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Double Rydberg Anions, Rydberg Radicals and Micro-solvated Cations with Ammonium-Water Kernels

Ernest Opoku, Filip Pawłowski and Joseph Vincent Ortiz*

Department of Chemistry and Biochemistry, Auburn University,
Auburn, AL 36849-5312, United States
ezo0009@auburn.edu, filip@auburn.edu, ortiz@auburn.edu

Supporting Information

Table S1: 1a $NH_4^+(H_2O)$ vertical electron attachment energies (VEAEs). Pole strengths are in parentheses. All energies are in eV.

Basis	KT	D2	D3	OVGF-A[a]	OVGF-B[a]	OVGF-C[a]	P3	P3+
aTZ	3.315	3.742 (0.988)	3.721 (0.986)	3.724 (0.987)	**3.725 (0.986)**	3.723 (0.986)	3.748 (0.986)	3.747 (0.986)
daTZ	3.324	3.744(0.988)	3.722(0.987)	3.726 (0.987)	3.727 (0.987)	**3.725 (0.987)**	3.749 (0.986)	3.748 (0.986)
taTZ	3.324	3.744 (0.988)	3.722(0.987)	3.726 (0.987)	3.727 (0.987)	**3.725 (0.987)**	3.749 (0.986)	3.748 (0.986)
qaTZ	3.324	3.744 (0.988)	3.722(0.987)	3.725 (0.986)	3.726 (0.986)	**3.724 (0.986)**	3.749 (0.986)	3.748 (0.986)
aQZ	3.318	3.751 (0.988)	3.720 (0.986)	3.725 (0.986)	3.725 (0.986)	**3.723 (0.986)**	3.753 (0.986)	3.753 (0.986)

[a]The numerically recommended OVGF version is in bold.

Table S2: $NH_4^+(H_2O)_2$ vertical electron attachment energies (VEAEs). Pole strengths are in parentheses. All energies are in eV.

2a $NH_4^+(H_2O)_2$	Basis	KT	D2	D3	OVGF-A[a]	OVGF-B[a]	OVGF-C[a]	P3	P3+
	aTZ	2.814	3.216 (0.988)	3.213 (0.987)	3.214 (0.987)	**3.218 (0.987)**	3.214 (0.987)	3.223 (0.986)	3.222 (0.986)
	daTZ	2.836	3.220(0.989)	3.217 (0.987)	**3.218 (0.988)**	3.221 (0.988)	**3.218 (0.988)**	3.226 (0.987)	3.226 (0.987)
	taTZ	2.836	3.220(0.989)	3.217 (0.987)	**3.218 (0.988)**	3.222 (0.988)	**3.218 (0.988)**	3.226 (0.987)	3.226 (0.987)
	qaTZ	2.836	3.220(0.989)	3.217 (0.987)	3.217 (0.987)	3.221 (0.987)	**3.217 (0.987)**	3.226 (0.987)	3.226 (0.987)
	aQZ	2.821	3.225 (0.988)	3.213 (0.987)	3.215 (0.987)	3.218 (0.987)	**3.214 (0.987)**	3.229 (0.986)	3.229 (0.986)
2b $NH_4^+(H_2O)_2$	**Basis**	**KT**	**D2**	**D3**	**OVGF-A[a]**	**OVGF-B[a]**	**OVGF-C[a]**	**P3**	**P3+**
	aTZ	2.954	3.359 (0.988)	3.346 (0.987)	3.348 (0.987)	3.350 (0.987)	**3.347 (0.987)**	3.366 (0.986)	3.366 (0.986)
	daTZ	2.969	3.361(0.988)	3.348 (0.987)	**3.350 (0.987)**	3.352 (0.987)	**3.350 (0.987)**	3.368 (0.986)	3.367 (0.987)
	taTZ	2.969	3.361(0.988)	3.348 (0.987)	3.351 (0.987)	3.352 (0.987)	**3.350 (0.988)**	3.368 (0.986)	3.367 (0.987)
	qaTZ	2.969	3.361(0.988)	3.348 (0.987)	**3.350 (0.987)**	3.352 (0.987)	3.349 (0.987)	3.368 (0.986)	3.367 (0.987)
	aQZ	2.959	3.368 (0.988)	3.346 (0.987)	3.349 (0.987)	3.350 (0.986)	3.348 (0.986)	3.372 (0.986)	3.372 (0.986)

[a]The numerically recommended OVGF version is in bold.

Table S3: $NH_4^-H_2O$ isomers and their vertical electron detachment energies (VEDEs). Pole strengths are in parentheses. All energies are in eV.

$H^-(NH_3)H_2O$	**KT**	**D2**	**D3**	**OVGF-A**[a]	**OVGF-B**[a]	**OVGF-C**[a]	**P3**	**P3+**
aTZ	2.512	1.958 (0.892)	2.211 (0.903)	2.093 (0.908)	2.243 (0.899)	**2.225 (0.900)**	1.977 (0.906)	1.975 (0.90)
daTZ	2.512	1.969 (0.893)	2.220 (0.907	2.101 (0.910)	2.252 (0.902)	**2.235 (0.904)**	1.987 (0.909)	1.985 (0.908)
taTZ	2.512	1.969 (0.893)	2.221 (0.907	2.102 (0.910)	2.253 (0.902)	**2.235 (0.904)**	1.988 (0.909)	1.986 (0.908)
qaTZ	2.512	1.970 (0.893)	2.221 (0.907)	2.102 (0.910)	2.253 (0.902)	**2.235 (0.904)**	1.988 (0.909)	1.986 (0.908)
aQZ	2.514	2.001 (0.892)	2.231 (0.905)	2.117 (0.908)	2.258 (0.901)	2.241 (0.902)	2.023 (0.907)	2.021 (0.906)
$[NH_4^-]H_2O$								
aTZ	0.112	0.652 (0.933)	0.553 (0.904)	0.479 (0.872)	0.602 (0.898)	**0.513 (0.883)**	0.612 (0.915)	0.616 (0.917)
daTZ	0.368	0.770 (0.877)	0.608 (0.854)	0.401 (0.673)	0.652 (0.851)	**0.533 (0.810)**	0.719 (0.851)	0.723 (0.854)
taTZ	0.382	0.756 (0.854)	0.613 (0.872)	0.391 (0.646)	0.652 (0.863)	**0.568 (0.892)**	0.736 (0.875)	0.738 (0.873)
qaTZ	0.382	0.756 (0.853)	0.613 (0.874)	0.391 (0.650)	0.652 (0.864)	0.569 (0.896)	0.737 (0.87)	0.739 (0.877)
aQZ	0.158	0.699 (0.929)	0.572 (0.899)	0.475 (0.860)	0.620 (0.894)	0.518 (0.870)	0.655 (0.908)	0.659 (0.910)
1a $NH_4^-(H_2O)$								
aTZ	0.151	0.374 (0.930)	0.303 (0.893)	0.251 (0.861)	0.360 (0.886)	**0.266 (0.863)**	0.331 (0.909)	0.334 (0.910)
daTZ	0.211	0.575 (0.872)	0.422 (0.834)	0.20887 (0.582)	**0.476 (0.830)**	0.311 (0.686)	0.511 (0.831)	0.517 (0.835)
taTZ	0.244	0.554 (0.828)	0.421 (0.848)	0.206 (0.338)	0.467 (0.836)	**0.365 (0.873)**	0.528 (0.848)	0.531 (0.846)
qaTZ	0.244	0.553 (0.824)	0.424 (0.859)	0.209 (0.339)	0.469 (0.845)	**0.373 (0.902)**	0.534 (0.869)	0.536 (0.865)
aQZ	0.088	0.434 (0.926)	0.336 (0.889)	0.260 (0.850)	0.392 (0.883)	**0.282 (0.847)**	0.387 (0.902)	0.391 (0.904)

[a]The numerically recommended OVGF version is in bold.

