Supporting information

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Figure S22-S25. Calculated equilibrium structures (in Å and degrees) of **$AmaH^+$(I,II)$(H_2O)_n$(I-VI)** in their ground electronic state (B3LYP-D3/cc-pVTZ). **(S22) H_2O**, **Ama**, **$AmaH^+$(I,II)**, and **$AmaH^+$(I,II)(H_2O)(I,II); (S23) $(H_2O)_2$**, **$AmaH^+$(I)$(H_2O)_2$(I-III)** and **$AmaH^+$(II)$(H_2O)_2$(I,II); (24) $AmaH^+$(I)$(H_2O)_3$(I-IV) (25) $AmaH^+$(I)$(H_2O)_4$(I,II)** and **$AmaH^+$(I)$(H_2O)_4$(IV-VI).**

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Figure S31. Plot of the calculated binding energies (D_0) for the observed **$AmaH^+$(I)$(H_2O)_n$** (crosses) as a function of the cluster size *n* (surface solvation). A linear line it is drawn to illustrate the decrease of the binding energies by increasing the number of water molecules. For comparison, the binding energies of **$AmaH^+$(I)$(H_2O)_{n=1-3}$** isomers are included, in which water is bound via cation-dipole forces to the adamantyl cage supported by weak CH···O contacts (interior ion solvation). The experimental value for the sublimation enthalpy of bulk ice suggests that D_0 of larger **$AmaH^+$(I)$(H_2O)_n$** clusters converges to this value.

Figure S32. Plots of various calculated and experimental properties of the O-H bonds of the most stable $AmaH^+(H_2O)_n$ clusters as a function of the cluster size *n*: calculated O-H bond lengths (r_{OH}); calculated second-order perturbation energies ($E^{(2)}$) of donor-acceptor orbital interactions involved in the H-bonds; calculated and experimental OH stretch frequencies (ν_{OH2}). Symbols denote individual data points, while the connected points correspond to the values of the assigned isomers. A colour code is used for different ν_{OH2} modes: $\nu_{OH2}{}^a$ (orange); $\nu_{OH2}{}^f$ (blue); $\nu_{OH2}{}^s$ (brown); $\nu_{OH2}{}^b$ ring (green); $\nu_{OH2}{}^b$ dimer (red); $\nu_{OH2}{}^b$ extended ring (magenta); $\nu_{OH2}{}^b$ trimer (cyan). Experimental observed peaks associated with ν_{OH2} modes are labeled (**K**, **M**, **S**, **T**, **W**, **X**, **Y**, **Z**).

Figure S33. Plot of the partial charge of the adamantly cage ($C_{10}H_{15}$) and C-N bond length for the identified $AmaH^+$(**I**)$(H_2O)_n$ clusters as a function of the cluster size *n*. The corresponding values of the neutral **Ama** are drawn as dashed lines. Linear extrapolations to larger clusters suggest that proton transfer could occur for *n*=11-13. However, the real trend will be nonlinear and thus this cluster size will only be a lower limit for proton transfer to solvent.

Cartesian coordinates (in Å) and energies (in hartree) of all relevant structures

Detailed description of the I-$(H_2O)_3$(I-IV) isomers

I-$(H_2O)_3$(I)

In **I-$(H_2O)_3$(I)** (C_s), three water molecules and the NH_3^+ group form a cyclic ring via two O-H···O H-bonds (1.932 Å, 162.1°) and two N-H···O H-bonds (1.765 Å, 162.5°) with a binding energy of 190.42 kJ mol^{-1}. Two H_2O ligands act as single-donor single-acceptor molecules in the NH···O and OH···O H-bonds, while the terminal water closes the ring as a double-acceptor ligand in OH···O H-bonds, resulting in less linear NH···O (162.1°) and OH···O H-bonds (162.5°). The NH_2 angles are increased to 109.1° and the N-H bonds involved are slightly more elongated at 1.038 Å compared to **I-$(H_2O)_2$(I)**. As result, the ν_{NH3}^{b} modes are more redshifted to 2982 and 2984 cm^{-1}. The remaining free N-H bond is a bit shorter with 1.018 Å compared to **I-$(H_2O)_2$(I)**, resulting in a blueshift of the ν_{NH3}^{f} mode by 10 cm^{-1} to 3307 cm^{-1}. Due to ring configuration of the three water molecules, the O-H bonds involved are slightly shorter compared to the O-H bonds of a bound $(H_2O)_2$ dimer, e.g., in **I-$(H_2O)_2$(II)** (0.971 vs. 0.979 Å), and consequently the ν_{OH}^{b} modes are less redshifted (ν_{OH2}^{b}=3509/3533 vs. 3379 cm^{-1}). The OH_2 angles are slightly smaller (107.4° vs. 107.8°), while the OH_2 angle of the terminal water is 105.6°, the same value as in **I-$(H_2O)_2$(II)**. The NBO charge analysis indicates a charge transfer from $AmaH^+$ to the water ligands of 78 m*e* and second order perturbative energy for the N-H···O H-bonds of $E^{(2)}$=67.3 kJ mol^{-1} and for O-H···O H-bonds of $E^{(2)}$=32.5/33.4 kJ mol^{-1}. Due to the three attached water molecules, the C-N bond is shortened even more by 28 mÅ to 1.516 Å compared to **I**, while the other C-C bonds and C-H bonds change only slightly (Δr_{CC}<3 mÅ, Δr_{CH}<3 mÅ).

I-$(H_2O)_3$(II)

The second isomer **I-$(H_2O)_3$(II)** (C_{3v}) has an energy difference of E_0=2.5 kJ mol^{-1} to the global minimum, however, free energy calculations at 300 K show that **I-$(H_2O)_3$(II)** is lower than the global minimum by ΔG=8.8 kJ mol^{-1}, which is due to entropic effects favoring the more flexible chain structures or singly bound water over the more rigid solvation ring of **I-$(H_2O)_3$(I)**. **I-$(H_2O)_3$(II)** has a fully solvated NH_3^+ group with N-H···O H-bond lengths of 1.840 Å, bond angles of 172.4°, and a total H_2O binding energy of 187.9 kJ mol^{-1}. The bond lengths and charge distribution indicate C_{3v} symmetry, although this could not be confirmed exactly by calculations. The N-H bonds are less stretched compared to isomers with one or two singly bonded H_2O molecules (r_{NH}=1.031 vs. 1.036 Å), e.g. **I-$(H_2O)_2$(I)**, resulting in lower redshifts of the ν_{NH3}^{b} modes to 3061, 3105, and 3107 cm^{-1}. Compared to **I-$(H_2O)_3$(I)**, the second order perturbative energies of the N-H···O H-bonds are lower with $E^{(2)}$= 50.3 kJ mol^{-1}, but the charge transfer to the H_2O ligands is larger with 84 m*e*. The bonded H_2O molecules have O-H bond lengths of 0.963 Å as in a single bonded H_2O, e.g., in **I-$(H_2O)_1$(I),** but the OH_2 bond angle is slightly smaller with 105.7°. This leads to three coupled three ν_{OH2}^{s} modes at 3745, 3745, and 3746 cm^{-1}, and three ν_{OH2}^{s} modes at 3656, 3657, and 3657 cm^{-1}. Due to fully solvated NH_3^+ group, the C-N bond is shortened even more by 29 mÅ to 1.515 Å compared to **I**, while the other C-C bonds and C-H bonds again change only slightly (Δr_{CC}<5 mÅ, Δr_{CH}<2 mÅ).

I-$(H_2O)_3$(III)

In **I-$(H_2O)_3$(III)** (E_0=4.4 kJ mol^{-1}), a water dimer and a single water are bound to the NH_3^+ group with a binding energy of D_0=186.0 kJ mol^{-1}. Just as with **I-$(H_2O)_3$(II)**, when considering the free energies ΔG= 1.2 kJ mol^{-1}, **I-$(H_2O)_3$(III)** is below the ring structure (**I-$(H_2O)_3$(I)**). The water dimer has a N-H···O H-bond length of

1.708 Å (172.6°) and a O-H···O H-bond length of 1.791 Å (168.9°) with second order perturbative energies of $E^{(2)}$= 88.0 kJ mol^{-1} and $E^{(2)}$=56.1 kJ mol^{-1}, respectively. The N-H bond involved is drastically stretched to 1.045 Å, resulting in a redshift of $\nu_{NH3}{}^{b}$ to 2872 cm^{-1} along with an increase in IR intensity. The N-H···O H-bond of the bonded single water is slightly longer (1.807 Å, 173.1°) and the N-H bond involved is shorter (1.034 Å, $E^{(2)}$=57.6 kJ mol^{-1}), resulting in a smaller redshift of the associated $\nu_{NH3}{}^{b}$ mode to 3045 cm^{-1}. The free N-H bond has a bond length of 1.019 Å and a corresponding $\nu_{NH3}{}^{f}$ mode at 3304 cm^{-1}. Due to the elongated O-H bond (0.977 Å) of the water dimer the $\nu_{OH2}{}^{b}$ mode is redshifted to 3408 cm^{-1}. The associated free O-H bond has a bond length of 0.961 Å, which leads to a $\nu_{OH2}{}^{f}$ mode at 3726 cm^{-1}. The terminal free water molecules have slightly longer O-H bond lengths of 0.963 Å and a larger OH_2 bond angle of 105.6°/105.8° than in bare water, resulting in slightly redshifted $\nu_{OH2}{}^{s}$ modes ($\nu_{OH2}{}^{s}$=3651/3654 cm^{-1}) and $\nu_{OH2}{}^{a}$ modes ($\nu_{OH2}{}^{a}$=3740/3743 cm^{-1}). The C-N bond (r_{CN}=1.518 Å) is slightly less shortened compared to **I-(H_2O)$_3$(I)** (Δr_{CN}=26 vs. 28 mÅ), but the charge transfer to water of 85 m*e* is greater.

I-(H_2O)$_3$(IV)

In **I-(H_2O)$_3$(IV)** (E_0=11.9 kJ mol^{-1}), a water trimer is bound to the $NH_3{}^{+}$ group with a N-H···O H-bond length of 1.625 Å and a bond angle of 173.6° and $E^{(2)}$=123.5 kJ mol^{-1}. The charge transfer to the bound water molecules is 75 m*e* and the binding energy is 178.5 kJ mol^{-1}. The N-H bond involved is drastically stretched by 37 mÅ to 1.059 Å, leading to a massive redshift of the $\nu_{NH3}{}^{b}$ mode to 2652 cm^{-1} together with a huge increase in IR intensity (1268 km mol^{-1}). The two remaining N-H bonds are slightly shorter than for **I**, with a length of 1.020 Å, resulting in $\nu_{NH3}{}^{s}$ at 3263 cm^{-1} and $\nu_{NH3}{}^{a}$ at 3322 cm^{-1}. The first O-H···O H-bond (1.702 Å, 168.5°, $E^{(2)}$= 82.7 kJ mol^{-1}) starting from the $NH_3{}^{+}$ group is much shorter and more linear than the second one (1.794 Å, 164.2°, $E^{(2)}$= 55.6 kJ mol^{-1}). Accordingly, the O-H bond involved (0.986 Å) of the first water is much longer than the O-H bond of the second water (0.977 Å), resulting in one $\nu_{OH2}{}^{b}$ mode being much more redshifted than the other ($\nu_{OH2}{}^{b}$=3243 vs. 3412 cm^{-1}). The free O-H bonds of these water molecules are slightly shortened to 0.960 and 0.961 Å, respectively, resulting in two $\nu_{OH2}{}^{f}$ modes at 3720 and 3727 cm^{-1}. The terminal water has a O-H bond length of 0.963 Å and a OH_2 bond angle of 105.7°, resulting in a typical $\nu_{OH2}{}^{s}$ mode at 3652 cm^{-1} and $\nu_{OH2}{}^{a}$ at 3742 cm^{-1}. The C-N bond (r_{CN}=1.523 Å) is less shortened than in the other isomers **I-(H_2O)$_3$(I-III).**

Detailed description of the I-$(H_2O)_4$(I-VI) isomers

I-$(H_2O)_4$(I,III)

The global minimum structure **I-$(H_2O)_4$(I)** and **I-$(H_2O)_4$(III)** (Figure S26) are generated by adding H_2O to the terminal H_2O of the eight-membered ring structure of **I-$(H_2O)_3$(I),** with binding energies of 243.7 and 241.1 kJ mol^{-1}, respectively. They differ mainly in orientation of the added H_2O, resulting in a small energy difference of 1.7 kJ mol^{-1}. However, if we consider the free energies, **I-$(H_2O)_3$(I)** is higher than **I-$(H_2O)_4$(III)** by ΔG=2.9 kJ mol^{-1}. The added H_2O shortens the intermolecular O-H···O H-bonds and the N-H···O H-bonds of the ring in **I-$(H_2O)_4$(I)** ($r_{OH...O}$=1.860 vs. 1.932 Å, $r_{NH...O}$=1.755 vs. 1.765 Å) and **I-$(H_2O)_4$(III)** ($r_{OH...O}$=1.837/1.850 vs. 1.932 Å, $r_{NH...O}$=1.747/1756 vs. 1.765 Å), while the N-H and O-H bonds involved in the H-bonds are further stretched (r_{OH}=0.976/0.977 vs. 0.971 Å, r_{NH} =1.040/1.041 vs. 1.038 Å). As a result, the corresponding ν_{NH3}^{b} and ν_{OH2}^{b} modes are more redshifted by $\Delta\nu_{NH3}^{b}$~40 cm^{-1} and $\Delta\nu_{OH2}^{b}$~100 cm^{-1} compared to **I-$(H_2O)_3$(I)** (**I-$(H_2O)_4$(I)**: ν_{NH3}^{b}= 2944/2948 vs. 2982/2984 cm^{-1}, ν_{OH2}^{b}=3421/3466 vs. 3509/3533 cm^{-1}; **I-$(H_2O)_4$(III)**: ν_{NH3}^{b}= 2937/2961 vs. 2982/2984 cm^{-1}, ν_{OH2}^{b}= 3404/3455 vs. 3509/3533 cm^{-1}). Moreover, the second order perturbative energies for the N-H···O H-bonds ($E^{(2)}$=72.4/72.7 vs. 67.3 kJ mol^{-1} and $E^{(2)}$=75.2/70.3 vs 67.3 kJ mol^{-1}, respectively) and for the O-H…O H-bonds ($E^{(2)}$=43.6/47.3 vs. 33.4/32.5 kJ mol^{-1} and $E^{(2)}$= 48.5/50.5 vs 33.4/32.5 kJ mol^{-1}, respectively) are also somewhat higher compared to **I-$(H_2O)_3$(I)**. In both isomers, the free O-H and N-H bonds (r_{OH}=0.961 Å, r_{NH}=1.018 Å) of the ring have the same bond lengths as in **I-$(H_2O)_3$(I)**, resulting in nearly equal frequencies of the corresponding modes (ν_{NH3}^{f}=3311 vs. 3307 cm^{-1}, ν_{OH2}^{f}=3725/3727 vs. 3727 cm^{-1}, ν_{OH2}^{f}=3727/2731 vs. 3730 cm^{-1}). In **I-$(H_2O)_4$(I),** the newly formed O-H···O H-bond ($E^{(2)}$=64.9 kJ mol^{-1}) is oriented toward the cage with a bond length of 1.752 Å and a bond angle of 173.0°, whereas in **I-$(H_2O)_4$(III)** the O-H···O H-bond ($E^{(2)}$=69.8 kJ mol^{-1}) is oriented away from the cage with a shorter bond length of 1.727 Å and a bond angle of 177.7°. The O-H bond of **I-$(H_2O)_4$(I)** involved is slightly less elongated compared to the O-H bond of **I-$(H_2O)_4$(III)** (r_{OH}=0.983 vs. 0.984 Å), resulting in a slightly smaller redshift of the ν_{OH2}^{b} mode (ν_{OH2}^{b}=3310 vs. 3291 cm^{-1}). The additional bound water increases the charge transfer to 92 m*e* and 88 m*e*, respectively. The C-N bond is shortened to 1.516 and 1.515 Å, respectively, while the lengths of the C-C bonds and C-N bonds change only slightly (Δr_{CC}<6 mÅ, Δr_{CH}<1 mÅ).

