626192	H	3.972996	0.344724	2.643434	H	3.996463	0.333208	2.671627	H	3.965092	0.255888	2.633428
H	-0.352950	-2.626192	3.958544	H	-0.344724	-2.643434	3.972996	H	-0.333208	-2.671627	3.996463	H	-0.255888	-2.633428	3.965092
H	2.626192	-3.958544	-0.352950	H	2.643434	-3.972996	-0.344724	H	2.671627	-3.996463	-0.333208	H	2.633428	-3.965092	-0.255888

Table S16. Cartesian coordinates (in Å) of all the studied $B(NH_3)_4@12NH_3^q$ species at CAM-B3LYP/aug-cc-pVTZ.

$[B(NH_3)_4@12NH_3]^{+}$				$[B(NH_3)_4@12NH_3]^{2+}$				$[B(NH_3)_4@12NH_3]^{3+}$			
B	0.000000	0.000000	0.000000	B	0.000000	0.000000	0.000000	B	0.000000	0.000000	0.000000
N	0.897804	-0.897804	0.897804	N	0.899494	-0.899494	0.899494	N	0.901734	-0.901734	0.901734
N	-0.897804	0.897804	0.897804	N	-0.899494	0.899494	0.899494	N	-0.901734	0.901734	0.901734
N	0.897804	0.897804	-0.897804	N	0.899494	0.899494	-0.899494	N	0.901734	0.901734	-0.901734
N	-0.897804	-0.897804	-0.897804	N	-0.899494	-0.899494	-0.899494	N	-0.901734	-0.901734	-0.901734
H	-1.539644	1.539644	0.381876	H	-1.542213	1.542213	0.384596	H	-1.546442	1.546442	0.389696
H	-0.381876	1.539644	1.539644	H	-0.384596	1.542213	1.542213	H	-0.389696	1.546442	1.546442
H	-1.539644	0.381876	1.539644	H	-1.542213	0.384596	1.542213	H	-1.546442	0.389696	1.546442
H	1.539644	0.381876	-1.539644	H	1.542213	0.384596	-1.542213	H	1.546442	0.389696	-1.546442
H	1.539644	1.539644	-0.381876	H	1.542213	1.542213	-0.384596	H	1.546442	1.546442	-0.389696
H	0.381876	1.539644	-1.539644	H	0.384596	1.542213	-1.542213	H	0.389696	1.546442	-1.546442
H	-0.381876	-1.539644	-1.539644	H	-0.384596	-1.542213	-1.542213	H	-0.389696	-1.546442	-1.546442
H	-1.539644	-1.539644	-0.381876	H	-1.542213	-1.542213	-0.384596	H	-1.546442	-1.546442	-0.389696
H	-1.539644	-0.381876	-1.539644	H	-1.542213	-0.384596	-1.542213	H	-1.546442	-0.389696	-1.546442
H	1.539644	-0.381876	1.539644	H	1.542213	-0.384596	1.542213	H	1.546442	-0.389696	1.546442
H	0.381876	-1.539644	1.539644	H	0.384596	-1.542213	1.542213	H	0.389696	-1.546442	1.546442
H	1.539644	-1.539644	0.381876	H	1.542213	-1.542213	0.384596	H	1.546442	-1.546442	0.389696
N	-2.859400	2.859400	-0.128059	N	-2.872055	2.872055	-0.124140	N	-2.881073	2.881073	-0.129996
N	0.128059	2.859400	2.859400	N	0.124140	2.872055	2.872055	N	0.129996	2.881073	2.881073
N	-2.859400	-0.128059	2.859400	N	-2.872055	-0.124140	2.872055	N	-2.881073	-0.129996	2.881073
N	2.859400	-0.128059	-2.859400	N	2.872055	-0.124140	-2.872055	N	2.881073	-0.129996	-2.881073
N	2.859400	2.859400	0.128059	N	2.872055	2.872055	0.124140	N	2.881073	2.881073	0.129996
N	-0.128059	2.859400	-2.859400	N	-0.124140	2.872055	-2.872055	N	-0.129996	2.881073	-2.881073
N	0.128059	-2.859400	-2.859400	N	0.124140	-2.872055	-2.872055	N	0.129996	-2.881073	-2.881073
N	-2.859400	-2.859400	0.128059	N	-2.872055	-2.872055	0.124140	N	-2.881073	-2.881073	0.129996
N	-2.859400	0.128059	-2.859400	N	-2.872055	0.124140	-2.872055	N	-2.881073	0.129996	-2.881073
N	2.859400	0.128059	2.859400	N	2.872055	0.124140	2.872055	N	2.881073	0.129996	2.881073
N	-0.128059	-2.859400	2.859400	N	-0.124140	-2.872055	2.872055	N	-0.129996	-2.881073	2.881073
N	2.859400	-2.859400	-0.128059	N	2.872055	-2.872055	-0.124140	N	2.881073	-2.881073	-0.129996
H	-3.235228	2.591740	-1.033890	H	-3.261241	2.605729	-1.023781	H	-3.280696	2.617841	-1.025085
H	1.033890	3.235228	2.591740	H	1.023781	3.261241	2.605729	H	1.025085	3.280696	2.617841