Table S4: $NH_4^+(H_2O)_n$ isomers and their relative energies are in eV. Calculations were executed with the **aug-cc-pVTZ** basis set.

n	**Isomer**	ΔE^{MP2}	ΔE_{ZPE}^{MP2}	ΔE^{CCSD}	$\Delta E^{CCSD(T)}$	$\Delta E_{ZPE-MP2}^{CCSD(T)}$
1	**1a** $NH_4^+(H_2O)$	-	-	-	-	-
2	**2a** $NH_4^+(H_2O)_2$	0.000	0.000	0.000	0.000	0.000
	2b $NH_4^+(H_2O)_2$	0.111	0.124	0.129	0.118	0.130
3	**3a** $NH_4^+(H_2O)_3$	0.000	0.054	0.006	0.000	0.047
	3b $NH_4^+(H_2O)_3$	0.015	0.000	0.000	0.022	0.000
	3c $NH_4^+(H_2O)_3$	0.085	0.091	0.085	0.097	0.096
4	**4a** $NH_4^+(H_2O)_4$	0.002	0.078	0.067	0.050	0.088
	4b $NH_4^+(H_2O)_4$	0.000	0.013	0.000	0.000	0.014
	4c $NH_4^+(H_2O)_4$	0.085	0.127	0.103	0.090	0.133
	4d $NH_4^+(H_2O)_4$	1.854	0.061	0.087	0.097	0.067
	4e $NH_4^+(H_2O)_4$	0.061	0.000	0.040	0.060	0.000

Table S5: $NH_4^+(H_2O)_n$ isomerization and vertical electron attachment energies (VEAEs). Pole strengths are in parentheses. All energies are in eV. Calculations were executed with the **d-aug-cc-pVTZ** basis set.

n	Isomer	$\Delta E_{MP2-ZPE}^{CCSD(T)}$	KT	D2	D3	OVGF-A[a]	OVGF-B[a]	OVGF-C[a]	P3	P3+	ΔCCSD(T)
1	**1a** $NH_4^+(H_2O)$	-	3.324	3.744(0.988)	3.722(0.987)	3.725 (0.987)	3.726 (0.986)	**3.724 (0.986)**	3.749 (0.986)	3.748 (0.986)	3.826
2	**2a** $NH_4^+(H_2O)_2$	0.000	2.836	3.220(0.989)	3.217 (0.987)	**3.218 (0.988**)	3.221 (0.987)	3.217 (0.987)	3.226 (0.987)	3.226 (0.987)	3.332
	2b $NH_4^+(H_2O)_2$	0.130	2.969	3.361(0.988)	3.348 (0.987)	**3.350 (0.987)**	3.352 (0.987)	3.349 (0.987)	3.368 (0.986)	3.367 (0.987)	3.456
3	**3a** $NH_4^+(H_2O)_3$	0.047	2.569	2.937 (0.989)	2.940 (0.988)	**2.940 (0.988)**	2.944 (0.987)	2.939 (0.987)	2.943 (0.987)	2.943 (0.987)	3.826
	3b $NH_4^+(H_2O)_3$	0.000	2.490	2.840 (0.990)	2.850 (0.988)	**2.849 (0.988)**	2.853 (0.988)	2.848 (0.988)	2.847 (0.988)	2.846 (0.988)	3.332
	3c $NH_4^+(H_2O)_3$	0.096	2.554	2.910 (0.989)	2.915 (0.988)	**2.915 (0.988)**	2.918 (0.988)	2.914 (0.988)	2.917 (0.987)	2.917 (0.987)	3.456
4	**4a** $NH_4^+(H_2O)_4$	0.088	2.362	2.698 (0.990)	2.706 (0.989)	**2.705 (0.989)**	2.709 (0.988)	**2.705 (0.989)**	2.706 (0.989)	2.705 (0.988)	3.071
	4b $NH_4^+(H_2O)_4$	0.014	2.301	2.638 (0.990)	2.649 (0.989)	**2.647 (0.989)**	2.652 (0.988)	**2.647 (0.988)**	2.645 (0.988)	2.645 (0.988)	2.972
	4c $NH_4^+(H_2O)_4$	0.133	2.385	2.734 (0.989)	2.742 (0.988)	2.740 (0.988)	2.745 (0.988)	**2.741(0.988)**	2.742 (0.987)	2.741 (0.988)	3.033
	4d $NH_4^+(H_2O)_4$	0.067	2.269	2.591(0.990)	2.607 (0.989)	2.604 (0.989)	2.609 (0.989)	**2.605 (0.989)**	2.599 (0.988)	2.599 (0.988)	2.834
	4e $NH_4^+(H_2O)_4$	0.000	2.256	2.574 (0.990)	2.591(0.989)	2.587 (0.989)	2.593 (0.989)	**2.589 (0.989)**	2.582 (0.988)	2.581(0.989)	2.785

[a]The numerically recommended OVGF version is in bold.

Table S6: $NH_4^+(H_2O)_n$ isomers and VEAEs obtained through total energy differences (indirect method). All energies are in eV.

n	**Isomer**	aug-cc-pVTZ			d-aug-cc-pVTZ		
		ΔCCSD	**ΔCCSD(T)**	**<S²> UHF**	**ΔCCSD**	**ΔCCSD(T)**	**<S²> UHF**
1	**1a** $NH_4^+(H_2O)$	3.769	3.821	0.751	3.773	3.826	0.751
2	**2a** $NH_4^+(H_2O)_2$	3.264	3.324	0.750	3.274	3.332	0.750
	2b $NH_4^+(H_2O)_2$	3.399	3.450	0.751	3.405	3.456	0.750
3	**3a** $NH_4^+(H_2O)_3$	2.992	3.052	0.750	3.005	3.071	0.750
	3b $NH_4^+(H_2O)_3$	2.893	2.958	0.750	2.909	2.972	0.750
	3c $NH_4^+(H_2O)_3$	2.962	3.021	0.750	2.976	3.033	0.750
4	**4a** $NH_4^+(H_2O)_4$	2.757	2.819	0.750	2.774	2.834	0.750
	4b $NH_4^+(H_2O)_4$	2.695	2.768	0.750	2.715	2.785	0.750
	4c $NH_4^+(H_2O)_4$	2.795	2.864	0.750	2.811	2.878	0.750
	4d $NH_4^+(H_2O)_4$	2.646	2.711	0.750	2.668	2.730	0.750
	4e $NH_4^+(H_2O)_4$	2.627	2.695	0.750	2.650	2.715	0.750

Table S7: $NH_4^-(H_2O)_n$ isomers and their relative energies are in eV. Calculations were executed with the **aug-cc-pVTZ** basis set.