I-$(H_2O)_4$(II)

I-$(H_2O)_4$(II) is also based on the structure of **I-$(H_2O)_3$(I)**, but here the added water is bound to the free N-H bond. The water binding energy is D_0=243.1 kJ mol^{-1} and the energy difference to the global minimum is E_0=0.6 kJ mol^{-1}, but the free energy *G* is much lower than the global minimum by 7.0 kJ mol^{-1}. The water ring has almost the same O-H···O H-bonds (1.932/1.940 vs. 1.932 Å, 162.8/162.4° vs. 162.1°) as in **I-$(H_2O)_3$(I)**, while N-H···O H-bonds (1.809/1.816 vs. 1.765 Å, 159.3/161.2° vs.162.5°) are longer. The NH_2 bond angle is reduced to 105.5° and the N-H bonds involved are less elongated to 1.033/1.031 Å compared to **I-$(H_2O)_3$(I)**. As result, the ν_{NH3}^{b} modes are less redshifted to 3049 and 3068 cm^{-1}. The O-H bonds involved have almost the same bond lengths with 0.971 and 0.970 Å as **I-$(H_2O)_3$(I)**, resulting in similar ν_{OH2}^{b} modes at 3519 and 3542 cm^{-1}. The newly formed N-H···O H-bond has a bond length of 1.849 Å and a bond angle of 171.4°. The N-H bond is stretched to 1.033 Å leading to a third redshifted ν_{NH3}^{b} mode at 3123 cm^{-1}. The NBO charge analysis shows a charge transfer from $AmaH^+$ to the water ligands of 92 m*e* and second order perturbative

energies for the N-H…O H-bonds of the ring of $E^{(2)}$=53.8/56.1 kJ mol^{-1} , for the N-H···O H-bond of individually bound water of $E^{(2)}$=48.2 and for O-H···O H-bonds of $E^{(2)}$=33.0/31.5 kJ mol^{-1} (Figure S25). The C-N bond is shortened even more by 32 mÅ to 1.512 Å by the fourth attached water compared to **I**, while the other C-C bonds and C-H bonds again change only slightly (Δr_{CC}<5 mÅ, Δr_{CH}<3 mÅ).

I-(H$_2$O)$_4$(IV)

I-(H$_2$O)$_4$(IV) (E_0=4.9 kJ mol^{-1}) has a fully solvated NH_3^+ group with two individually bound water molecules and a water dimer with a binding energy of D_0=238.8 kJ mol^{-1}. Considering the free energies G, **I-(H$_2$O)$_4$(IV)** is the global minimum, being ΔG=13.2 kJ mol^{-1} lower than **I-(H$_2$O)$_4$(I)**. The two individually bound water molecules have O-H···O H-bond lengths of 1.844 and 1.853 Å and bond angles of 172.8° and 171.1°, respectively. The attached water dimer has a O-H···O H-bond length of 1.757 Å and a bond angle of 171.4°. The N-H bonds are stretched to 1.030 and 1.038 Å, resulting in a more redshifted $\nu_{NH3}{}^b$ mode at 2979 cm^{-1} and two less redshifted $\nu_{NH3}{}^b$ modes at 3095 and 3126 cm^{-1}. The O-H···O H-bond of the water dimer has bond length of 1.806 Å and a bond angle of 169.3°. The O-H bond involved is stretched to 0.976 Å, resulting in a $\nu_{OH2}{}^b$ mode at 3434 cm^{-1}. The NBO charge analysis shows a charge transfer from AmaH$^+$ to the water ligands of 98 m*e* and second order perturbative energies for the N-H…O H-bonds of the individual bound water molecules of $E^{(2)}$=47.6/49.2 kJ mol^{-1} , for the N-H···O H-bond of the water dimer of $E^{(2)}$=70.8 kJ mol^{-1}, and for O-H···O H-bond of $E^{(2)}$=52.6 kJ mol^{-1} (Figure S25). The free O-H bonds have similar bond lengths (r_{OH}=0.960-0.963 Å) as in the isomers before, resulting in three $\nu_{OH2}{}^a$ modes at 3747, 3746, and 3743 cm^{-1}, three $\nu_{OH2}{}^s$ modes at 3657, 3656, and 3653 cm^{-1} and one $\nu_{OH2}{}^f$ mode at 3730 cm^{-1}. The C-N bond is shortened to 1.513 Å by the fourth attached water compared to **I**, while the other C-C bonds and C-H bonds again change only slightly (Δr_{CC}<5 mÅ, Δr_{CH}<3 mÅ).

I-(H$_2$O)$_4$(V)

I-(H$_2$O)$_4$(V) (E_0=7.1 kJ mol^{-1}) again has a water ring structure as in **I-(H$_2$O)$_4$(I)**, but here the added water is not bound to the terminal water of the ring but to an intermediate water, with a water binding energy of D_0=236.7 kJ mol^{-1}. Due to the laterally bound water, the O-H···O H-bond and N-H···O H-bonds of the ring strongly change compared to the original structure **I-(H$_2$O)$_3$(I)** ($r_{NH...O}$=1.690/1.781 vs. 1.765 Å, $E^{(2)}{}_{NH...O}$=104.8/63.4 kJ mol^{-1}, $r_{OH...O}$=2.016/1.913 vs. 1.932 Å, $E^{(2)}{}_{OH...O}$=22.6/35.3 kJ mol^{-1}). The intermolecular bond angles are also very different, while they are approximately the same for **I-(H$_2$O)$_3$(I)** (ϕ_{NHO}=169.2 vs.161.5°, ϕ_{NHO}=158.9° vs. 161.5°, ϕ_{OHO}=163.5° vs.162.1°, ϕ_{NHO}=157.0° vs. 162.1°). In addition, the N-H bond closer to the added water is significantly more elongated than the other N-H bond involved (r_{NH}=1.051 vs 1.037 Å), resulting in a strongly redshifted $\nu_{NH3}{}^b$ mode at 2776 cm^{-1} and one less redshifted $\nu_{NH3}{}^b$ mode at 3008 cm^{-1}. The same applies to the involved O-H bonds of the ring. While one O-H bond involved of the ring has almost the same bond length of 0.972 Å as in **I-(H$_2$O)$_3$(I)**, the other O-H bond involved is much shorter with 0.968 Å, resulting in a more redshifted $\nu_{OH2}{}^b$ mode at 3505 cm^{-1} and a less redshifted $\nu_{OH2}{}^b$ mode at 3598 cm^{-1}. The newly formed OH···O H-bond is much longer ($r_{OH...O}$=1.837 vs. 1.752/1.727 Å) and is less linear (ϕ_{OHO}=164.6° vs. 173.0°/177.7°) compared to **I-(H$_2$O)$_4$(I)** or **I-(H$_2$O)$_4$(III)**. Therefore, the involved O-H bond ($E^{(2)}$=46.6 kJ mol^{-1}) is less stretched and the corresponding $\nu_{OH2}{}^b$ mode is less redshifted to 3456 cm^{-1}. The free O-H bonds have bond lengths of 0.961, 0.963, and 0.964 Å, resulting

in two ν_{OH2}^{a} modes at 3740 and 3725 cm^{-1}, two ν_{OH2}^{s} modes at 3642 and 3651 cm^{-1}, and one ν_{OH2}^{f} mode at 3728 cm^{-1}. The free N-H bond length remains the same as in **I-$(H_2O)_3$(I)**, resulting in a ν_{NH3}^{f} mode at 3311 cm^{-1}. The charge transfer to the water ligands is larger than in **I-$(H_2O)_4$(I)** or **I-$(H_2O)_4$(III)** with Δq=103 m*e* (Figure S25). The C-N bond is shortened to 1.512 Å, while the other C-C bonds and C-H bonds again change only slightly (Δr_{CC}<4 mÅ, Δr_{CH}<3 mÅ).

I-$(H_2O)_4$(VI)

In **I-$(H_2O)_4$(VI)** (C_s) two $(H_2O)_2$ dimers are bound to the NH_3^+ group via almost linear NH···O H-bonds (1.728 Å, 172.0°, $E^{(2)}$=80.0 kJ mol^{-1}). The energy difference from the global minimum is ΔE_0= 7.2 kJ mol^{-1}, however, the free energy is ΔG=-7.7 kJ mol^{-1} below the global minimum, so that this isomer must also be considered when assigning experimental bands. The N-H bonds involved are stretched to 1.042 Å, resulting in two redshifted ν_{NH3}^{b} modes at 2913 and 2929 cm^{-1}. Due to the noncooperative effects, the remaining N-H bond is shortened to 1.018 Å, leading to a ν_{NH3}^{f} mode at 3307 cm^{-1}. The attached $(H_2O)_2$ dimers have slightly shorter OH···O H-bonds and are slightly less linear (169.0° vs. 169.3°) compared to the bound $(H_2O)_2$ dimer of **I-$(H_2O)_4$(IV)** ($r_{OH..O}$=1.800 vs. 1.806 Å), while the involved O-H bonds have the same bond lengths of 0.976 Å, resulting in two ν_{OH2}^{b} modes at 3418 and 3427 cm^{-1}. The NBO charge analysis shows a charge transfer from $AmaH^+$ to the water ligands of 96 m*e* and second order perturbative energies for the O-H···O H-bonds of $E^{(2)}$=54.3 kJ mol^{-1} (Figure S25). The free O-H bonds have similar bond lengths of r_{OH}=0.960 and 0.963 Å as in the isomers before, resulting in two ν_{OH2}^{a} modes at 3741 and 3743 cm^{-1}, two ν_{OH2}^{s} modes at 3652 and 3653 cm^{-1}, and two ν_{OH2}^{f} modes at 3730 cm^{-1}. The C-N bond (r_{CN}=1.515 Å) is slightly less shortened compared to isomers **I-$(H_2O)_4$(II-VI)**, while the other C-C and C-H bonds again change only slightly (Δr_{CC}<4 mÅ, Δr_{CH}<3 mÅ).

Table S1. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of **Ama** compared to calculated vibrational frequencies of **$AmaH^+$(I-IV)**. In bold are the convoluted calculated bands. Stretching (ν), bending (β), torsing (τ), wagging (γ), rocking (ρ).

Mode of Ama	**Ama**	Mode of $AmaH^+$	**$AmaH^+$(I)**	**$AmaH^+$(II)**	**$AmaH^+$(III)**	**$AmaH^+$(IV)**
τ_{CH2}, γ_{CH2}	**1256** 1256 (4) 1274 (0.0) 1277 (0.2) 1279 (0.0)	τ_{CH2}, ρ_{CH2}	**1117** 1117 (6) 1117 (6) 1118 (0) 1127 (0)	**1113** 1112 (0.3) 1113 (15)	**1106** 1106 (8) 1116 (1) 1123 (2)	**1117** 1108 (0.7) 1117 (22) 1134 (2)
		τ_{CH2},		**1156** (2)	**1150** (4)	**1151** (0.8)
		τ_{CH2}	**1206** 1206 (4) 1206 (4)	**1203** 1199 (0.2) 1203 (15)	**1192** 1192 (29) 1203 (2) 1214 (0.1)	
γ_{CH2}	**1308** 1308 (5) 1311 (1) 1313 (1) 1319 (0.0) 1320 (0.0)	τ_{CH2}		**1251** 1248 (2) 1253 (2)	**1235** (15)	**1220** 1197 (0.9) 1220 (5)
		τ_{CH2}, γ_{CH2},	**1294** 1278 (0.02) 1278 (0.02) 1285 (0) 1294 (27) 1297 (0.5) 1297 (0.5) 1321 (0.1) 1321 (0.1) 1325 (0)	**1297** 1283 (3) 1297 (14) 1302 (2) 1314 (1.4) 1324 (2) 1330 (1)	**1281** 1281 (10) 1285 (1) 1300 (0.8) **1307** 1307 (4) 1314 (1) 1327 (0.4)	**1279** 1261 (1) 1267 (0.2) 1279 (3) 1299 (3) **1324** 1315 (2) 1324 (10) 1334 (1) 1340 (8)
τ_{CH2}, γ_{CH2}, τ_{NH2}	**1360** 1342 (0.2) 1351 (1) 1358 (3) 1364 (2) 1373 (0.1)	τ_{CH2}, γ_{CH2},	**1359** 1355 (0.7) 1355 (0.7) 1359 (18) 1371 (0.7) 1371 (0.7)	**1346** 1346 (13) 1355 (1) 1356 (2) 1369 (1)	**1349** 1338 (0.5) 1349 (2) 1357 (0.5) 1369 (0.4)	
β_{CH2}	**1461** 1446 (0.0) 1448 (0.0) 1461 (8) 1461 (10) 1463 (8) 1486 (0.1)	ρ_{NH2} γ_{CH3} (umbrella), γ_{CH2}, β_{CH2}		**1415** 1390 (16) 1393 (2) 1409 (12) 1417 (23)	**1396** 1392 (4) 1397 (10)	**1384** 1356 (1) 1364 (3) 1365 0.1) 1368 (1) 1382 (33) 1395 (6) 1399 (19) 1401 (0.3)
		$\gamma_{NH3\ (umbrella)}$, β_{CH2}	**1441** 1441 (130) 1450 (0.1) 1450 (0.1)		**1441** 1436 (17) 1443 (21)	**1455** 1452 (4) 1452 (13) 1459 (2) 1469 (12) 1476 (5)
		β_{CH3}, β_{CH2}	**1469** 1463 (13) 1463 (13) 1472 (39)	**1462** 1450 (4) 1453 (10) 1463 (8)	**1467** 1455 (0.2) 1462 (8) 1465 (6)	

			1493 (7)	1465 (10) 1476 (9)	1469 (16) 1474 (7)	
β_{NH2}	**1609** (34)	β_{NH3}	**1611** 1611 (39) 1611 (39)			
		ν_{CN} [b]		**1534** (7)	**1541** (3)	**1534** (5)
		β_{NH2} [b]		**1664** (219)	**1669** (206)	**1665** (203)
ν_{CH}, ν_{CH2}	**2890** 2880 (15) 2885 (28) 2890 (60) 2891 (4) 2892 (19) 2893 (28)	ν_{CH}		**2848** (60)		
		$\nu_{CH/CH2}$	**2899** 2892 (11) 2892 (12) 2899 (47) 2916 (25) 2916 (25) 2917 (0.3) 2930 (0)		**2882** 2883 (24) 2884 (9)	**2874** 2871 (8) 2876 (11)
	2917 2913 (113) 2914 (68) 2916 (92) 2922 (28) 2926 (12) 2926 (46) 2932 (100) 2936 (5) 2941 (81)	ν_{CH2}		**2913** 2885 (5) 2891 (10) 2908 (19) 2910 (4) 2915 (37) 2917 (9)	**2917** 2904 (6) 2913 (0.4) 2915 (33) 2919 (9) 2929 (17)	**2916** 2911 (3) 2913 (20) 2914 (22) 2924 (10) 2930 (17)
		ν_{CH2}	**2956** 2935 (34) 2935 (34) 2953 (38) 2953 (38) 2955 (0) 2958 (1) 2958 (1) 2964 (43)	**2952** 2942 (10) 2944 (19) 2952 (6) 2953 (14) 2954 (26) 2955 (7) 2966 (13)	**2972** 2954 (0.3) 2955 (8) 2666 (17) 2969 (25) 2971 (9) 2972 (9) 2974 (9) 2977 (21) 2983 (16)	**2948** 2944 (20) 2946 (2) 2948 (0.6) 2948 (14) 2949 (6) 2950 (31) 2966 (15)
		ν_{CH3}		**2977** 2977 (25) 2982 (18)		**2998** 2979 (16) 2998 (50)
ν_{NH} [s]	**3285** (3)	ν_{NH3} [s]	**3214** (26)			
		ν_{NH2} [s]		**3331** (136)	**3330** (129)	**3329** (129)
ν_{NH} [a]	**3359** (0.2)	ν_{NH3} [a]	**3301** 3301 (52) 3301 (52)			
		ν_{NH2} [a]		**3435** (77)	**3433** (76)	**3432** (78)

[a] IR intensities in km/mol are given in parentheses. [b] Coupled β_{NH2}/ν_{CN} modes.

Table S2. Various energies of the **AmaH$^+$(I-IV)** isomers calculated at the B3LYP-D3/cc-pVTZ level. Energies are given in kJ/mol.

	E_0	E_e	G
AmaH$^+$(I)	0	0	0
AmaH$^+$(II)	3.03	15.72	-4.73
AmaH$^+$(III)	27.39	39.42	18.09
AmaH$^+$(IV)	29.50	42.50	20.76
TS I-IV	262.90	287.47	259.58
TS III-IV	43.48	56.33	35.97

Table S3. Various energies of the **AmaH$^+$(I-IV)H_2O(I-IV)** isomers calculated at the B3LYP-D3/cc-pVTZ level. Energies are given in kJ/mol.