H	-2.591740	-1.033890	3.235228	H	-2.605729	-1.023781	3.261241	H	-2.617841	-1.025085	3.280696
H	2.591740	-1.033890	-3.235228	H	2.605729	-1.023781	-3.261241	H	2.617841	-1.025085	-3.280696
H	3.235228	2.591740	1.033890	H	3.261241	2.605729	1.023781	H	3.280696	2.617841	1.025085
H	-1.033890	3.235228	-2.591740	H	-1.023781	3.261241	-2.605729	H	-1.025085	3.280696	-2.617841
H	1.033890	-3.235228	-2.591740	H	1.023781	-3.261241	-2.605729	H	1.025085	-3.280696	-2.617841
H	-3.235228	-2.591740	1.033890	H	-3.261241	-2.605729	1.023781	H	-3.280696	-2.617841	1.025085
H	-2.591740	1.033890	-3.235228	H	-2.605729	1.023781	-3.261241	H	-2.617841	1.025085	-3.280696
H	2.591740	1.033890	3.235228	H	2.605729	1.023781	3.261241	H	2.617841	1.025085	3.280696
H	-1.033890	-3.235228	2.591740	H	-1.023781	-3.261241	2.605729	H	-1.025085	-3.280696	2.617841
H	3.235228	-2.591740	-1.033890	H	3.261241	-2.605729	-1.023781	H	3.280696	-2.617841	-1.025085
H	-3.658658	2.965808	0.491040	H	-3.666347	2.990257	0.497856	H	-3.675404	3.011902	0.488143
H	-0.491040	3.658658	2.965808	H	-0.497856	3.666347	2.990257	H	-0.488143	3.675404	3.011902
H	-2.965808	0.491040	3.658658	H	-2.990257	0.497856	3.666347	H	-3.011902	0.488143	3.675404
H	2.965808	0.491040	-3.658658	H	2.990257	0.497856	-3.666347	H	3.011902	0.488143	-3.675404
H	3.658658	2.965808	-0.491040	H	3.666347	2.990257	-0.497856	H	3.675404	3.011902	-0.488143
H	0.491040	3.658658	-2.965808	H	0.497856	3.666347	-2.990257	H	0.488143	3.675404	-3.011902
H	-0.491040	-3.658658	-2.965808	H	-0.497856	-3.666347	-2.990257	H	-0.488143	-3.675404	-3.011902
H	-3.658658	-2.965808	-0.491040	H	-3.666347	-2.990257	-0.497856	H	-3.675404	-3.011902	-0.488143
H	-2.965808	-0.491040	-3.658658	H	-2.990257	-0.497856	-3.666347	H	-3.011902	-0.488143	-3.675404
H	2.965808	-0.491040	3.658658	H	2.990257	-0.497856	3.666347	H	3.011902	-0.488143	3.675404
H	0.491040	-3.658658	2.965808	H	0.497856	-3.666347	2.990257	H	0.488143	-3.675404	3.011902
H	3.658658	-2.965808	0.491040	H	3.666347	-2.990257	0.497856	H	3.675404	-3.011902	0.488143
H	-2.456373	3.785976	-0.239623	H	-2.472975	3.798319	-0.244642	H	-2.490095	3.809164	-0.256313
H	0.239623	2.456373	3.785976	H	0.244642	2.472975	3.798319	H	0.256313	2.490095	3.809164
H	-3.785976	-0.239623	2.456373	H	-3.798319	-0.244642	2.472975	H	-3.809164	-0.256313	2.490095
H	3.785976	-0.239623	-2.456373	H	3.798319	-0.244642	-2.472975	H	3.809164	-0.256313	-2.490095
H	2.456373	3.785976	0.239623	H	2.472975	3.798319	0.244642	H	2.490095	3.809164	0.256313
H	-0.239623	2.456373	-3.785976	H	-0.244642	2.472975	-3.798319	H	-0.256313	2.490095	-3.809164
H	0.239623	-2.456373	-3.785976	H	0.244642	-2.472975	-3.798319	H	0.256313	-2.490095	-3.809164
H	-2.456373	-3.785976	0.239623	H	-2.472975	-3.798319	0.244642	H	-2.490095	-3.809164	0.256313
H	-3.785976	0.239623	-2.456373	H	-3.798319	0.244642	-2.472975	H	-3.809164	0.256313	-2.490095
H	3.785976	0.239623	2.456373	H	3.798319	0.244642	2.472975	H	3.809164	0.256313	2.490095
H	-0.239623	-2.456373	3.785976	H	-0.244642	-2.472975	3.798319	H	-0.256313	-2.490095	3.809164
H	2.456373	-3.785976	-0.239623	H	2.472975	-3.798319	-0.244642	H	2.490095	-3.809164	-0.256313