N	Isomer	ΔE^{MP2}	ΔE^{MP2}_{ZPE}	ΔE^{CCSD}	$\Delta E^{CCSD(T)}$	$\Delta E^{CCSD(T)}_{MP2\,ZPE}$
1	$H^-(NH_3)H_2O$	0.000	0.000	0.000	0.000	0.000
	$[NH_4^-]H_2O$	1.154	1.311	1.148	1.123	1.148
	1a $NH_4^-(H_2O)$	1.214	1.446	1.194	1.147	1.194
2	$H^-(NH_3)(H_2O)_2$	0.000	0.000	0.000	0.000	0.000
	$[NH_4^-](H_2O)_2$	1.669	1.686	1.667	1.656	1.667
	2a $NH_4^-(H_2O)_2$	1.649	1.819	1.641	1.573	1.641
	2b $NH_4^-(H_2O)_2$	1.572	1.733	1.557	1.506	1.557
3	$H^-(NH_3)(H_2O)_3$	0.000	0.000	0.000	0.000	0.000
	$[NH_4^-](H_2O)_3$	1.912	1.933	1.923	1.906	1.923
	3a $NH_4^-(H_2O)_3$	1.939	2.131	1.925	1.837	1.925
	3b $NH_4^-(H_2O)_3$	1.958	2.109	1.971	1.891	1.971
	3c $NH_4^-(H_2O)_3$	1.832	2.034	1.809	1.743	1.809
4	$H^-(NH_3)(H_2O)_4$	0.000	0.000	0.000	0.000	0.000
	$[NH_4^-](H_2O)_4$	2.068	2.067	2.061	2.054	2.061
	4a $NH_4^-(H_2O)_4$	2.153	2.298	2.126	2.061	2.126
	4b $NH_4^-(H_2O)_4$	2.188	2.297	2.195	2.117	2.195
	4c $NH_4^-(H_2O)_4$	2.206	2.324	2.178	2.109	2.178
	4d $NH_4^-(H_2O)_4$	2.267	2.349	2.264	2.194	2.264
	4e $NH_4^-(H_2O)_4$	2.347	2.404	2.318	2.256	2.318

Table S8: $NH_4^-(H_2O)_n$ isomers and their vertical electron detachment energies (VEDEs). Pole strengths are in parentheses. All energies are in eV. Calculations were executed with the **d-aug-cc-pVTZ** basis set.

n	Isomer	KT	D2	D3	OVGF-A[a]	OVGF-B[a]	OVGF-C[a]	P3	P3+	BD-T1
1	$H^-(NH_3)H_2O$	2.512	1.969 (0.893)	2.220 (0.907	2.102 (0.910)	2.252 (0.903)	**2.235 (0.904)**	1.987 (0.909)	1.985 (0.908)	2.172 (0.882)
	$[NH_4^-]H_2O$	0.368	0.770 (0.877)	0.608 (0.854)	0.402 (0.674)	0.652 (0.851)	**0.534 (0.810)**	0.719 (0.851)	0.723 (0.854)	0.684 (0.881)
	1a $NH_4^-(H_2O)$	0.211	0.575 (0.872)	0.422 (0.834)	0.208 (0.582)	**0.476 (0.830)**	0.312 (0.686)	0.511 (0.831)	0.517 (0.835)	0.495 (0.862)
2	$H^-(NH_3)(H_2O)_2$	3.135	2.574 (0.903)	2.812 (0.908)	2.695 (0.913)	2.835 (0.905)	**2.819 (0.906)**	2.576 (0.909)	2.576 (0.908)	2.771 (0.831)
	$[NH_4^-](H_2O)_2$	0.490	0.954 (0.881)	0.789 (0.867)	0.613 (0.757)	0.824 (0.864)	**0.742 (0.854)**	0.917 (0.864)	0.920 (0.866)	0.886 (0.894)
	2a $NH_4^-(H_2O)_2$	0.186	0.607 (0.873)	0.451 (0.835)	0.274 (0.680)	**0.498 (0.831)**	0.362 (0.731)	0.552 (0.826)	0.558 (0.835)	0.539 (0.870)
	2b $NH_4^-(H_2O)_2$	0.238	0.621 (0.862)	0.454 (0.832)	0.226 (0.568)	**0.497 (0.829)**	0.369 (0.753)	0.562 (0.826)	0.568 (0.829)	0.552 (0.864)
3	$H^-(NH_3)(H_2O)_3$	3.980	3.352 (0.908)	3.600 (0.908)	3.479 (0.915)	**3.603 (0.906)**	3.594 (0.907)	3.366 (0.908)	3.364 (0.908)	3.567 (0.900)
	$[NH_4^-](H_2O)_3$	0.632	1.138 (0.886)	0.970 (0.876)	0.807 (0.791)	0.999 (0.872)	**0.935 (0.870)**	1.109 (0.73)	1.112 (0.874)	1.075 (0.899)
	3a $NH_4^-(H_2O)_3$	0.143	0.534 (0.860)	0.372 (0.812)	0.179 (0.601)	**0.420 (0.811)**	0.252 (0.528)	0.464 (0.806)	0.471 (0.812)	0.459 (0.856)
	3b $NH_4^-(H_2O)_3$	0.169	0.575 (0.857)	0.396 (0.814)	0.204 (0.625)	**0.435 (0.814)**	0.286 (0.595)	0.506 (0.804)	0.513 (0.809)	0.498 (0.856)
	3c $NH_4^-(H_2O)_3$	0.186	0.574 (0.863)	0.428 (0.829)	0.239 (0.618)	**0.475 (0.925)**	0.344 (0.731)	0.519 (0.823)	0.525 (0.827)	0.537 (0.868)
4	$H^-(NH_3)(H_2O)_4$	4.192	3.543 (0.908)	3.781 (0.907)	3.665 (0.914)	**3.785 (0.906)**	3.776 (0.906)	3.551 (0.906)	3.551 (0.903)	3.756 (0.896)
	$[NH_4^-](H_2O)_4$	0.730	1.240 (0.889)	1.071 (0.878)	0.910 (0.798)	1.100 (0.875)	**1.035 (0.872)**	1.210 (0.876)	1.213 (0.877)	1.177 (0.900)
	4a $NH_4^-(H_2O)_4$	0.141	0.523 (0.861)	0.376 (0.819)	0.199 (0.623)	**0.421 (0.817)**	0.275 (0.632)	0.464 (0.811)	0.470 (0.817)	0.473 (0.860)
	4b $NH_4^-(H_2O)_4$	0.148	0.522 (0.838)	0.331 (0.793)	0.113 (0.522)	**0.368 (0.795)**	0.368 (0.795)	0.444 (0.779)	0.452 (0.785)	0.432 (0.853)
	4c $NH_4^-(H_2O)_4$	0.162	0.521 (0.840)	0.348 (0.800)	0.117 (0.434)	**0.390 (0.800)**	0.243 (0.616)	0.449 (0.789)	0.457 (0.795)	0.455 (0.858)
	4d $NH_4^-(H_2O)_4$	0.173	0.586 (0.848)	0.404 (0.811)	0.202 (0.603)	**0.439 (0.811)**	0.314 (0.676)	0.523 (0.798)	0.529 (0.803)	0.515 (0.859)
	4e $NH_4^-(H_2O)_4$	0.183	0.566 (0.839)	0.393 (0.807)	0.183 (0.538)	**0.427 (0.807)**	0.312 (0.696)	0.503 (0.794)	0.509 (0.799)	0.534 (0.863)

[a]The numerically recommended OVGF version is in bold.