	E_0	E_e	E_0^{total}	G^{total}	D_0
I-H_2O(I)	0	0	0	0	70.87
I-H_2O(II)	44.78	47.46	44.78	41.47	26.09
II-H_2O(I)	0	0	8.34	3.28	65.56
II-H_2O(II)	22.32	23.45	30.67	23.75	43.23
II-H_2O(III)	35.12	36.94	43.46	35.19	30.44
II-H_2O(IV)	44.18	47.68	52.52	47.34	21.38
III-H_2O(I)	0	0	31.96	26.02	66.30
III-H_2O(II)	25.86	27.55	57.85	49.50	40.45
III-H_2O(III)	35.76	38.28	67.72	58.57	30.54
IV-H_2O(I)	0	0	34.80	29.01	65.58
IV-H_2O(II)	22.03	23.36	56.82	50.18	43.55
IV-H_2O(III)	35.53	38.56	70.33	57.16	30.05
IV-H_2O(IV)	36.78	36.78	71.58	61.66	28.80

Table S4. Various energies of the **AmaH$^+$(I-IV)$(H_2O)_2$(I-VIII)** isomers calculated at the B3LYP-D3/cc-pVTZ level. Energies are given in kJ/mol.

	E_0	E_e	E_0^{total}	G^{total}	D_0
I-$(H_2O)_2$(I)	0	0	0	0	133.14
I-$(H_2O)_2$(II)	4.85	1.97	4.85	6.84	128.45
I-$(H_2O)_2$(III)	7.00	3.95	7.00	12.17	126.30
I-$(H_2O)_2$(IV)	38.03	40.48	38.03	29.84	95.27
I-$(H_2O)_2$(V)	38.77	40.58	38.77	37.72	94.53
I-$(H_2O)_2$(VI)	69.80	68.80	69.80	73.13	63.50
I-$(H_2O)_2$(VII)	74.23	74.23	74.23	65.24	59.07
II-$(H_2O)_2$(I)	0	0	13.52	12.65	122.66
II-$(H_2O)_2$(II)	5.07	2.73	18.59	12.41	117.58
II-$(H_2O)_2$(III)	18.34	20.20	31.86	20.09	104.31
II-$(H_2O)_2$(IV)	25.49	24.47	39.01	28.35	97.16
II-$(H_2O)_2$(V)	31.04	33.77	44.56	39.46	91.61
II-$(H_2O)_2$(VI)	32.76	32.12	46.27	40.27	89.90
II-$(H_2O)_2$(VII)	50.60	54.84	64.12	45.00	72.05
III-$(H_2O)_2$(I)	0	0	36.15	33.94	124.39
III-$(H_2O)_2$(II)	5.40	3.53	41.55	40.57	118.99
III-$(H_2O)_2$(III)	7.76	5.97	43.90	40.84	116.63
III-$(H_2O)_2$(IV)	20.23	21.96	56.37	52.06	104.16
III-$(H_2O)_2$(V)	22.31	24.80	58.45	52.52	102.08
III-$(H_2O)_2$(VI)	29.63	32.18	65.77	60.54	94.76
III-$(H_2O)_2$(VII)	53.64	54.02	89.79	87.59	70.75
III-$(H_2O)_2$(VIII)	54.28	58.16	90.43	83.87	70.11
III-$(H_2O)_2$(IX)	54.88	59.69	91.02	83.36	69.51
IV-$(H_2O)_2$(I)	0	0	39.12	36.15	123.53
IV-$(H_2O)_2$(II)	6.08	3.96	45.20	42.20	117.44
IV-$(H_2O)_2$(III)	7.28	5.27	46.40	43.22	116.25
IV-$(H_2O)_2$(IV)	9.44	7.03	48.56	47.12	114.08
IV-$(H_2O)_2$(V)	18.35	20.45	57.47	51.78	105.17
IV-$(H_2O)_2$(VI)	23.43	22.46	62.54	62.06	100.10
IV-$(H_2O)_2$(VII)	26.64	29.02	65.76	64.09	96.88

Table S5. Various energies of the **AmaH$^+$(I-IV)(H$_2$O)$_3$(I-X)** isomers calculated at the B3LYP-D3/cc-pVTZ level. Energies are given in kJ/mol.

	E_0	E_e	E_0^{total}	G^{total}	D_0
I-(H$_2$O)$_3$(I)	0	0	0	0	190.42
I-(H$_2$O)$_3$(II)	2.48	9.79	2.48	-8.83	187.94
I-(H$_2$O)$_3$(III)	4.42	8.54	4.42	-1.16	186.00
I-(H$_2$O)$_3$(IV)	11.94	13.80	11.94	12.82	178.48
I-(H$_2$O)$_3$(V)	12.78	13.78	12.78	14.37	177.64
I-(H$_2$O)$_3$(VI)	15.79	19.30	15.79	9.77	174.62
I-(H$_2$O)$_3$(VII)	32.78	42.14	32.78	18.12	157.64
I-(H$_2$O)$_3$(VIII)	35.29	44.92	35.29	22.77	155.13
I-(H$_2$O)$_3$(IX)	39.34	46.22	39.34	29.97	151.08
II-(H$_2$O)$_3$(I)	0	0	21.46	13.38	171.99
II-(H$_2$O)$_3$(II)	2.68	3.06	24.14	11.83	169.32
II-(H$_2$O)$_3$(III)	5.84	2.60	27.30	24.48	166.15
II-(H$_2$O)$_3$(IV)	5.86	2.95	27.32	22.93	166.13
II-(H$_2$O)$_3$(V)	10.15	10.11	31.61	21.65	161.84
II-(H$_2$O)$_3$(VI)	11.59	6.35	33.04	31.15	160.40
II-(H$_2$O)$_3$(VII)	12.41	7.57	33.87	32.13	159.59
II-(H$_2$O)$_3$(VIII)	12.87	7.46	34.33	29.82	159.12
II-(H$_2$O)$_3$(IX)	13.83	17.99	35.29	22.92	158.16
III-(H$_2$O)$_3$(I)	0	0	44.24	34.83	173.57
III-(H$_2$O)$_3$(II)	2.24	2.89	46.49	33.18	171.33
III-(H$_2$O)$_3$(III)	7.46	4.76	51.70	46.95	166.11
III-(H$_2$O)$_3$(IV)	9.84	10.52	54.08	42.06	163.73
III-(H$_2$O)$_3$(V)	14.90	18.74	59.14	45.76	158.67
III-(H$_2$O)$_3$(VI)	18.71	19.96	62.95	52.74	154.86
III-(H$_2$O)$_3$(VII)	20.89	23.53	65.13	50.04	152.68
III-(H$_2$O)$_3$(VIII)	21.21	23.15	65.45	54.24	152.36
III-(H$_2$O)$_3$(IX)	22.66	27.62	66.90	52.41	150.92
III-(H$_2$O)$_3$(X)	29.31	32.82	73.56	57.68	144.26
IV-(H$_2$O)$_3$(I)	0	0	47.37	36.71	172.55
IV-(H$_2$O)$_3$(II)	2.50	1.56	49.87	39.79	170.05
IV-(H$_2$O)$_3$(III)	2.75	15.5	50.13	40.39	169.80
IV-(H$_2$O)$_3$(IV)	5.67	2.63	53.05	46.16	166.87
IV-(H$_2$O)$_3$(V)	6.09	2.48	53.47	49.02	166.46
IV-(H$_2$O)$_3$(VI)	7.39	6.01	54.77	41.67	165.16
IV-(H$_2$O)$_3$(VII)	7.51	4.79	74.88	49.30	165.04
IV-(H$_2$O)$_3$(VIII)	8.97	5.71	56.35	50.55	163.57

IV-$(H_2O)_3$(IX)	10.75	10.26	58.13	47.66	161.79
IV-$(H_2O)_3$(X)	11.61	8.68	58.99	51.91	160.93

Table S6. Various energies of the **AmaH$^+$(I-IV)(H$_2$O)$_4$(I-X)** isomers calculated at the B3LYP-D3/cc-pVTZ level. Energies are given in kJ/mol.

	E_0	E_e	E_0^{total}	G^{total}	D_0
I-(H$_2$O)$_4$(I)	0	0	0	0	243.71
I-(H$_2$O)$_4$(II)	0.63	4.94	0.63	-7.01	243.08
I-(H$_2$O)$_4$(III)	1.74	2.93	1.74	-2.92	241.97
I-(H$_2$O)$_4$(IV)	4.92	14.76	4.92	-13.17	238.79
I-(H$_2$O)$_4$(V)	7.05	9.28	7.05	2.97	236.65
I-(H$_2$O)$_4$(VI)	7.20	12.99	7.20	-7.69	236.51
I-(H$_2$O)$_4$(VII)	9.04	13.11	9.04	2.42	234.67
I-(H$_2$O)$_4$(VIII)	9.65	5.59	9.65	14.61	234.05
I-(H$_2$O)$_4$(IX)	9.79	14.73	9.79	1.52	233.91
I-(H$_2$O)$_4$(X)	10.48	14.57	10.48	5.78	233.23
II-(H$_2$O)$_4$(I)	0	0	18.65	16.76	228.09
II-(H$_2$O)$_4$(II)	0.70	1.31	19.35	16.79	227.39
II-(H$_2$O)$_4$(III)	2.95	4.39	21.60	17.49	225.14
II-(H$_2$O)$_4$(IV)	9.19	17.11	27.84	14.64	218.90
II-(H$_2$O)$_4$(V)	9.23	17.20	27.88	14.31	218.86
II-(H$_2$O)$_4$(VI)	10.38	19.04	29.03	11.85	217.71
II-(H$_2$O)$_4$(VII)	13.52	23.17	32.17	6.49	214.57
II-(H$_2$O)$_4$(VIII)	15.36	25.59	34.01	15.61	212.73
II-(H$_2$O)$_4$(IX)	16.84	22.57	35.49	26.16	211.25
II-(H$_2$O)$_4$(X)	16.93	19.05	35.58	32.73	211.16
III-(H$_2$O)$_4$(I)	0	0	51.35	48.02	219.75
III-(H$_2$O)$_4$(II)	0.07	7.09	51.43	38.48	219.67
III-(H$_2$O)$_4$(III)	0.82	8.31	52.17	34.83	218.93
III-(H$_2$O)$_4$(IV)	7.89	12.74	59.25	50.72	211.85
III-(H$_2$O)$_4$(V)	8.29	14.39	59.64	45.66	211.46
III-(H$_2$O)$_4$(VI)	11.59	14.94	62.94	55.71	208.16
III-(H$_2$O)$_4$(VII)	11.64	18.98	62.99	48.19	208.11
III-(H$_2$O)$_4$(VIII)	12.53	24.16	63.88	45.08	207.22
III-(H$_2$O)$_4$(IX)	15.36	23.14	66.71	52.99	204.39
III-(H$_2$O)$_4$(X)	15.56	27.75	66.91	44.31	204.19
IV-(H$_2$O)$_4$(I)	0	0	51.29	47.29	221.92
IV-(H$_2$O)$_4$(II)	2.33	7.45	53.62	40.66	219.59
IV-(H$_2$O)$_4$(III)	3.07	9.08	54.36	37.66	218.85
IV-(H$_2$O)$_4$(IV)	4.85	10.80	56.14	39.25	217.07
IV-(H$_2$O)$_4$(V)	6.73	8.68	58.02	49.51	215.19
IV-(H$_2$O)$_4$(VI)	9.28	16.44	60.57	43.32	212.64

IV-$(H_2O)_4$(VII)	9.39	12.88	60.68	50.24	212.53
IV-$(H_2O)_4$(VIII)	13.67	16.05	64.96	55.95	208.25
IV-$(H_2O)_4$(IX)	13.97	20.13	65.26	53.03	207.95
IV-$(H_2O)_4$(X)	14.23	19.85	65.52	45.73	207.69

Table S7. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of **AmaH$^+$(I-IV)** compared to experimental values of AmaH$^+$Ar (Figure 1 and 2).[a] Maxima of convoluted bands are given in bold. The experimental values are given with peak width (fwhm in parenthesis) and are assigned to the most dominant vibrations.

Mode[b]	**AmaH$^+$(I)** C_{3v}	**AmaH$^+$(II)** C_s	**AmaH$^+$(III)** C_s	**AmaH$^+$(IV)** C_S	AmaH$^+$Ar
ν_{CH}		**2848** (60)			**C** 2853 (10)
$\nu_{CH/CH2}$	**2899** 2892 (11) 2892 (12) 2899 (47) 2916 (25) 2916 (25) 2917 (0.3) 2930 (0)		**2882** 2883 (24) 2884 (9)	**2874** 2871 (8) 2876 (11)	**D** 2872 (7)
ν_{CH2}		**2913** 2885 (5) 2891 (10) 2908 (19) 2910 (4) 2915 (37) 2917 (9)	**2917** 2904 (6) 2913 (0.4) 2915 (33) 2919 (9) 2929 (17)	**2916** 2911 (3) 2913 (20) 2914 (22) 2924 (10) 2930 (17)	**E** 2921 (14)
ν_{CH2}	**2956** 2935 (34) 2935 (34) 2953 (38) 2953 (38) 2955 (0) 2958 (1) 2958 (1) 2964 (43)	**2952** 2942 (10) 2944 (19) 2952 (6) 2953 (14) 2954 (26) 2955 (7) 2966 (13)		**2948** 2944 (20) 2946 (2) 2948 (0.6) 2948 (14) 2949 (6) 2950 (31) 2966 (15)	**F** 2949 (17)
ν_{CH3}		**2977** 2977 (25) 2982 (18)	**2972** 2954 (0.3) 2955 (8) 2666 (17) 2969 (25) 2971 (9) 2972 (9) 2974 (9) 2977 (21) 2983 (16)	**2998** 2979 (16) 2998 (50)	**G** 2973 (5)
$2\beta_{NH3}$	3222				**L** 3164 (7) **M** 3185 (5)
ν_{NH3}^{s}	**3214** (26)				**N** 3238 (13)
ν_{NH3}^{a}	**3301** 3301 (52) 3301 (52)				**P** 3317 (21)
ν_{NH2}^{s}		**3331** (136)	**3330** (129)	**3329** (129)	**Q** 3344 (7)
$2\beta_{NH2}$[c]		3328	3338	3330	**U** 3428 (11)
ν_{NH2}^{a}		**3435** (77)	**3433** (76)	**3432** (78)	**V** 3451 (10)

[a] IR intensities in km mol^{-1} are given in parentheses. [b] Stretching (ν), bending (β), [c] Coupled β_{NH2}/ν_{CN} modes.

Table S8. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of **I-$(H_2O)_2$(I-III)** and **II-$(H_2O)_2$(I,II)** compared to experimental values of $AmaH^+(H_2O)_2$ (Figure 5).[a] The experimental values (peak maxima) are given with peak width (fwhm in parenthesis) and are assigned to the most dominant vibrations.

$AmaH^+(H_2O)_2$	Mode [b]	**I-$(H_2O)_2$(I)** C_s	**I-$(H_2O)_2$(II)**	**I-$(H_2O)_2$(III)**	**II-$(H_2O)_2$(I)**	**II-$(H_2O)_2$(II)**
A 2754 (24)	ν_{NH3} [b]		2745 (1139)			
C 2863 (16)	$\nu_{CH/CH2}$	2892 (7)	2891 (16)	2891 (11)	2870 (39)	2884 (39)
		2896 (40)	2899 (19)	2895 (22)	2887 (3)	2890 (2)
			2903 (38)	2900 (48)	2892 (7)	2898 (18)
D 2871 (14)	$\nu_{CH/CH2}$	2906 (27)	2913 (26)	2910 (28)	2902 (20)	2904 (18)
		2910 (32)	2914 (17)	2913 (24)	2905 (12)	2907 (9)
		2912 (28)	2915 (13)	2914 (8)	2912 (48)	2912 (44)
		2912 (2)			2912 (6)	2915 (14)
E 2911 (13)	$\nu_{CH/CH2}$	2938 (2)	2930 (26)	2929 (22)	2936 (15)	2938 (25)
		2941 (24)		2937 (19)	2940 (31)	
F 2939 (20)	$\nu_{CH/CH2}$, FR [c]	2944 (55)	2943 (63)	2944 (41)	2944 (29)	2945 (31)
		2945 (25)	2945 (20)	2947 (44)	2946 (17)	2947 (14)
		2947 (52)	2949 (24)	2949 (17)	2959 (24)	2948 (82)
		2948 (1)	2952 (2)	2950 (10)	2973 (28)	2954 (90)
		2951 (5)	2953 (1)	2953 (4)	2973 (4)	2961 (25)
		2953 (8)	2954 (3)	2954 (5)	2974 (4)	2973 (33)
	ν_{NH2} [b]					2914 (1010)
G 2977 (11)	ν_{CHn}	2958 (65)	2958 (43)	2959 (65)	2975 (23)	2976 (33)
			2958 (64)			2986 (8)
	ν_{NH3} [b]	3007 (487)		2953 (688)		
J 3069 (39)	ν_{NH3} [b]	3007 (487)				
		3033 (790)				
	ν_{NH2} [b]				3088 (760)	
K 3127 (24)	ν_{NH3} [b]	3033 (790)		3188 (156)		
	$2\beta_{OH2}$, FR [c]		3116			
	ν_{NH2} [b]				3178 (857)	
M 3230 (40)	$2\beta_{OH2}$	3200	3243			
		3208				
	$2\beta_{NH3}$	3293	3257			
		3348	3258			
N 3288 (5)	ν_{NH3} [s]		3262 (51)			
O 3315 (12)	ν_{NH3} [f]	3297 (38)		3309 (61)		
P 3331 (3)	ν_{NH3} [a]		3320 (35)			
T 3403 (39)	ν_{OH2} [b]		3379 (541)			3399 (544)
	ν_{NH2} [f]					3390 (68)
X 3638 (22)	ν_{OH2} [s]	3653 (56)	3648 (36)	3615 (99)	3652 (43)	3650 (31)
		3654 (37)		3640 (25)	3653 (40)	
Y 3683 (8)	ν_{OH2} [f]		3725 (123)			3725 (124)
Z 3716 (27)	ν_{OH2} [a]	3740 (49)	3735 (101)	3723 (104)	3740 (45)	3738 (95)
		3741 (162)		3736 (147)	3741 (162)	

[a] IR intensities in km/mol are given in parentheses. [b] Stretching (ν), bending (β). [c] FR = Fermi resonance with ν_{NH3} [b].