Table S9: $NH_4^-(H_2O)_n$ isomers and VEDEs obtained through total energy differences (indirect method). All energies are in eV.

n	**Isomer**	aug-cc-pVTZ			d-aug-cc-pVTZ		
		ΔCCSD	**ΔCCSD(T)**	**<S²> UHF**	**ΔCCSD**	**ΔCCSD(T)**	**<S²> UHF**
1	$H^-(NH_3)H_2O$	2.032	2.080	0.755	2.036	2.085	0.755
	$[NH_4^-]H_2O$	0.518	0.606	0.751	0.594	0.675	0.751
	1a $NH_4^-(H_2O)$	0.280	0.378	0.751	0.407	0.491	0.751
2	$H^-(NH_3)(H_2O)_2$	2.634	2.689	0.753	2.637	2.693	0.753
	$[NH_4^-](H_2O)_2$	0.745	0.850	0.751	0.787	0.886	0.751
	2a $NH_4^-(H_2O)_2$	0.343	0.464	0.751	0.449	0.553	0.751
	2b $NH_4^-(H_2O)_2$	0.359	0.472	0.751	0.456	0.556	0.751
3	$H^-(NH_3)(H_2O)_3$	3.412	3.466	0.754	3.416	3.470	0.754
	$[NH_4^-](H_2O)_3$	0.940	1.055	0.751	0.971	1.081	0.751
	3a $NH_4^-(H_2O)_3$	0.237	0.380	0.750	0.360	0.481	0.750
	3b $NH_4^-(H_2O)_3$	0.296	0.432	0.751	0.396	0.517	0.751
	3c $NH_4^-(H_2O)_3$	0.339	0.463	0.751	0.444	0.551	0.754
4	$H^-(NH_3)(H_2O)_4$	3.598	3.655	0.754	3.601	3.659	0.754
	$[NH_4^-](H_2O)_4$	1.045	1.160	0.751	1.073	1.183	0.751
	4a $NH_4^-(H_2O)_4$	0.250	0.379	0.751	0.372	0.481	0.751
	4b $NH_4^-(H_2O)_4$	0.206	0.349	0.751	0.313	0.439	0.751
	4c $NH_4^-(H_2O)_4$	0.242	0.388	0.751	0.314	0.474	0.751
	4d $NH_4^-(H_2O)_4$	0.305	0.449	0.751	0.402	0.530	0.751
	4e $NH_4^-(H_2O)_4$	0.345	0.495	0.751	0.429	0.564	0.751

Table S10: Twenty vertical electron affinities (EAs) and radical excitation energies (EEs) of **3b** $NH_4^+(H_2O)_3$. All energies are in eV. The numbers in second column refer to Figure 5 in the main text.

l	Dyson #	Final State	KT	KT EEs	D2	D2 EEs	D3	D3 EEs	OVGF-B	OVGF-B EEs	P3	P3 EEs	P3+	P3+ EEs
s	1	1^2A	2.490	0.000	2.840	0.000	2.850	0.000	2.849	0.000	2.847	0.000	2.846	0.000
p	2,3	1^2E	1.937	0.553	2.144	0.696	2.154	0.696	2.153	0.696	2.152	0.695	2.152	0.694
	4	2^2A	1.864	0.626	2.012	0.828	2.023	0.827	2.021	0.828	2.019	0.828	2.018	0.828
d	5,6	2^2E	1.377	1.113	1.477	1.363	1.483	1.367	1.482	1.367	1.483	1.364	1.482	1.364
	7	3^2A	1.327	1.163	1.434	1.406	1.438	1.412	1.438	1.411	1.439	1.408	1.438	1.408
	8,9	3^2E	1.246	1.244	1.307	1.533	1.314	1.536	1.314	1.535	1.312	1.535	1.312	1.534
s	10	4^2A	1.151	1.339	1.261	1.579	1.264	1.586	1.264	1.585	1.263	1.584	1.263	1.583
p	11,12	4^2E	0.880	1.610	0.991	1.849	0.995	1.855	0.995	1.854	0.994	1.853	0.994	1.852
	13	5^2A	0.892	1.598	0.980	1.860	0.984	1.866	0.983	1.866	0.983	1.864	0.983	1.863
f	14,15	5^2E	0.739	1.751	0.799	2.041	0.802	2.048	0.801	2.048	0.803	2.044	0.803	2.043
	16	6^2A	0.635	1.855	0.699	2.141	0.704	2.146	0.704	2.145	0.704	2.143	0.703	2.143
	17,18	6^2E	0.578	1.912	0.650	2.190	0.656	2.194	0.655	2.194	0.655	2.192	0.654	2.192
	19	7^2A	0.492	1.998	0.599	2.241	0.602	2.248	0.602	2.247	0.603	2.244	0.602	2.244
	20	8^2A	0.528	1.962	0.595	2.245	0.601	2.249	0.599	2.250	0.599	2.248	0.598	2.248

Table S11: Eighteen vertical electron affinities (EAs) and radical excitation energies (EEs) for **4e** $NH_4^+(H_2O)_4$. All energies are in eV. The numbers in second column refer to Figure 6 in the main text.

l	Dyson #	Final State	KT	KT EEs	D2	D2 EEs	D3	D3 EEs	OVGF-B	OVGF-B EEs	P3	P3 EEs	P3+	P3+ EEs
s	1	1^2A_1	2.256	0.000	2.574	0.000	2.591	0.000	2.589	0.000	2.582	0.000	2.581	0.000
p	2	1^2B	1.807	0.449	1.995	0.579	2.008	0.583	2.006	0.583	2.004	0.578	2.003	0.578
	3,4	1^2E	1.800	0.456	1.988	0.586	2.001	0.590	1.999	0.590	1.996	0.586	1.996	0.585
d	5	2^2B	1.311	0.945	1.406	1.168	1.413	1.178	1.412	1.177	1.412	1.170	1.411	1.170
	6,7	2^2E	1.290	0.966	1.382	1.192	1.389	1.202	1.387	1.202	1.387	1.195	1.387	1.194
	8	2^2A	1.236	1.020	1.302	1.272	1.310	1.281	1.310	1.279	1.308	1.274	1.307	1.274
	9	3^2B	1.190	1.066	1.248	1.326	1.256	1.335	1.256	1.333	1.253	1.329	1.253	1.328
s	10	3^2A	1.109	1.147	1.233	1.341	1.237	1.354	1.237	1.352	1.234	1.348	1.234	1.347
p	11,12	3^2E	0.853	1.403	0.941	1.633	0.946	1.645	0.945	1.644	0.944	1.638	0.943	1.638
	13	4^2B	0.812	1.444	0.928	1.646	0.934	1.657	0.933	1.656	0.931	1.651	0.931	1.650
	14	4^2A	0.706	1.550	0.773	1.801	0.777	1.814	0.776	1.813	0.778	1.804	0.777	1.804
	15	5^2A	0.688	1.568	0.749	1.825	0.753	1.838	0.752	1.837	0.753	1.829	0.753	1.828
d	16,17	4^2E	0.588	1.668	0.640	1.934	0.647	1.944	0.646	1.943	0.646	1.936	0.645	1.936
	18	5^2B	0.495	1.761	0.595	1.979	0.602	1.989	0.601	1.988	0.598	1.984	0.598	1.983

I. Sample Inputs for Electron Propagator Calculations of Vertical Electron Binding Energies

A. *Sample input for calculation of vertical electron affinities (VEAs) of 1a $NH_4^+(H_2O)$ to Gaussian 16 Program.*

****

#p ept gfinput gfprint iop(6/7=3,9/11=30100) daug-cc-pVTZ

Title: Diagonal EPT calculations for VEAs of 1a $NH_4^+(H_2O)$

+1 1

H	1.6871400000	-0.5171200000	-0.8070700000
H	0.2861700000	0.0026100000	-0.0003000000
H	1.6866500000	-0.4397700000	0.8519600000
H	1.6920900000	0.9554200000	-0.0446800000
N	1.3405900000	-0.0001900000	0.0000400000
O	-1.3568500000	0.0002400000	-0.0001000000
H	-1.9392600000	-0.7683200000	0.0002900000
H	-1.9421700000	0.7665700000	0.0002900000

9 12

****

The option ept invokes the electron propagator theory (EPT) calculations and the IOP 9/3=30100 requests the program to carry out EPT calculations with the diagonal P3+, P3, OVGF, D3, D2 and KT methods and to read an additional line (the last line of the input) containing orbitals for which electron binding energies (vertical electron affinities in this case) will be calculated.
In this case, diagonal EPT calculations are carried out on $NH_4^+(H_2O)$ which has 20 electrons in 10 molecular orbitals. As the standard frozen-core approximation is a default in Gaussian calculations, the 2 lowest-energy occupied orbitals are therefore frozen. The last line of the input (9 12) therefore requests a calculation of vertical electron affinities (VEAs) for LUMO, LUMO +1, LUMO +2 and LUMO+3 orbitals.
The p, gfinput, gfprint, and IOP 6/7=3 are necessary to use the Gaussian output file as an input to Molden.

B. *Sample input for calculation of vertical electron detachment energies (VEDEs) of 1a $NH_4^-(H_2O)$ to Gaussian 16 Program.*

****

#p ept gfinput gfprint iop(6/7=3,9/11=30100) daug-cc-pVTZ

Title: Diagonal EPT calculations for VEAs of 1a $NH_4^-(H_2O)$

-1 1

H	-0.9319990000	-0.7827910000	-0.0245850000
H	0.4611630000	1.9566870000	0.0249990000
H	-2.1493760000	-0.0933860000	0.7770270000
H	-1.1521280000	0.7762710000	-0.1550320000
N	-1.6826470000	-0.1039260000	-0.1242420000
O	1.5557310000	-0.2103940000	0.1080620000
H	2.0051560000	-0.1690020000	-0.7427290000
H	1.0998660000	0.7228570000	0.1255150000

7 9

****

See the previous example for the detailed explanation of keywords.
In this case, diagonal EPT calculations are carried out on $NH_4^-(H_2O)$ which has 22 electrons in 11 molecular orbitals. As the standard frozen-core approximation is a default in Gaussian calculations, the 2 lowest-energy occupied orbitals are therefore frozen. The last line of the input (7 9) therefore requests a calculation of vertical electron detachment energies (VEDEs) for HOMO-2, HOMO-1, and HOMO orbitals.
Results will be reported for diagonal P3+, P3, OVGF, D3, D2 and KT methods.

II. Cartesian Coordinates of all the Optimized $OH_3^{\pm}(H_2O)_n$ geometries

A. Optimized geometries of the $NH_4^+(H_2O)_n$ Cations

$NH_4^+(H_2O)_n$:

1a $NH_4^+(H_2O)$

H	1.6871400000	-0.5171200000	-0.8070700000
H	0.2861700000	0.0026100000	-0.0003000000
H	1.6866500000	-0.4397700000	0.8519600000
H	1.6920900000	0.9554200000	-0.0446800000
N	1.3405900000	-0.0001900000	0.0000400000
O	-1.3568500000	0.0002400000	-0.0001000000
H	-1.9392600000	-0.7683200000	0.0002900000
H	-1.9421700000	0.7665700000	0.0002900000

$NH_4^+(H_2O)_2$ isomers:

2a $NH_4^+(H_2O)_2$

H	0.8593500000	0.4589200000	-0.0000100000
H	-0.8524200000	0.4757300000	-0.0000200000
H	0.0138600000	1.6557700000	0.8262700000
H	0.0138400000	1.6557600000	-0.8263000000
N	0.0090200000	1.0622400000	-0.0000100000
O	-2.2576300000	-0.5112800000	-0.0000200000
H	-2.7675100000	-0.8006200000	0.7650100000
H	-2.7657000000	-0.8031600000	-0.7652900000
O	2.2548000000	-0.5301400000	0.0000300000
H	3.1779700000	-0.2532600000	-0.0011800000
H	2.2800900000	-1.4934900000	0.0015000000

2b $NH_4^+(H_2O)_2$

H	-2.8259800000	-0.1999100000	0.8288300000
H	-2.8257900000	-0.1999500000	-0.8291700000
H	-1.3586700000	0.1265200000	-0.0000100000
H	-2.0841400000	-1.4263900000	-0.0000500000
N	-2.2804000000	-0.4272500000	-0.0001000000
O	2.3038100000	-0.4480500000	-0.0000200000
H	2.8849700000	-0.5184900000	-0.7651100000
H	2.8849500000	-0.5186700000	0.7650800000
O	-0.0171700000	0.8785200000	0.0001200000
H	0.8718400000	0.4533900000	0.0000700000
H	0.1225500000	1.8305000000	0.0002300000

$NH_4^+(H_2O)_3$ isomers:

3a $NH_4^+(H_2O)_3$

H	-1.4703000000	-0.8324400000	0.0000300000
H	-2.6875800000	0.0000600000	0.8292500000
H	-1.4702900000	0.8324400000	-0.0000700000
H	-2.6875900000	-0.0000600000	-0.8292800000

N	-2.1003100000	0.0000000000	-0.0000200000
O	2.1405000000	0.0000000000	-0.0000200000
H	2.7314800000	0.0002400000	0.7635500000
H	2.7315300000	-0.0002300000	-0.7635400000
O	-0.0806000000	1.8002200000	0.0000600000
H	0.0655900000	2.7513000000	-0.0002000000
H	0.7946800000	1.3786600000	-0.0001800000
O	-0.0806000000	-1.8002200000	-0.0000200000
H	0.0655900000	-2.7513000000	0.0002200000
H	0.7946800000	-1.3786600000	0.0001600000

3b $NH_4^+(H_2O)_3$

H	0.7670000000	0.6072200000	0.3685900000
H	0.0000000000	0.0000100000	1.7226200000
H	-0.9093700000	0.3606400000	0.3685900000
H	0.1423600000	-0.9678500000	0.3686000000
N	0.0000000000	0.0000100000	0.7066100000
O	0.3736100000	-2.6196900000	-0.2243700000
H	-0.0283200000	-3.4308200000	0.1053800000
H	0.9949600000	-2.9076500000	-0.9019500000
O	-2.4555300000	0.9862900000	-0.2243800000
H	-2.9569700000	1.7400000000	0.1052900000
H	-3.0156500000	0.5920600000	-0.9018400000
O	2.0819200000	1.6334000000	-0.2243700000
H	2.0205500000	2.3157200000	-0.9017100000
H	2.9854300000	1.6906400000	0.1051000000

3c $NH_4^+(H_2O)_3$

H	-0.2644300000	0.4826500000	0.3715700000
H	-0.8765100000	1.5497500000	-0.7899400000
H	-1.9287800000	0.4648800000	-0.0665300000
H	-1.2934600000	1.7581500000	0.7946800000
N	-1.0942000000	1.0658700000	0.0774100000
O	3.3768100000	-0.0713300000	-0.5255400000
H	3.7539800000	-0.7199800000	-1.1293200000
H	4.1315800000	0.4153200000	-0.1776400000
O	-3.3189900000	-0.5515700000	-0.3149800000
H	-4.2486500000	-0.2988700000	-0.3320700000
H	-3.3130900000	-1.4988800000	-0.4904800000
O	1.0243100000	-0.4131200000	0.7661100000
H	1.1332300000	-0.9925400000	1.5260900000
H	1.9084500000	-0.3333900000	0.3470900000