Table S9. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of **I-$(H_2O)_3$(I-IV)** compared to experimental values of $AmaH^+(H_2O)_3$ (Figure 7).[a] The experimental values (peak maxima) are given with peak width (fwhm in parenthesis) and are assigned to the most dominant vibrations.

$AmaH^+(H_2O)_3$	Mode [b]	**I-$(H_2O)_3$(I)** C_s	**I-$(H_2O)_3$(II)** C_{3v}	**I-$(H_2O)_3$(III)**	**I-$(H_2O)_3$(IV)**
A 2712 (13)	ν_{NH3}[b]				2652 (1268)
B 2823 (11)	ν_{NH3}[b]			2872 (614)	
C 2862 (17)	$\nu_{CH/CH2}$	2892 (10)	2902 (12)	2894 (6)	2890 (12)
		2896 (42)	2902 (11)	2900 (45)	2896 (24)
					2902 (36)
D 2870 (16)	$\nu_{CH/CH2}$	2910 (14)	2907 (43)	2910 (19)	2911 (27)
		2911 (29)	2909 (31)	2911 (166)	2913 (20)
		2913 (4)	2910 (30)	2912 (22)	2918 (14)
			2910 (4)	2913 (123)	
E 2911 (7)	$\nu_{CH/CH2}$	2931 (8)	2940 (52)	2938 (1)	2929 (29)
		2934 (29)	2940 (56)	2940 (87)	
			2940 (1)		
F 2936 (25)	$\nu_{CH/CH2}$, FR [c]	2942 (59)	2943 (21)	2941 (44)	2944 (59)
		2943 (54)	2944 (18)	2945 (13)	2946 (42)
		2946 (6)	2945 (30)	2949 (3)	2948 (10)
		2949 (2)	2949 (14)	2950 (2)	2950 (4)
		2951 (5)	2950 (12)	2953 (11)	2953 (21)
		2953 (20)	2955 (73)	2956 (60)	2958 (45)
		2956 (74)		2958 (66)	2966 (2)
					2970 (27)
I 3009 (39)	ν_{NH3}[b]	2982 (692)			
		2984 (593)			
J 3118 (46)	ν_{NH3}[b]		3061 (308)	3045 (629)	
K 3170 (21)	ν_{NH3}[b]		3105 (602)		
			3107 (600)		
	$2\beta_{OH2}$, FR [c]	3169		3173	3161
	ν_{OH2}[b]				3243 (858)
M 3268 (30)	$2\beta_{OH2}$[d]		3208	3200	3204
		3237		3240	3242
	$2\beta_{NH3}$[d]	3244			3270
				3280	3282
	ν_{NH3}[s]				3263 (18)
O 3317 (10)	ν_{NH3}[f]	3307 (49)		3304 (38)	
	ν_{NH3}[a]				3322 (33)
T 3432 (52)	ν_{OH2}[b]			3408 (498)	3412 (422)
W 3552 (11)	ν_{OH2}[b-ring]	3509 (209)			
		3533 (586)			
X 3639 (12)	ν_{OH2}[s]	3637 (17)	3656 (47)	3651 (34)	
			3657 (46)	3654 (42)	3652 (28)
			3657 (26)		
Y 3680 (9)	ν_{OH2}[f]				
Z 3712 (42)	ν_{OH2}[f]	3727 (223)		3726 (110)	3720 (103)
		3730 (26)			3727 (108)
	ν_{OH2}[a]	3721 (117)	3745 (17)	3740 (96)	3742 (95)
			3745 (143)	3743 (104)	
			3746 (131)		

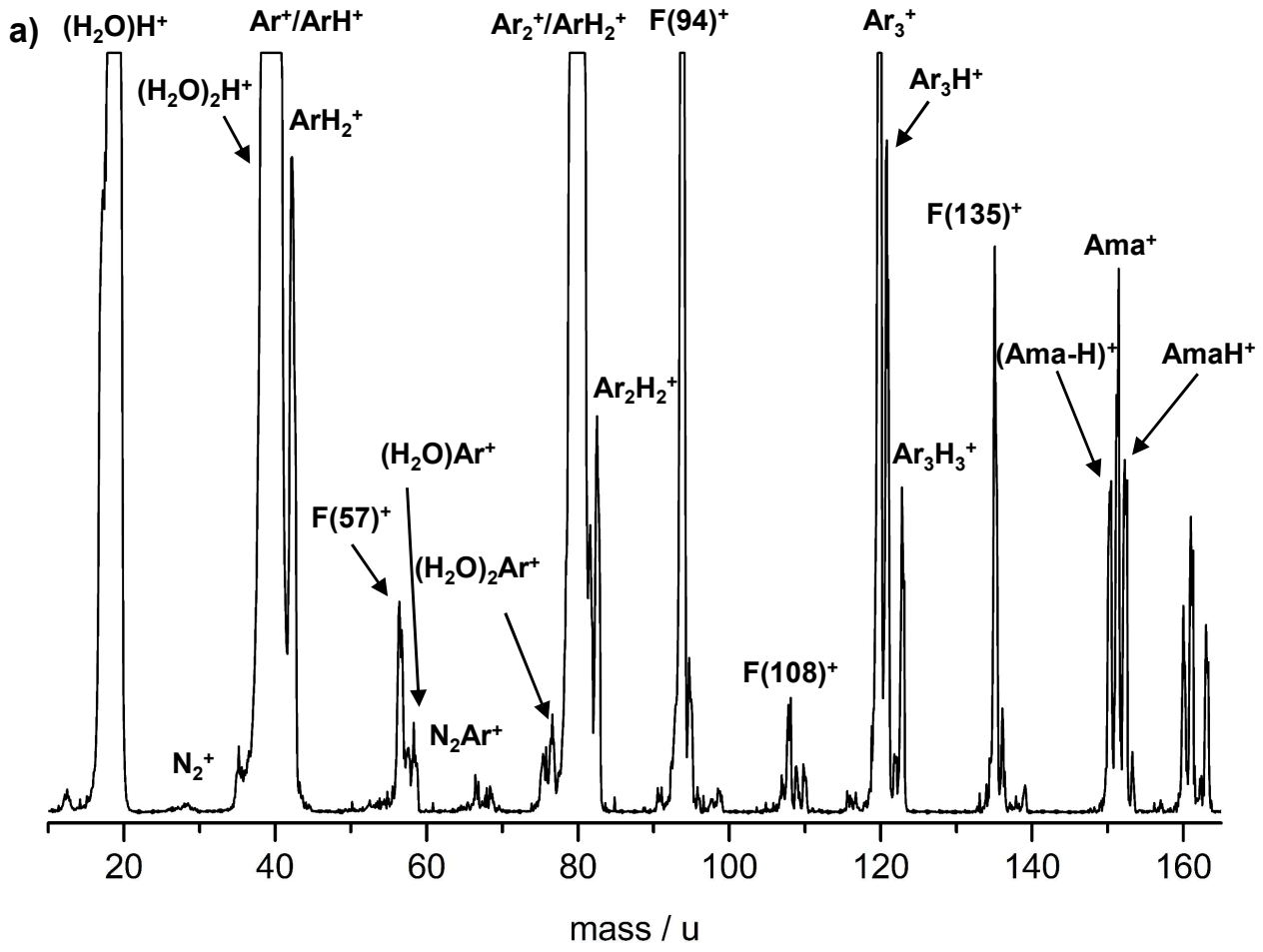
[a] IR intensities in km/mol are given in parentheses. [b] Stretching (ν), bending (β). [c] FR = Fermi resonance with ν_{NH3}[b]. [d] Coupled β_{NH3}/β_{OH2}.

Table S10. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of **I-$(H_2O)_4$(I-IV)** compared to experimental values of $AmaH^+(H_2O)_4$ (Figure 9).[a] The experimental values (peak maxima) are given with peak width (fwhm in parenthesis) and are assigned to the most dominant vibrations.

$AmaH^+(H_2O)_4$	Mode [b]	**I-$(H_2O)_4$(I)**	**I-$(H_2O)_4$(II)**	**I-$(H_2O)_4$(III)**	**I-$(H_2O)_4$(IV)**	**I-$(H_2O)_4$(V)**	**I-$(H_2O)_4$(VI)** C_s
A 2680 (11)	ν_{NH3} [b]					2776 (938)	
C 2860 (10)	$\nu_{CH/CH2}$	2893 (7)	2900 (15)	2891 (9)	2903 (17)	2892 (10)	2896 (2)
		2897 (44)	2902 (25)	2896 (43)		2898 (43)	2901 (50)
D 2867 (4)	$\nu_{CH/CH2}$	2908 (13)	2908 (24)	2909 (24)	2909 (18)	2909 (19)	2909 (17)
		2908 (27)	2908 (27)	2910 (27)	2909 (16)	2910 (27)	2910 (25)
		2911 (21)	2909 (15)	2910 (11)	2911 (19)	2911 (16)	2914 (13)
			2912 (19)	2915 (10)	2913 (12)	2918 (15)	2919 (13)
					2915 (32)		
E 2905 (3)	$\nu_{CH/CH2}$	2925 (11)	2937 (55)	2933 (9)	2935 (75)	2933 (11)	2936 (61)
		2935 (3)	2939 (59)	2938 (8)	2937 (53)	2937 (75)	2938 (49)
		2937 (27)	2939 (17)	2939 (66)			
		2939 (55)					
F 2933 (23)	ν_{NH3} [b]						2913 (443)
	$\nu_{CH/CH2,}$ FR [c]	2943 (59)	2942 (8)	2942 (57)	2941 (19)	2940 (40)	2941 (44)
		2945 (10)	2943 (28)	2945 (12)	2942 (20)	2944 (40)	2947 (2)
		2947 (1)	2946 (1)	2948 (1)	2947 (10)	2945 (1)	2949 (23)
		2948 (9)	2947 (19)	2949 (4)	2949 (6)	2949 (4)	2954 (177)
		2953 (82)	2952 (32)	2954 (85)	2953 (65)	2949 (12)	2954 (63)
		2970 (3)	2952 (71)	2957 (8)	2954 (14)	2954 (72)	2960 (20)
					2958 (32)	2959 (31)	2962 (67)
H 2974 (18)	ν_{NH3} [b]	2944 (505)		2937 (659)	2979 (655)		2929 (1039)
		2948 (762)		2961 (740)			
I 3058 (17)	ν_{NH3} [b]		3049 (493)			3008 (608)	
J 3144 (42)	ν_{NH3} [b]		3068 (355)		3095 (462)		
K 3188 (6)	ν_{NH3} [b]		3123 (668)		3126 (579)		
	$2\beta_{OH2}$, FR [c]	3173	3174	3179	3174	3175	
		3192	3180	3183	3192	3188	
M 3271 (30)	$2\beta_{OH2}$ [d]	3226	3200	3221	3200	3212	
		3249	3236	3254	3241	3221	
	$2\beta_{NH3}$ [d]	3262	3310	3264		3257	
	ν_{OH2} [b]	3310 (800)		3291 (1460)			
	ν_{NH3} [f]	3311 (43)		3311 (43)		3311 (43)	3307 (37)
S 3387 (13)	ν_{OH2} [b]	3421 (349)		3404 (389)			3418 (471)
	$2\beta_{NH3}$ [e]	3367	3370	3374	3321		
					3351	3375	
T 3452 (55)	ν_{OH2} [b]	3466 (467)		3455 (413)	3434 (458)	3456 (333)	3427 (497)
						3505 (379)	
W 3554 (10)	ν_{OH2} [b-ring]		3519 (204)			3598 (527)	
			3542 (532)				
X 3642 (13)	ν_{OH2} [s]	3655 (34)	3639 (15)	3662 (29)	3653 (33)		3652 (44)
			3657 (38)		3656 (40)	3642 (13)	3653 (20)
					3657 (33)	3651 (22)	
Y 3683 (8)	ν_{OH2} [f]	3703 (92)		3698 (83)			
Z 3705 (49)	ν_{OH2} [f]	3725 (156)	3730 (206)	3727 (141)	3730 (103)	3728 (113)	3730 (25)
		3727 (67)	3732 (26)	3731 (57)			3730 (187)
	ν_{OH2} [a]	3745 (99)	3724 (114)	3751 (108)	3743 (90)	3725 (108)	3741 (93)
			3747 (98)		3746 (77)	3740 (92)	3743 (99)
					3747 (116)		

[a] IR intensities in km/mol are given in parentheses. [b] Stretching (ν), bending (β), [c] FR = Fermi resonance with ν_{NH3} [b]. [d] Coupled β_{NH3}/β_{OH2}.