$NH_4^+(H_2O)_4$ isomers:

4a $NH_4^+(H_2O)_4$

H	2.2002700000	0.8328900000	-0.3168900000
H	3.0548600000	-0.0000100000	-1.5186800000

H	3.6325900000	0.0000000000	0.0357100000
H	2.2002800000	-0.8328900000	-0.3168800000
N	2.7937500000	0.0000000000	-0.5370700000
O	0.8966200000	1.7752600000	0.1511900000
H	0.7409500000	2.7188000000	0.2514300000
H	0.0887100000	1.3132500000	0.4476500000
O	0.8966200000	-1.7752600000	0.1511900000
H	0.0887100000	-1.3132400000	0.4476600000
H	0.7409600000	-2.7188000000	0.2514700000
O	-3.3339600000	0.0000000000	-0.6733900000
H	-3.8785200000	-0.7647000000	-0.8868300000
H	-3.8785600000	0.7646800000	-0.8867700000
O	-1.1102000000	0.0000000000	0.8835900000
H	-1.4038100000	0.0000000000	1.8017700000
H	-1.9354200000	0.0000000000	0.3492900000

4b $NH_4^+(H_2O)_4$

H	0.5530100000	0.8264100000	0.6542600000
H	2.0007100000	-0.0000200000	0.2959200000
H	1.3880800000	-0.0000400000	1.8519600000
H	0.5530200000	-0.8264600000	0.6542300000
N	1.1408200000	-0.0000300000	0.8673300000
O	-0.8191000000	1.8125400000	0.1898400000
H	-1.6394100000	1.3762500000	-0.0914400000
H	-0.9865400000	2.7591700000	0.1552600000
O	-0.8191200000	-1.8125600000	0.1898000000
H	-1.6394200000	-1.3762500000	-0.0914700000
H	-0.9865500000	-2.7591800000	0.1551200000
O	3.5268800000	0.0000200000	-0.6340500000
H	4.0226000000	-0.7637000000	-0.9481800000
H	4.0222000000	0.7637700000	-0.9487300000
O	-2.9265900000	0.0000200000	-0.5339600000
H	-3.2369700000	0.0000400000	-1.4478800000
H	-3.7329900000	0.0000300000	-0.0035300000

4c $NH_4^+(H_2O)_4$

H	2.7005500000	-1.7055900000	0.2891400000
H	2.0700200000	-0.1445200000	0.0879400000
H	2.3777900000	-1.1554600000	-1.2376900000
H	1.1000400000	-1.5117600000	-0.1996800000
N	2.0709500000	-1.1364200000	-0.2693600000
O	1.7300100000	1.3350100000	0.6626600000
H	0.9298500000	1.7020900000	0.2316100000
H	2.2613700000	2.0738500000	0.9728600000
O	-0.5291200000	-1.9688000000	-0.0375800000
H	-1.2751800000	-1.3609300000	0.1048200000
H	-0.8952900000	-2.8573800000	0.0099200000
O	-0.5453700000	1.7643400000	-0.7036500000
H	-1.3487500000	1.3369200000	-0.3693900000
H	-0.8403500000	2.5315800000	-1.2041100000

O	-2.5711200000	-0.0048500000	0.3429400000
H	-3.3858600000	-0.1118600000	-0.1633900000
H	-2.8659900000	0.1523900000	1.2484900000

4d $NH_4^+(H_2O)_4$

H	-1.5368400000	-0.7359200000	-0.3650600000
H	-1.1862300000	0.9169000000	-0.3290300000
H	0.0506500000	-0.2137200000	-0.0397000000
H	-0.6172000000	-0.0404200000	-1.5693200000
N	-0.8249300000	-0.0183700000	-0.5754700000
O	1.4829200000	-0.4878800000	0.7939200000
H	1.5988300000	-0.9007900000	1.6545700000
H	2.3832700000	-0.3543500000	0.4332600000
O	3.9156200000	-0.0483500000	-0.3665000000
H	4.5024000000	0.6798100000	-0.1373100000
H	4.4946000000	-0.7366500000	-0.7101400000
O	-1.8179400000	2.5312300000	0.1252900000
H	-1.4770000000	3.0934300000	0.8291400000
H	-2.4898200000	3.0634000000	-0.3141600000
O	-2.7778300000	-1.9792600000	-0.0084700000
H	-3.6388200000	-1.8429300000	0.4011400000
H	-2.7314400000	-2.9260900000	-0.1790500000

4e $NH_4^+(H_2O)_4$

H	0.5964700000	0.4968900000	0.6769100000
H	-0.5949500000	-0.6776700000	0.4975700000
H	-0.5963500000	0.6776300000	-0.4960300000
H	0.5948400000	-0.4967100000	-0.6784000000
N	0.0000000000	0.0000400000	0.0000200000
O	1.6551400000	-1.3666400000	-1.8739200000
H	1.5758000000	-2.2817600000	-2.1634600000
H	2.4365300000	-1.0319000000	-2.3265700000
O	-1.6593700000	1.8716700000	-1.3647100000
H	-1.5815700000	2.1612400000	-2.2799600000
H	-2.4409100000	2.3233300000	-1.0290100000
O	1.6597000000	1.3669500000	1.8697500000
H	1.5807700000	2.2819500000	2.1597800000
H	2.4425100000	1.0324300000	2.3200900000
O	-1.6554800000	-1.8720200000	1.3688600000
H	-1.5749800000	-2.1620400000	2.2837400000
H	-2.4381500000	-2.3233200000	1.0353200000

B. Optimized geometries of the $NH_4^-(H_2O)_n$ Anions

$NH_4^-(H_2O)$ isomers:

$H^-(NH_3)H_2O$

H	-0.9319990000	-0.7827910000	-0.0245850000
H	0.4611630000	1.9566870000	0.0249990000
H	-2.1493760000	-0.0933860000	0.7770270000
H	-1.1521280000	0.7762710000	-0.1550320000
N	-1.6826470000	-0.1039260000	-0.1242420000
O	1.5557310000	-0.2103940000	0.1080620000
H	2.0051560000	-0.1690020000	-0.7427290000
H	1.0998660000	0.7228570000	0.1255150000

$[NH_4^-]H_2O$

H	2.6369490000	-0.0191020000	0.8651790000
H	1.4467180000	-0.8496710000	-0.0306810000
H	1.4475700000	0.8508990000	0.0063190000
H	2.6720490000	0.0180980000	-0.8406110000
N	2.0549290000	0.0000580000	0.0000190000
O	-2.3812710000	-0.0007050000	0.0001890000
H	-1.7648620000	-0.7450360000	-0.0011310000
H	-1.7727600000	0.7500440000	-0.0007210000

1a $NH_4^-(H_2O)$

H	1.9281200000	0.0000900000	-0.8738400000
H	0.3492700000	0.0000000000	-0.2090300000
H	1.6010300000	-0.8454600000	0.5592200000
H	1.6009900000	0.8453800000	0.5593700000
N	1.3733800000	0.0000000000	0.0012100000
O	-1.4858100000	0.0000000000	-0.1230000000
H	-1.6032700000	-0.7627200000	0.4698900000
H	-1.6032700000	0.7627200000	0.4699000000

$NH_4^-(H_2O)_2$ isomers:

$H^-(NH_3)(H_2O)_2$

H	0.3432350000	-0.0440850000	1.8417490000
H	-1.2566730000	0.1414290000	0.7677080000
H	-1.2443520000	1.0092740000	-0.5711780000
N	-1.7840680000	0.2857600000	-0.1043550000
O	0.5884860000	-1.6831460000	-0.1206080000
H	0.5786070000	-1.1504440000	0.7296580000
H	-0.2816060000	-1.4509190000	-0.4725550000
O	1.2484670000	1.3474700000	-0.1112390000
H	1.3946950000	0.5336040000	-0.6107620000
H	0.9306210000	0.9422850000	0.7495880000
H	-2.6716710000	0.7039420000	0.1510520000

[NH_4^-]($(H_2O)_2$

H	0.8576730000	2.4026500000	-0.0139020000
H	0.0022270000	1.2096370000	0.8575590000
N	0.0000530000	1.8041100000	-0.0008540000
O	-3.1970450000	-1.0698580000	0.0008050000
H	-2.2464060000	-1.2436090000	-0.0066520000
H	-3.2170700000	-0.1041890000	0.0061940000
O	3.1968880000	-1.0700250000	0.0003860000
H	3.2180530000	-0.1045070000	0.0164280000
H	2.2461200000	-1.2424460000	-0.0165570000
H	0.0008240000	1.1743040000	-0.8341530000
H	-0.8605290000	2.3984460000	-0.0124630000

2a $NH_4^-(H_2O)_2$

H	0.8436300000	0.7163300000	0.0000000000
H	-0.8436000000	0.7163900000	0.0000100000
H	0.0000500000	1.9257200000	0.8422300000
H	0.0000400000	1.9257100000	-0.8422400000
N	0.0000300000	1.3342100000	0.0000000000
O	-2.0307100000	-0.6255000000	0.0000000000
H	-1.7274600000	-1.1538200000	0.7614000000
H	-1.7274900000	-1.1538300000	-0.7614000000
O	2.0306700000	-0.6255300000	0.0000000000
H	1.7274600000	-1.1538700000	0.7614000000
H	1.7274600000	-1.1538600000	-0.7614100000

2b $NH_4^-(H_2O)_2$

H	-1.5973600000	-0.9770400000	0.9484200000
H	-2.7849300000	-0.3494200000	-0.0889700000
H	-1.1883200000	0.2693100000	-0.1254300000
H	-1.5177800000	-1.3001700000	-0.7064800000
N	-1.7795700000	-0.5836300000	0.0021100000
O	1.8027500000	-0.7566700000	0.0025500000
H	1.4078100000	-1.2986200000	-0.7026400000
H	1.4290200000	-1.1638900000	0.8036800000
O	0.1635500000	1.5324600000	-0.1108300000
H	0.8668200000	0.8485500000	-0.0786600000
H	0.1113500000	1.8503700000	0.8016000000

$NH_4^-(H_2O)_3$ isomers:

$H^-(NH_3)(H_2O)_3$

H	1.9935880000	0.0094690000	1.0710220000
H	-0.0646310000	-0.0270580000	1.4095780000
H	2.8350650000	0.8546990000	-0.0015540000
N	2.8561130000	-0.0148650000	0.5213060000
O	-0.3098430000	1.6368280000	-0.5606280000
H	-0.1054080000	0.9108120000	-1.1649960000

H	-0.1791890000	1.1593020000	0.3036080000
O	-2.5313940000	-0.2170140000	0.5955800000
H	-1.6614430000	-0.2233720000	1.0761580000
H	-2.3805890000	0.5378830000	0.0121900000
O	0.0523990000	-1.4086390000	-0.7296140000
H	0.1113120000	-0.9372080000	0.1536520000
H	-0.9034220000	-1.5353080000	-0.7801420000
H	2.6726280000	-0.7345520000	-0.1713540000

$[NH_4^-](H_2O)_3$

H	-1.0483920000	1.5717780000	-0.7494680000
H	-1.1396210000	1.5801330000	0.9446180000
N	-1.0094730000	2.1858230000	0.0987800000
O	3.7223340000	-0.1493450000	-0.3188500000
H	3.4473500000	0.7569170000	-0.4892040000
H	2.8857160000	-0.5773050000	-0.0629600000
O	1.1637830000	-1.2471750000	0.4179670000
H	0.5490050000	-1.0565500000	-0.3065450000
H	0.8113390000	-0.6851670000	1.1246270000
O	-3.6577180000	-1.2100840000	-0.2228060000
H	-3.1186370000	-0.9640220000	0.5406200000
H	-3.3036630000	-0.6234890000	-0.9041380000
H	-1.7684040000	2.9006420000	0.0526800000
H	-0.0755770000	2.6491310000	0.1478240000

3a $NH_4^-(H_2O)_3$

H	0.8329100000	-1.2581800000	-0.1379600000
H	-0.0690900000	-2.6955400000	-0.3094000000
H	-0.8568200000	-1.2093700000	-0.0238400000
H	-0.1263700000	-1.5181300000	-1.5084600000
N	-0.0514700000	-1.6848100000	-0.4917500000
O	0.0551900000	1.6841800000	-0.4498500000
H	0.0625600000	2.6573300000	-0.4153500000
H	-0.1012800000	1.4814900000	-1.3964800000
O	-1.9894200000	0.0040700000	0.6475800000
H	-2.7281800000	0.0655600000	0.0228700000
H	-1.4324700000	0.7732300000	0.4110300000
O	2.0767700000	-0.0838400000	0.4521900000
H	2.0793100000	-0.0405000000	1.4184500000
H	1.5593100000	0.7024700000	0.1820300000

3b $NH_4^-(H_2O)_3$

H	-0.5979500000	0.7611100000	0.7877500000
H	0.0501400000	0.0530800000	2.1921700000
H	-0.2557600000	-0.8790800000	0.8029200000
H	1.0039300000	0.2356000000	0.7943100000
N	0.0539800000	0.0451600000	1.1707000000
O	2.4313500000	0.4821900000	-0.3353100000

H	2.5698300000	-0.4018000000	-0.7184600000
H	1.9963300000	0.9590100000	-1.0664400000
O	-0.7727800000	-2.2229400000	-0.2923900000
H	-1.6418900000	-1.9277400000	-0.6216200000
H	-0.1912000000	-2.0703900000	-1.0618600000
O	-1.6342300000	1.7511300000	-0.3264400000
H	-2.3943200000	1.1731200000	-0.5206100000
H	-1.1117900000	1.6980100000	-1.1498500000

3c $NH_4^-(H_2O)_3$

H	0.7635500000	1.3651200000	-0.1725800000
H	-0.2043000000	2.0065800000	-1.4267000000
H	-0.9078000000	1.1567300000	-0.1503800000
H	-0.2663300000	2.6929700000	0.1095500000
N	-0.1461100000	1.8157400000	-0.4155100000
O	0.3165600000	-1.8773400000	-0.3961200000
H	-0.5229900000	-1.5051500000	-0.0631600000
H	0.2167600000	-1.8101800000	-1.3555700000
O	-1.9136100000	-0.2789600000	0.4042600000
H	-2.7421400000	-0.2497700000	-0.1124700000
H	-2.1851500000	-0.0716000000	1.3205200000
O	2.0192600000	0.1736800000	0.3966700000
H	1.9740600000	0.2054200000	1.3616300000
H	1.5194400000	-0.6393300000	0.1592800000

$NH_4^-(H_2O)_4$ isomers:

$H^-(NH_3)(H_2O)_4$

H	-0.4897310000	0.5800880000	-1.5510710000
H	1.3849140000	0.6256070000	-1.3431630000
H	2.3603410000	1.5763050000	-0.4668160000
N	2.3344920000	0.6850340000	-0.9502670000
O	1.3998430000	-1.0773940000	1.1993630000
H	1.9230140000	-0.6170240000	0.5169200000
H	0.6648570000	-1.4500020000	0.6723580000
O	-0.7183810000	-1.7356780000	-0.5754980000
H	-0.5573550000	-0.8719510000	-1.0652820000
H	-1.5791090000	-1.5363790000	-0.1824460000
O	-0.1986520000	1.4392200000	0.9306160000
H	0.2932950000	0.6707750000	1.2651790000
H	-0.2844060000	1.2150170000	-0.0308070000
O	-2.8090240000	0.4825050000	-0.1923250000
H	-2.1176940000	0.5573350000	-0.8903970000
H	-2.3107380000	0.8383390000	0.5578270000
H	2.9808710000	0.7474260000	-1.7276820000

$[NH_4^-](H_2O)_4$

H	1.8191220000	2.2250390000	0.7357750000
H	3.0173250000	3.2472410000	0.0599260000

N	2.6562050000	2.2692350000	0.1128100000
O	-4.1419300000	0.6990930000	0.0876590000
H	-3.8542450000	1.3361540000	0.7463830000
H	-3.3009000000	0.3169030000	-0.2315920000
O	-1.6753810000	-0.3109920000	-0.8123880000
H	-1.1067820000	0.3824260000	-1.1669060000
H	-1.1024100000	-0.7517130000	-0.1502410000
O	0.0837880000	-1.4203610000	1.0537950000
H	0.3400990000	-0.6447900000	1.5699120000
H	0.8912710000	-1.6035910000	0.5318610000
O	2.4321120000	-1.6819920000	-0.5020260000
H	2.2492380000	-1.0254570000	-1.1933070000
H	3.0891640000	-1.2142560000	0.0387470000
H	2.3832060000	1.9315190000	-0.8400760000
H	3.3927690000	1.6298880000	0.4935310000

4a $NH_4^-(H_2O)_4$

H	0.8453700000	-0.8593800000	-1.1480000000
H	0.0000200000	0.5224200000	-1.5558900000
H	-0.0000100000	-0.7800600000	-2.6265800000
H	-0.8453900000	-0.8593500000	-1.1479900000
N	0.0000000000	-0.5094500000	-1.6433200000
O	2.0373300000	-1.0931100000	0.2217300000
H	2.7548100000	-0.4579300000	0.0863200000
H	1.4857600000	-0.6734300000	0.9124300000
O	-2.0373600000	-1.0930500000	0.2217000000
H	-1.4857700000	-0.6733900000	0.9124000000
H	-2.7548200000	-0.4578600000	0.0863000000
O	0.0000400000	2.0533100000	-0.4214700000
H	-0.7762600000	2.6377400000	-0.5390000000
H	0.7763500000	2.6377300000	-0.5390200000
O	-0.0000100000	0.2444300000	1.6560700000
H	-0.0001000000	0.5931200000	2.5581700000
H	0.0000200000	1.0439300000	1.0798600000

4b $NH_4^-(H_2O)_4$

H	-0.2311900000	0.8438600000	-1.1882500000
H	-1.5523300000	-0.0008200000	-0.5581000000
H	-1.2729000000	-0.0007600000	-2.2289800000
H	-0.2305000000	-0.8446000000	-1.1882100000
N	-0.8282400000	-0.0006300000	-1.3115700000
O	0.9366100000	2.0733800000	-0.5835600000
H	1.3246100000	1.4987400000	0.1088000000
H	0.4247400000	2.7161700000	-0.0699900000
O	0.9392000000	-2.0723200000	-0.5833500000
H	1.3253100000	-1.4969100000	0.1094600000
H	0.4284600000	-2.7164500000	-0.0703700000
O	-2.5565600000	-0.0011500000	0.8905900000

H	-2.2309500000	-0.7608300000	1.4121000000
H	-2.2316600000	0.7590300000	1.4118500000
O	1.5592300000	0.0008100000	1.2446300000
H	0.7420600000	0.0010700000	1.7917200000
H	2.2741300000	0.0001600000	1.9045000000

4c $NH_4^-(H_2O)_4$

H	0.4478000000	0.8702800000	1.7807800000
H	-0.3008500000	1.6389200000	0.4619100000
H	0.8744400000	2.4472100000	1.4002800000
H	1.3254800000	1.1688900000	0.3723200000
N	0.5838800000	1.5453700000	1.0062200000
O	-1.7104400000	1.4498100000	-0.6569700000
H	-1.9229800000	0.5056300000	-0.4649400000
H	-1.3871200000	1.4404600000	-1.5657700000
O	2.2893100000	0.2350700000	-0.7997600000
H	1.8399300000	-0.6193300000	-0.6277700000
H	3.1708400000	0.1069000000	-0.4196400000
O	-2.0738900000	-1.1740100000	0.0522400000
H	-1.1650600000	-1.5334100000	-0.0050700000
H	-2.2354800000	-1.1732400000	1.0068300000
O	0.6787700000	-1.8996400000	0.1417600000
H	0.9673500000	-2.8224200000	0.0184800000
H	0.8285600000	-1.7374400000	1.1008500000

4d $NH_4^-(H_2O)_4$

H	-0.9423200000	-1.3115200000	0.2721700000
H	-0.6032600000	-0.3885900000	-1.0418300000
H	0.6679000000	-1.2824100000	-0.3485400000
H	-0.5748800000	-2.0575900000	-1.2019200000
N	-0.3507300000	-1.2780900000	-0.5760900000
O	2.3995700000	-1.1301300000	-0.0742100000
H	2.8338100000	-1.1370600000	-0.9377400000
H	2.4220600000	-0.1804400000	0.1935600000
O	2.1904800000	1.5432400000	0.5752400000
H	1.4866400000	1.6074600000	1.2453200000
H	1.7497300000	1.9191400000	-0.2090500000
O	-1.8215500000	1.1457100000	-1.0196900000
H	-2.0050500000	1.4236600000	-1.9347200000
H	-1.2067800000	1.8323800000	-0.6834300000
O	-2.3827100000	-0.5125700000	1.2847000000
H	-2.5280500000	0.1473900000	0.5815600000
H	-1.9310000000	0.0042000000	1.9689400000

4e $NH_4^-(H_2O)_4$

H	1.1555800000	-0.5054800000	-0.9570400000
H	0.4476000000	0.9987900000	-0.6414900000

H	-0.3682500000	-0.1104800000	-1.6427900000
H	-0.2180000000	-0.3901800000	-0.0081000000
N	0.2592700000	-0.0034000000	-0.8461900000
O	-1.1288000000	-0.9159700000	1.4776700000
H	-0.9638400000	-0.1508800000	2.0670100000
H	-0.5569600000	-1.6167300000	1.8490500000
O	-2.7355800000	-0.3319500000	-0.9021400000
H	-2.4630500000	-0.6807500000	-0.0365400000
H	-3.0037700000	0.5718800000	-0.6928600000
O	2.7287900000	-1.3311200000	-0.3462000000
H	2.3793700000	-2.0412300000	0.2206900000
H	3.0279200000	-0.6746200000	0.3080800000
O	0.8050500000	2.5402700000	0.2427200000
H	1.4055000000	2.2121200000	0.9389800000
H	-0.0126600000	2.7214100000	0.7418900000