Figure S1


a)
(H2O)H+
(H2O)2H+
Ar+/ArH+
ArH2+
Ar2+/ArH2+
F(94)+
Ar3+
Ar3H+
F(135)+
Ama+
(Ama-H)+
AmaH+
Ar2H2+
Ar3H3+
(H2O)Ar+
F(57)+
(H2O)2Ar+
F(108)+
N2+
N2Ar+
20
40
60
80
100
120
140
160
mass / u

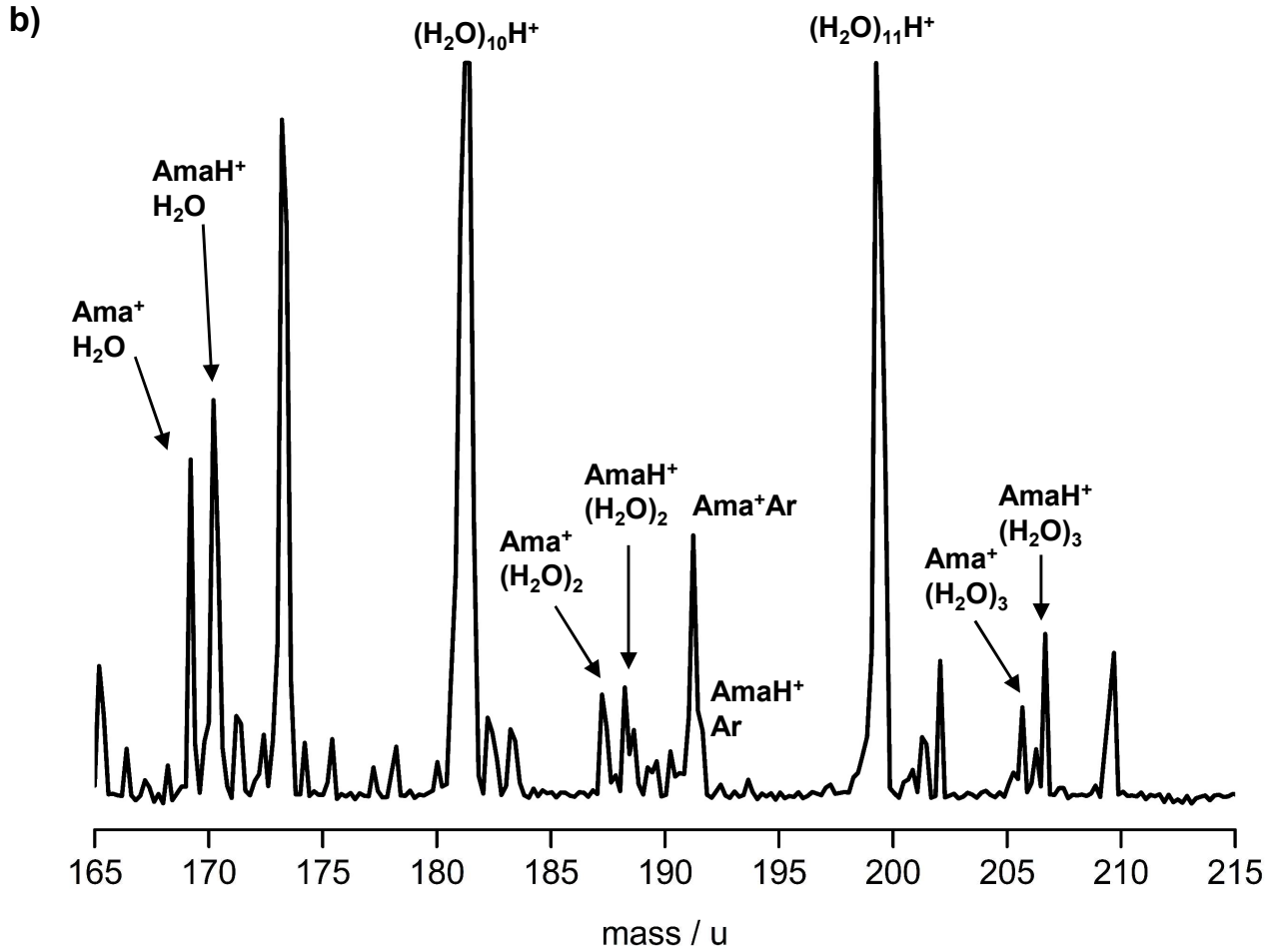
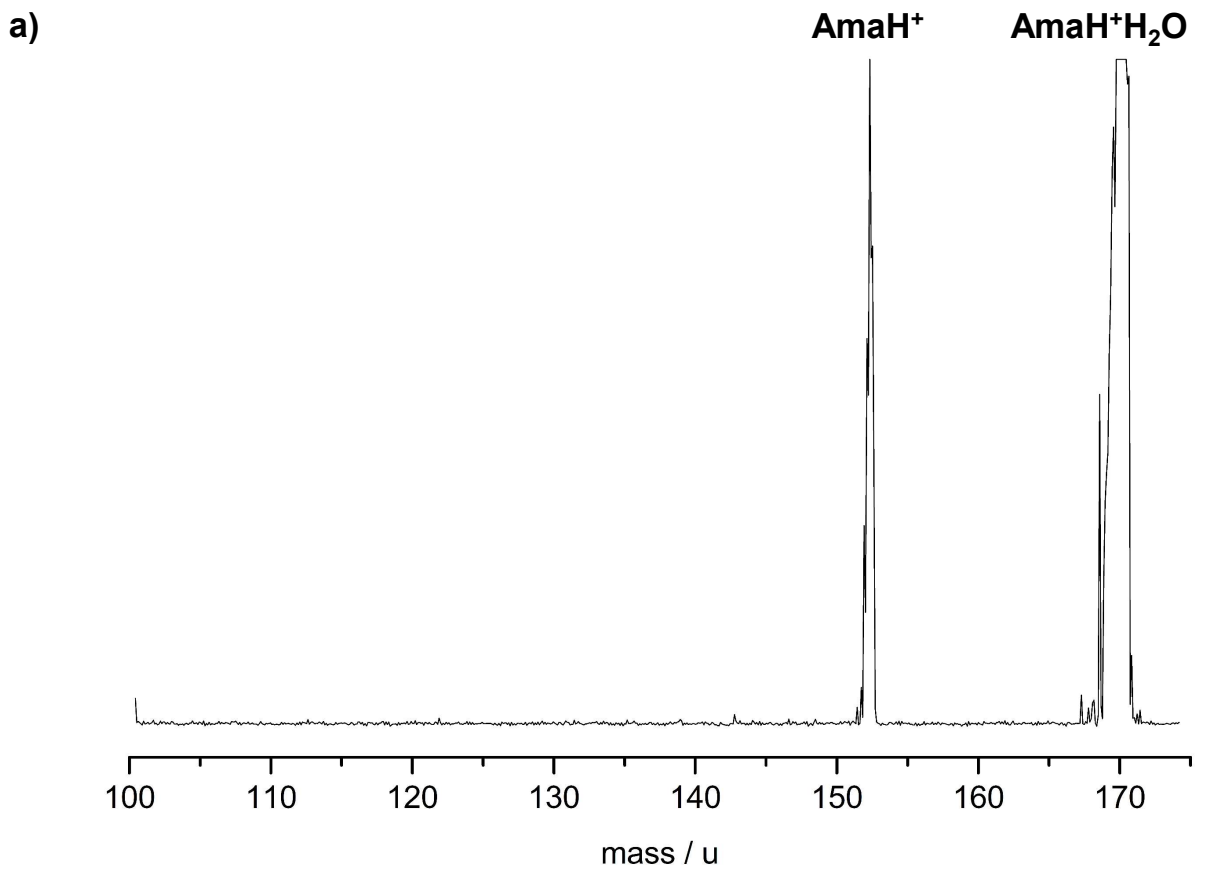

b)
(H2O)10H+
(H2O)11H+
AmaH+
H2O
Ama+
H2O
AmaH+
(H2O)2
Ama+Ar
Ama+
(H2O)2
AmaH+
(H2O)3
Ama+
(H2O)3
AmaH+
Ar
165
170
175
180
185
190
195
200
205
210
215
mass / u

Figure S2


a)
AmaH+
AmaH+H2O
100
110
120
130
140
150
160
170
mass / u

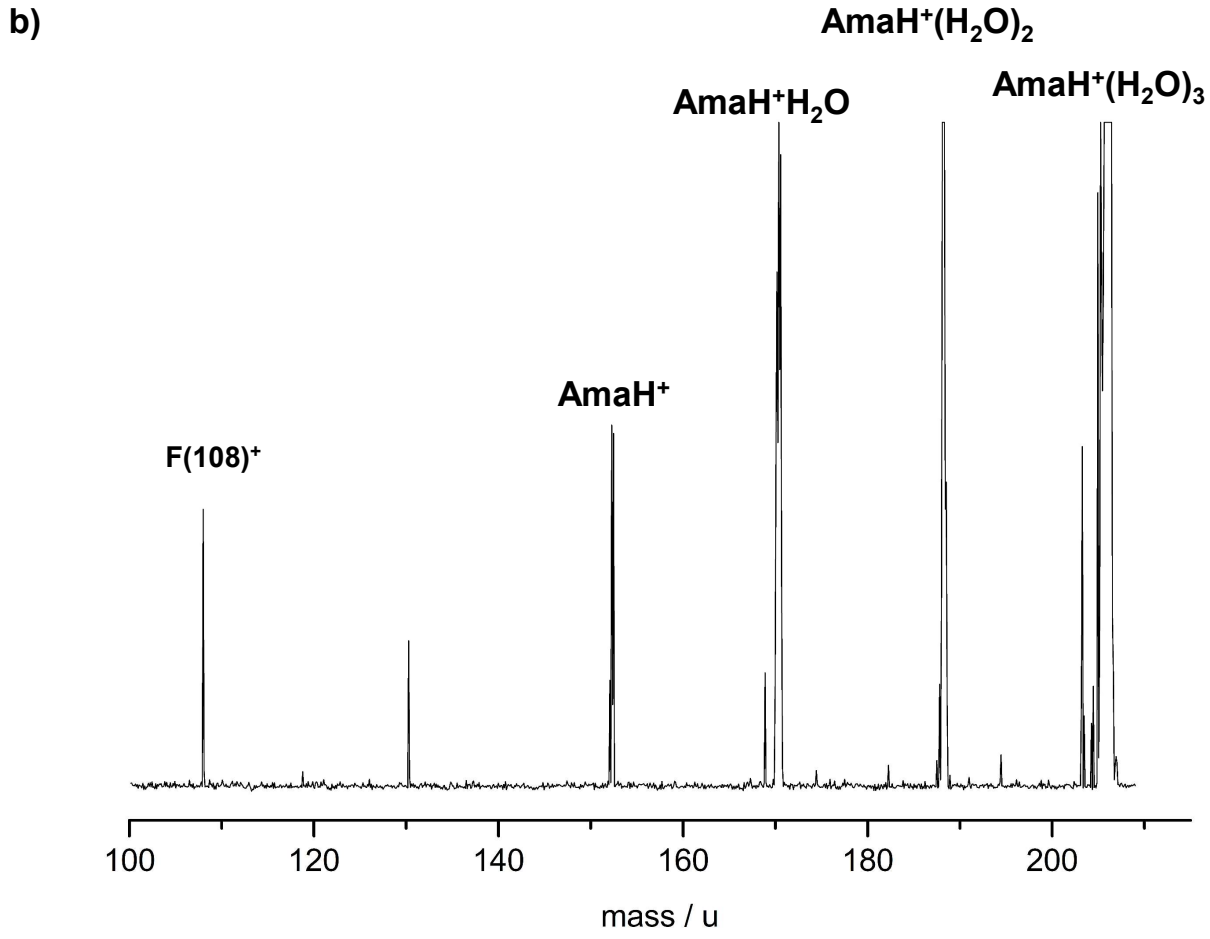

b)
AmaH+(H2O)2
AmaH+H2O
AmaH+(H2O)3
AmaH+
F(108)+
100
120
140
160
180
200
mass / u

Figure S3

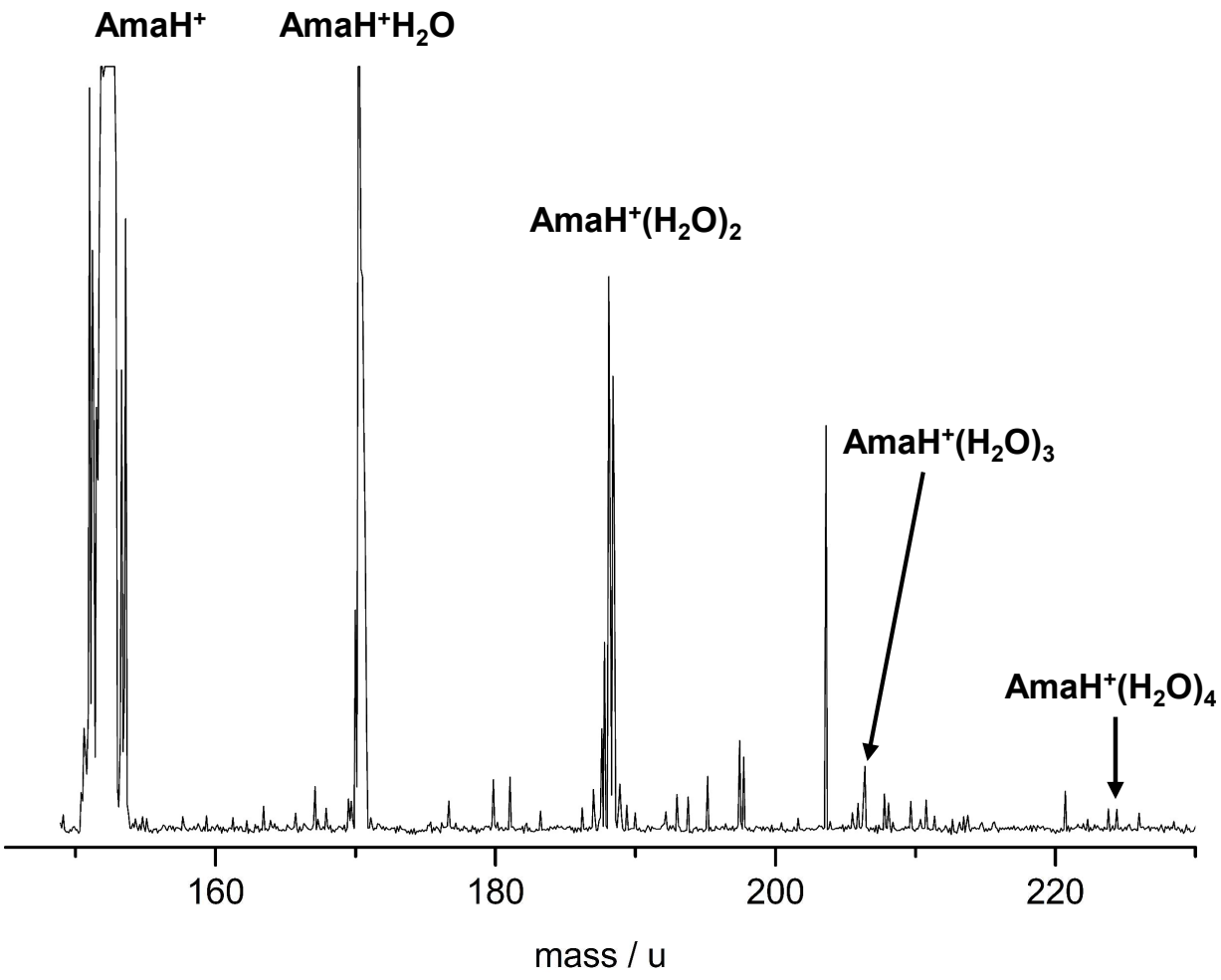
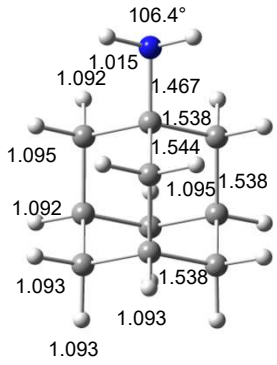
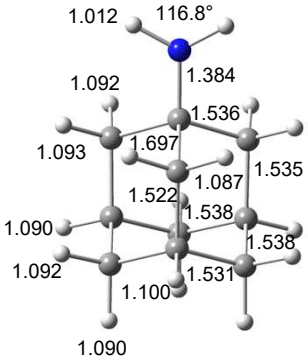

AmaH+
AmaH+H2O
AmaH+(H2O)2
AmaH+(H2O)3
AmaH+(H2O)4
160
180
200
220
mass / u

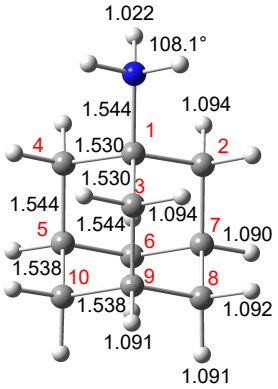
Figure S4



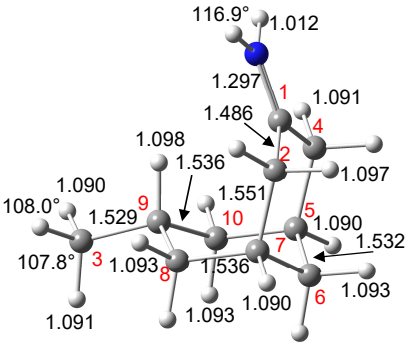
Ama (C_s)



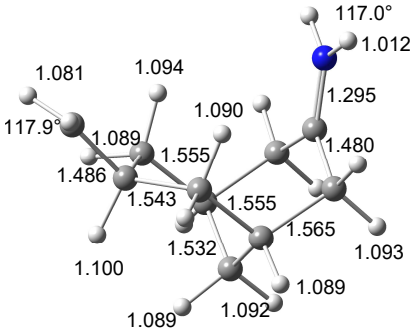
Ama$^+$(I) (C_s)



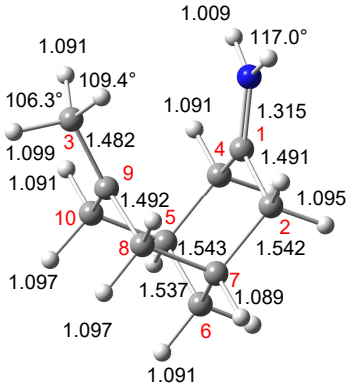
AmaH$^+$(I) (C_{3v})



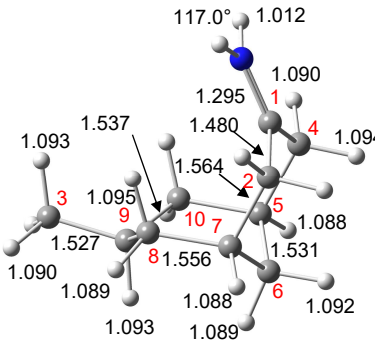
AmaH$^+$(II) (C_s)



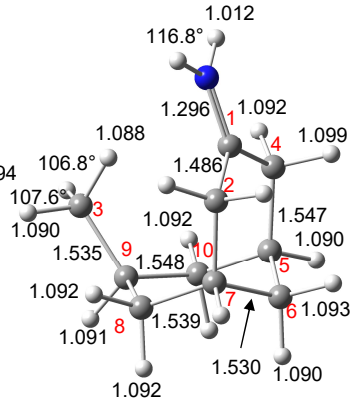
Ama$^+$(II) (C_s)



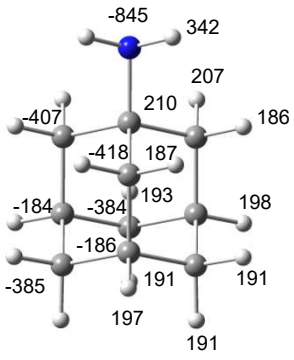
Ama$^+$(III) (C_s)



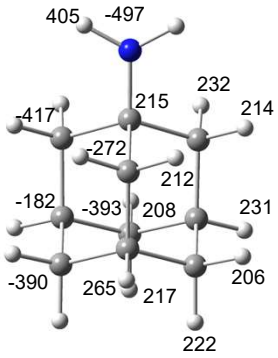
AmaH$^+$(III) (C_s)



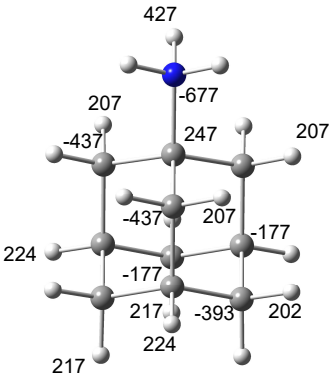
AmaH$^+$(IV) (C_s)



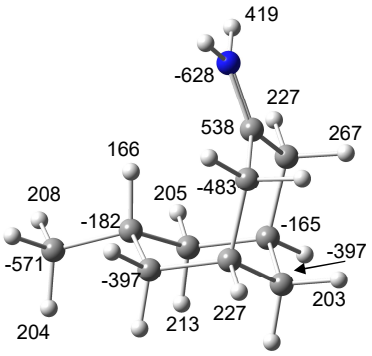
Ama (C_s)



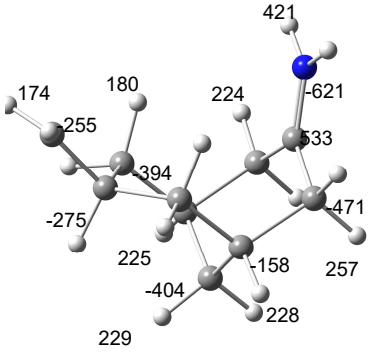
Ama$^+$(I) (C_s)



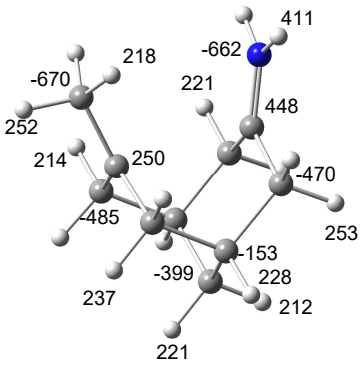
AmaH$^+$(I) (C_{3v})



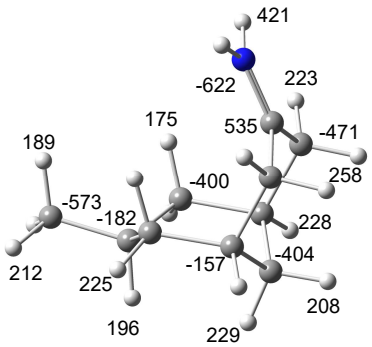
AmaH$^+$(II) (C_s)



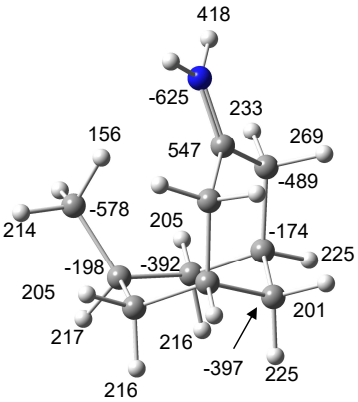
Ama$^+$(II) (C_s)



Ama$^+$(III) (C_s)



AmaH$^+$(III) (C_s)



AmaH$^+$(IV) (C_s)

Figure S5

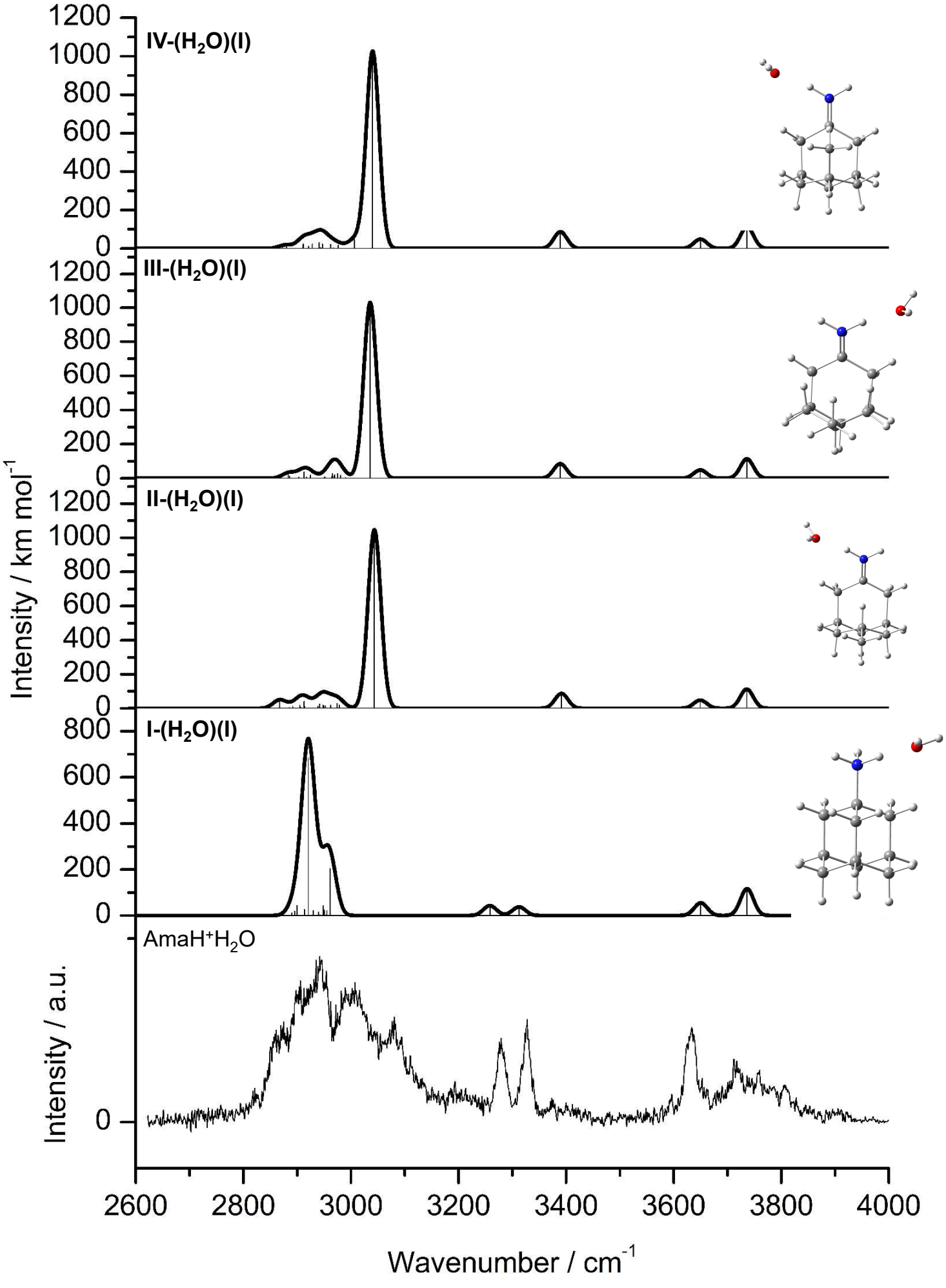

IV-(H2O)(I)
III-(H2O)(I)
II-(H2O)(I)
I-(H2O)(I)
AmaH+H2O
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
0
200
400
600
800
1000
1200
2600
2800
3000
3200
3400
3600
3800
4000

Figure S6

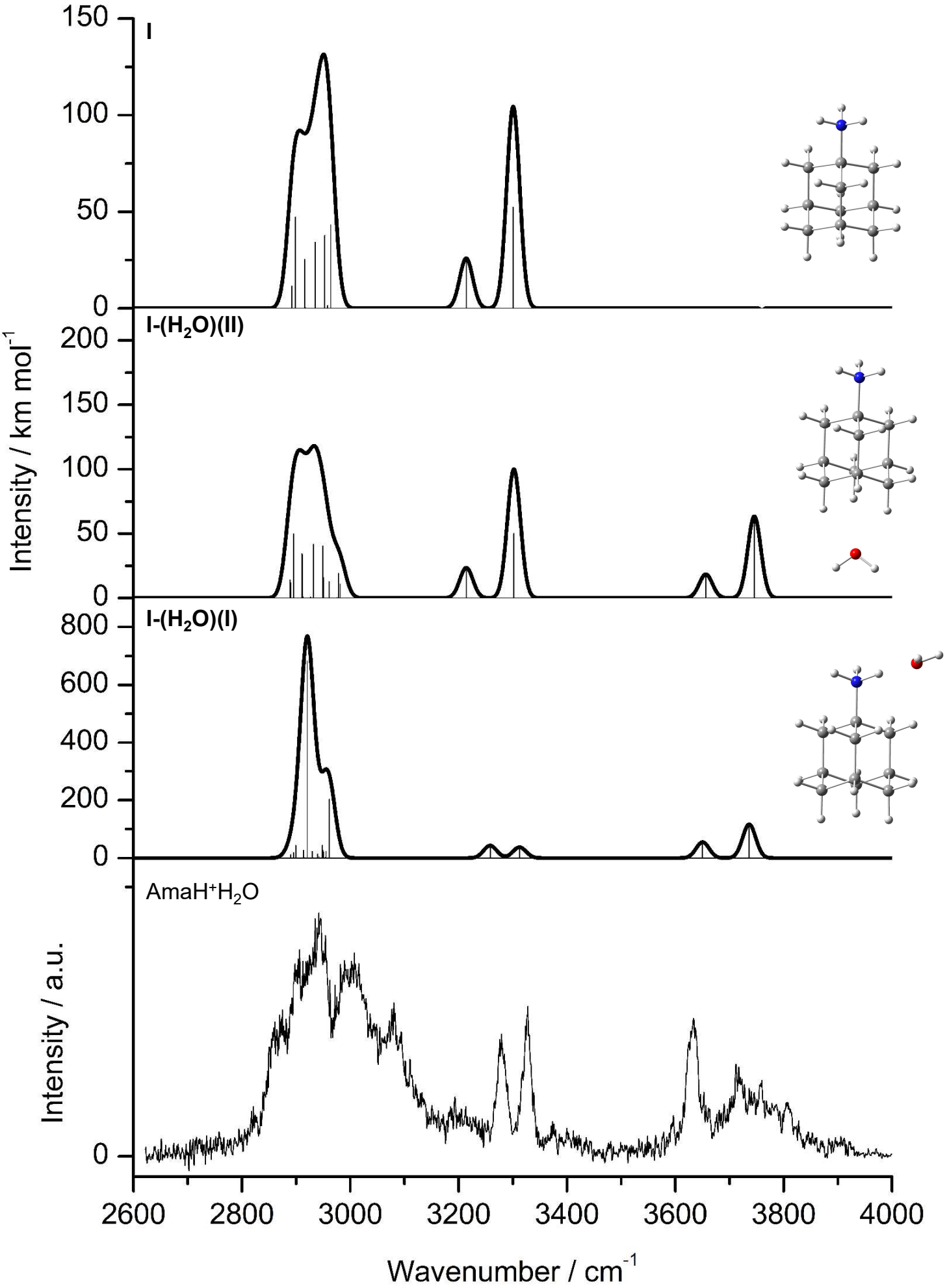

I
I-(H2O)(II)
I-(H2O)(I)
AmaH+H2O
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
150
100
50
0
200
150
100
50
0
800
600
400
200
0
0
2600
2800
3000
3200
3400
3600
3800
4000

Figure S7

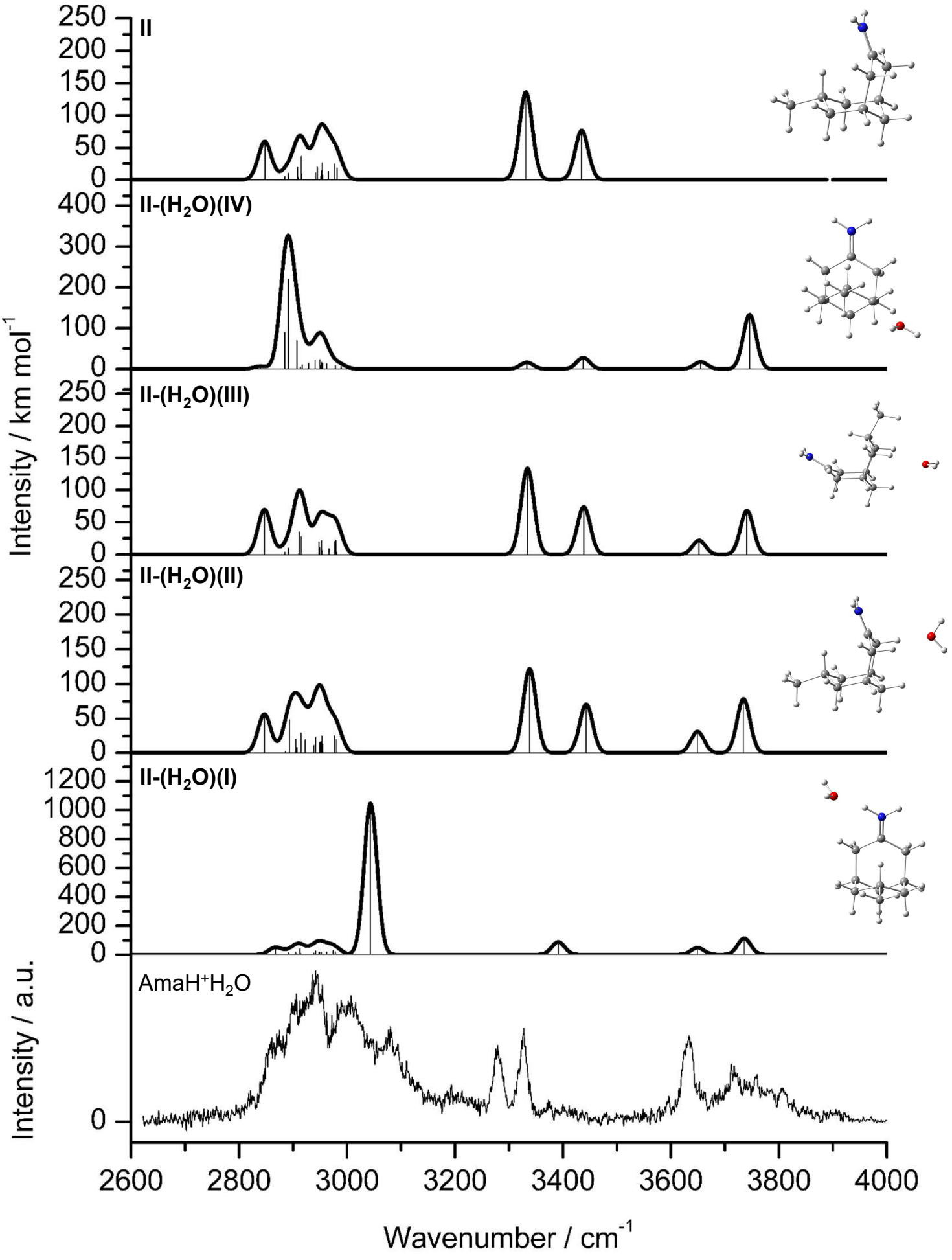

II
II-(H2O)(IV)
II-(H2O)(III)
II-(H2O)(II)
II-(H2O)(I)
AmaH+H2O
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
2600
2800
3000
3200
3400
3600
3800
4000

Figure S8

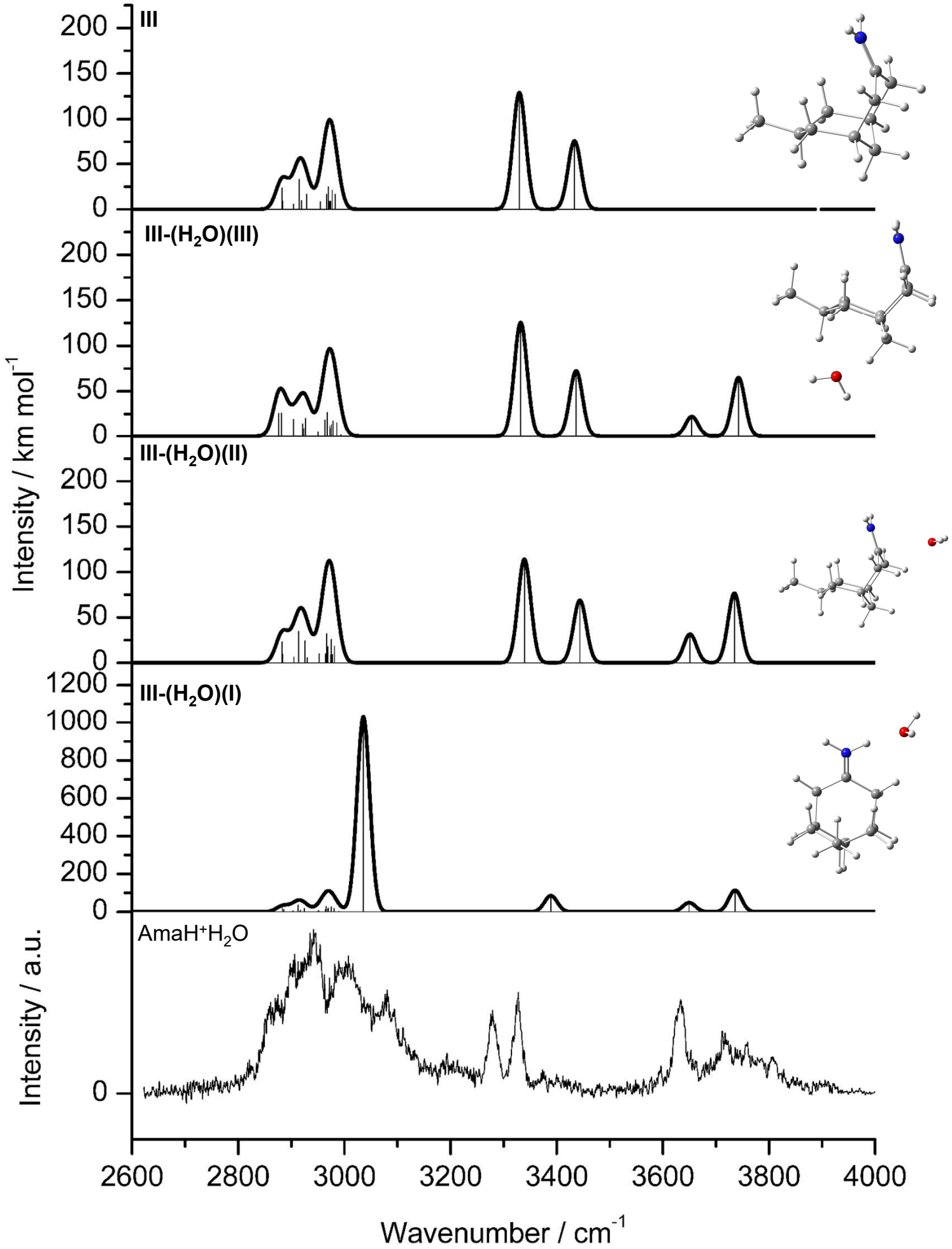

III
III-(H2O)(III)
III-(H2O)(II)
III-(H2O)(I)
AmaH+H2O
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
200
150
100
50
0
1200
1000
800
600
400
200
2600
2800
3000
3200
3400
3600
3800
4000

Figure S9

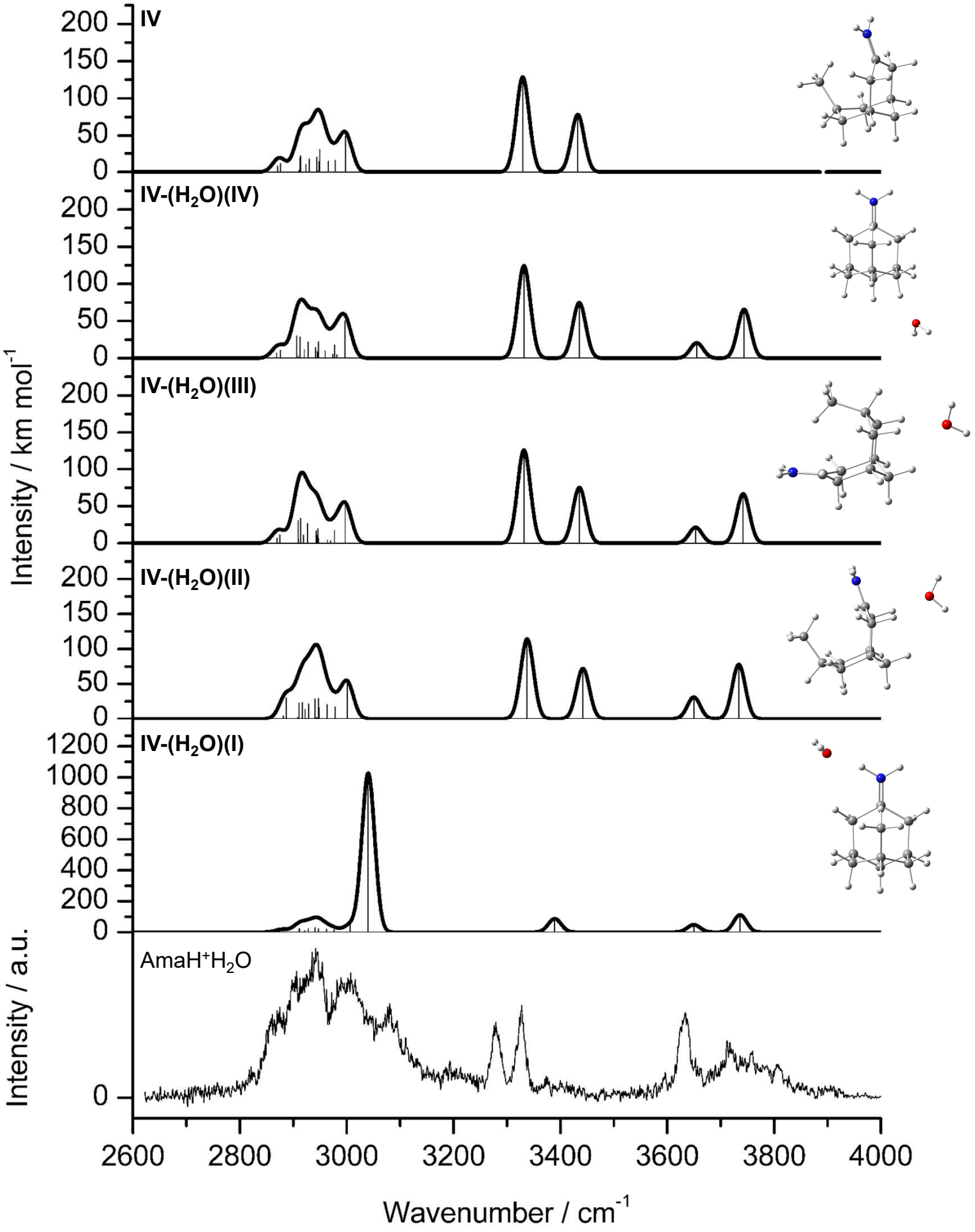

IV
IV-(H2O)(IV)
IV-(H2O)(III)
IV-(H2O)(II)
IV-(H2O)(I)
AmaH+H2O
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
200
150
100
50
0
1200
1000
800
600
400
200
2600
2800
3000
3200
3400
3600
3800
4000

Figure S10

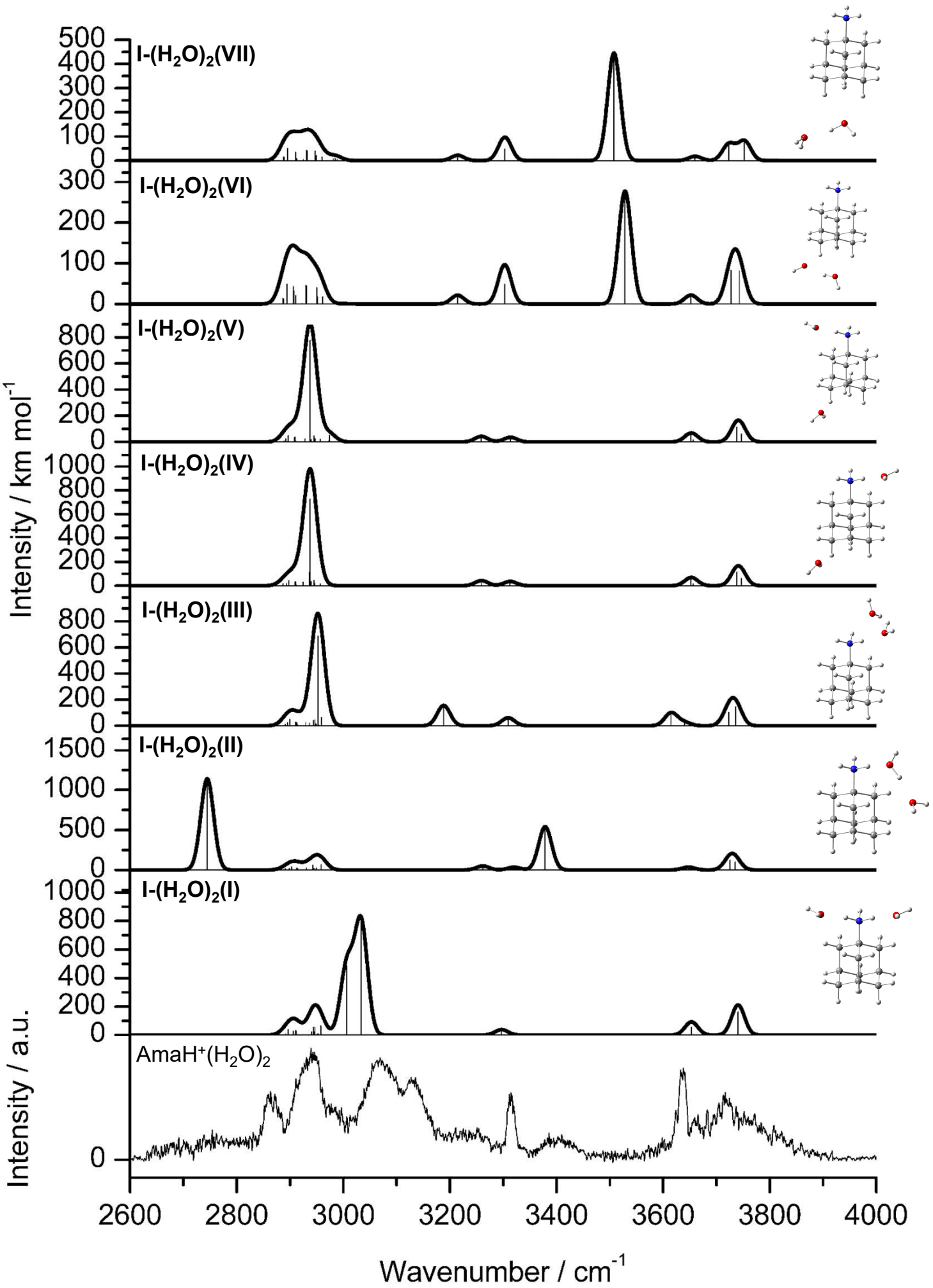

I-(H2O)2(VII)
I-(H2O)2(VI)
I-(H2O)2(V)
I-(H2O)2(IV)
I-(H2O)2(III)
I-(H2O)2(II)
I-(H2O)2(I)
AmaH+(H2O)2
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
2600
2800
3000
3200
3400
3600
3800
4000

Figure S11

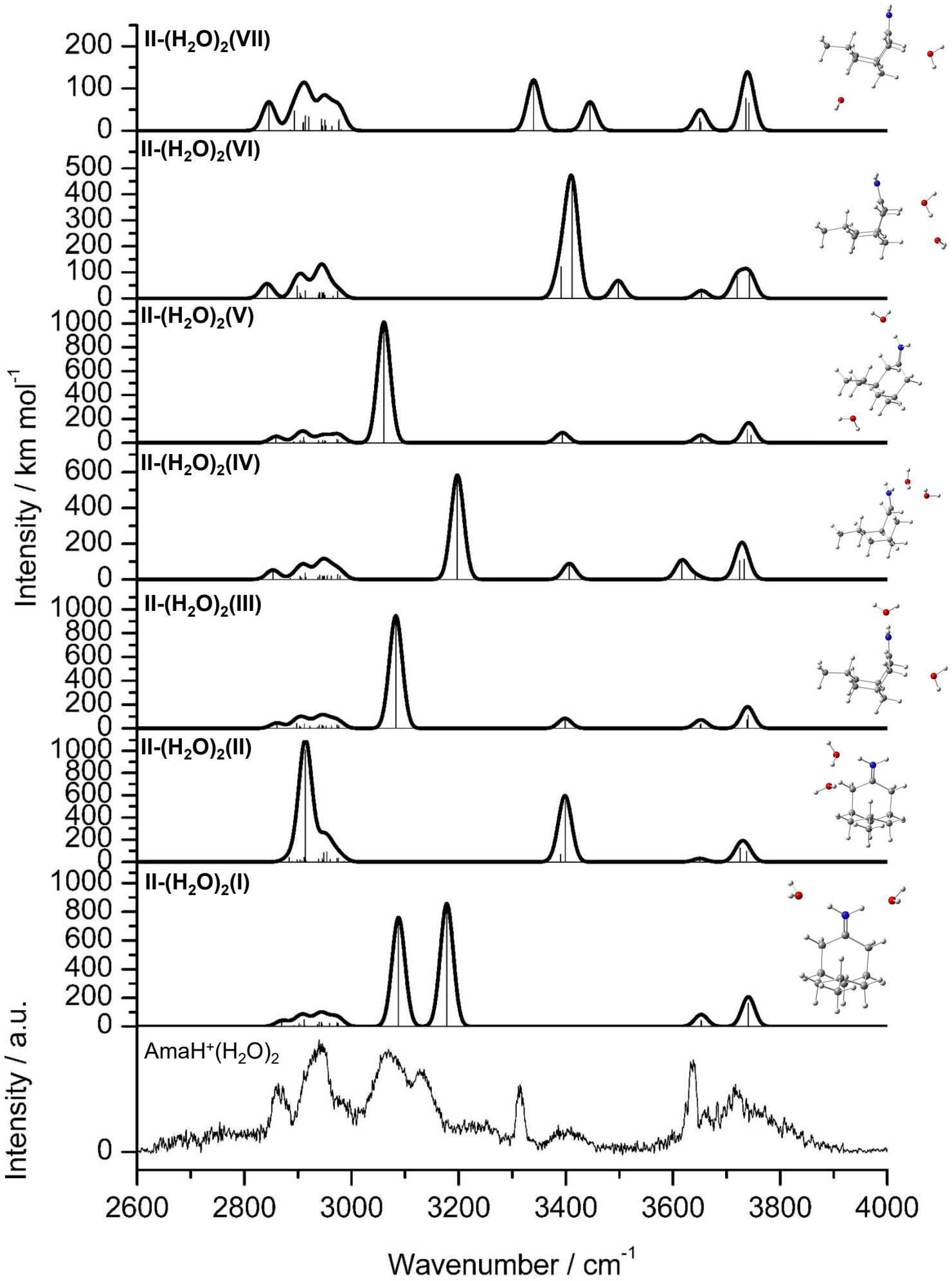

II-(H2O)2(VII)
II-(H2O)2(VI)
II-(H2O)2(V)
II-(H2O)2(IV)
II-(H2O)2(III)
II-(H2O)2(II)
II-(H2O)2(I)
AmaH+(H2O)2
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1

Figure S12

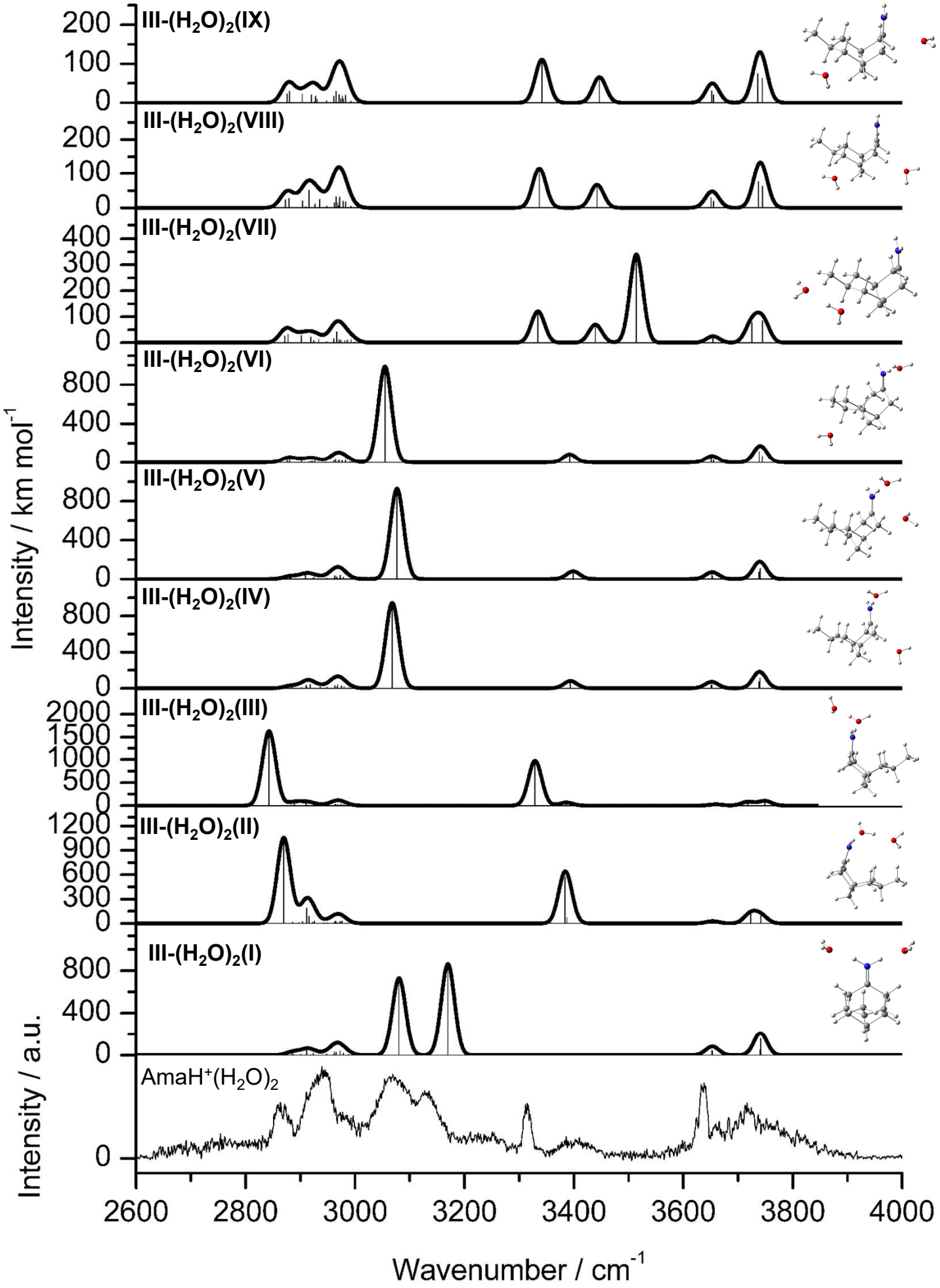

III-(H2O)2(IX)
III-(H2O)2(VIII)
III-(H2O)2(VII)
III-(H2O)2(VI)
III-(H2O)2(V)
III-(H2O)2(IV)
III-(H2O)2(III)
III-(H2O)2(II)
III-(H2O)2(I)
AmaH+(H2O)2
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
2600
2800
3000
3200
3400
3600
3800
4000

Figure S13

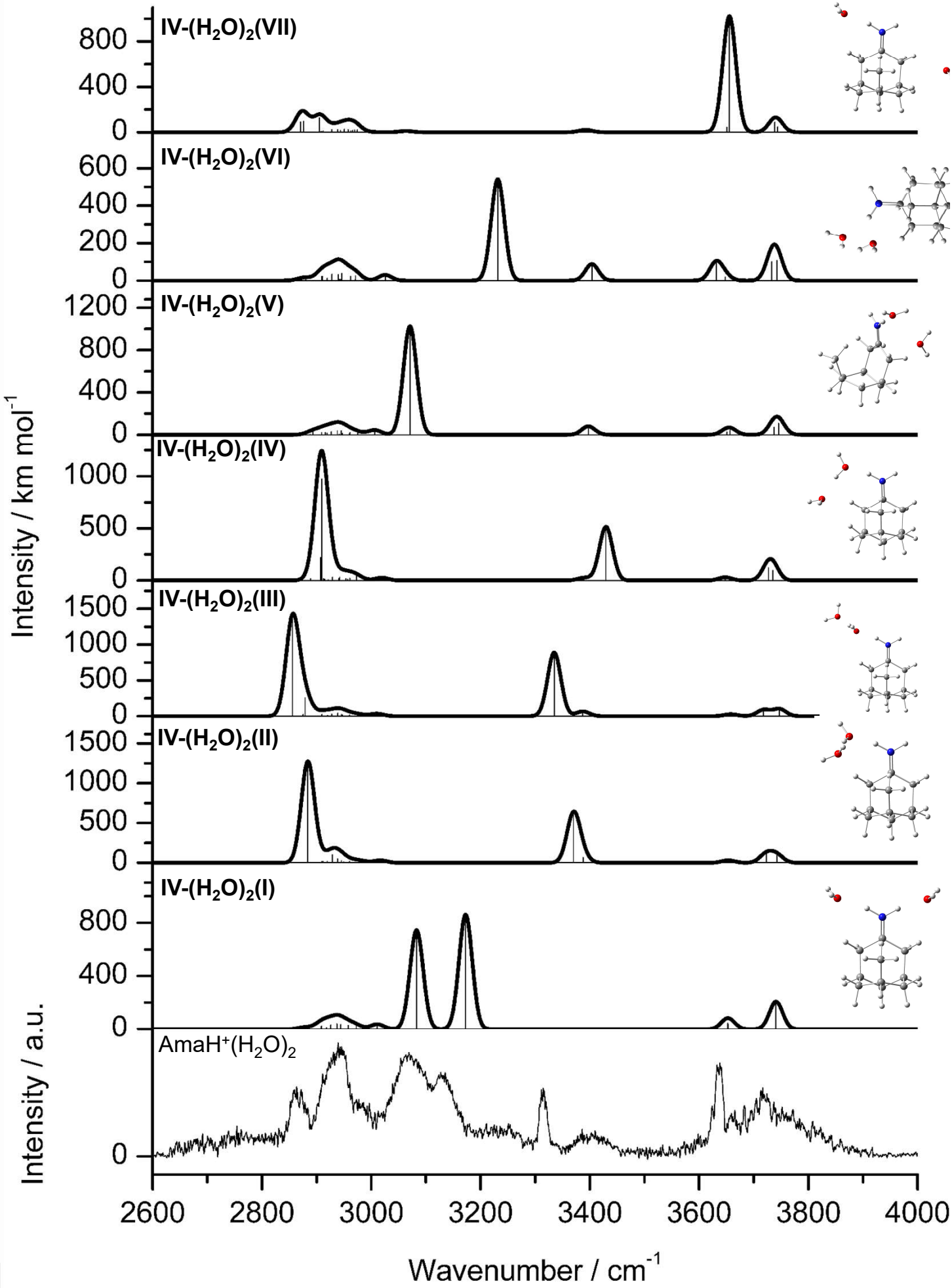

IV-(H2O)2(VII)
IV-(H2O)2(VI)
IV-(H2O)2(V)
IV-(H2O)2(IV)
IV-(H2O)2(III)
IV-(H2O)2(II)
IV-(H2O)2(I)
AmaH+(H2O)2
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
2600
2800
3000
3200
3400
3600
3800
4000

Figure S14

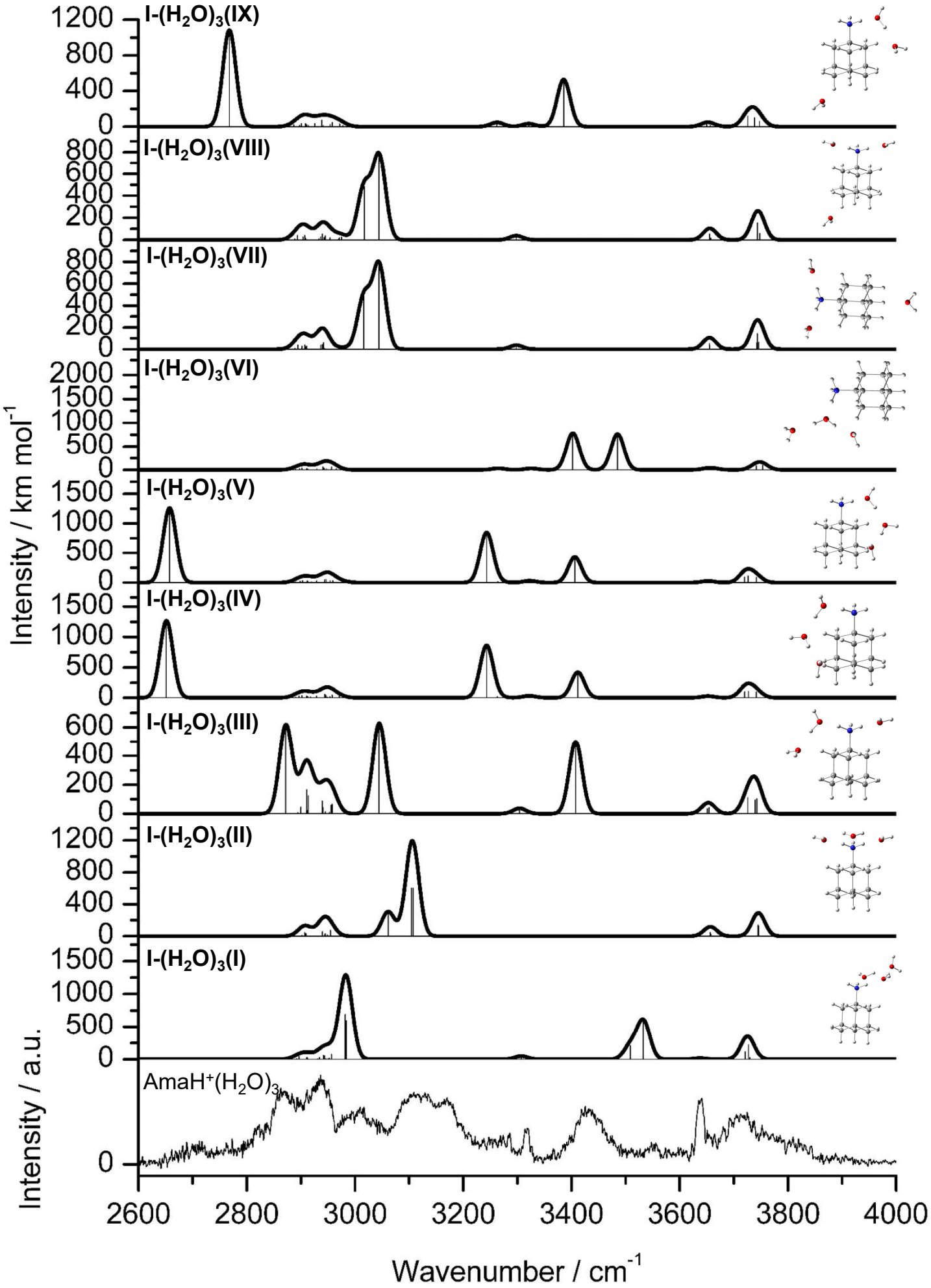

I-(H2O)3(IX)
I-(H2O)3(VIII)
I-(H2O)3(VII)
I-(H2O)3(VI)
I-(H2O)3(V)
I-(H2O)3(IV)
I-(H2O)3(III)
I-(H2O)3(II)
I-(H2O)3(I)
AmaH+(H2O)3
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
2600
2800
3000
3200
3400
3600
3800
4000

Figure S15

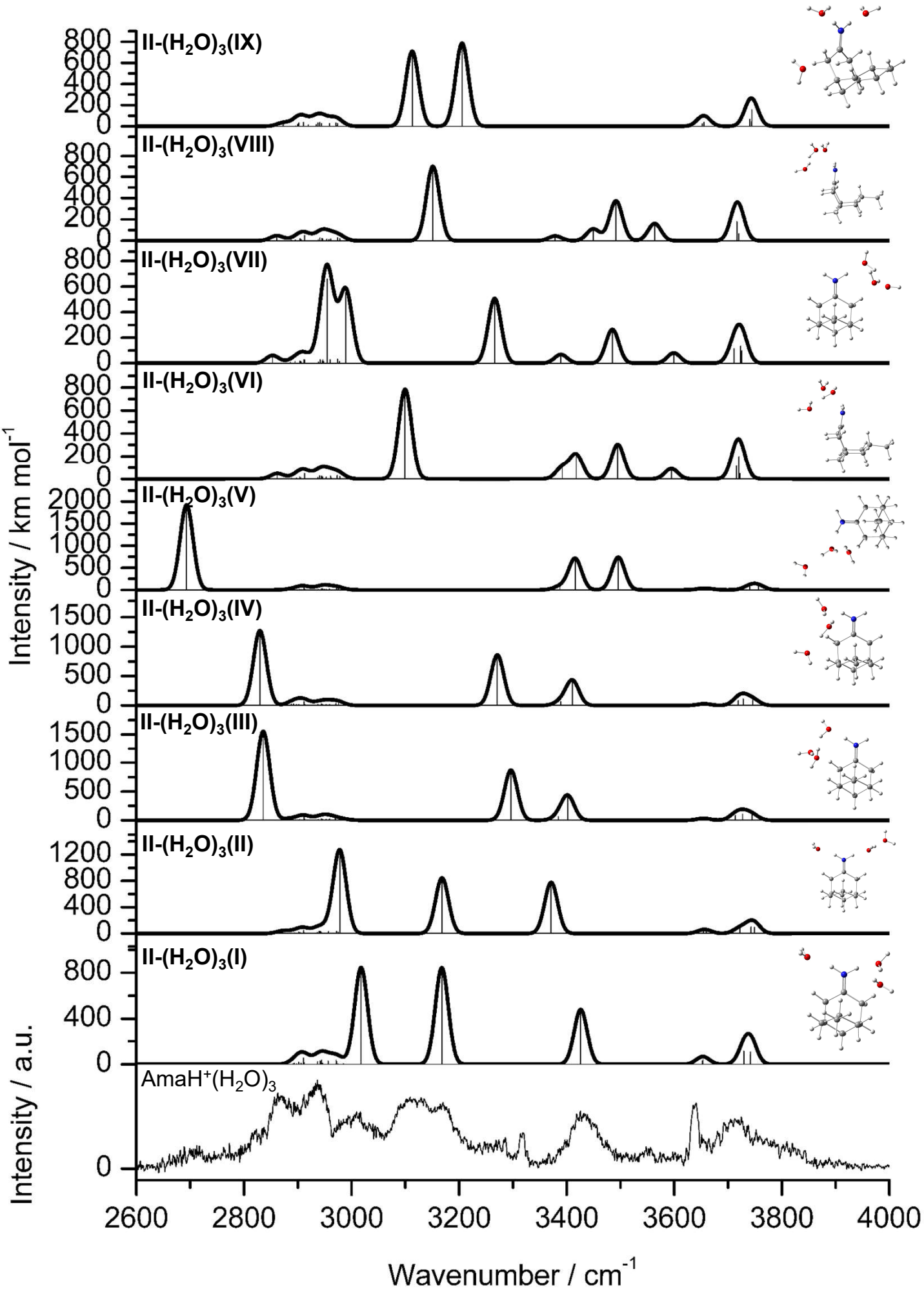

II-(H2O)3(IX)
II-(H2O)3(VIII)
II-(H2O)3(VII)
II-(H2O)3(VI)
II-(H2O)3(V)
II-(H2O)3(IV)
II-(H2O)3(III)
II-(H2O)3(II)
II-(H2O)3(I)
AmaH+(H2O)3
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
2600
2800
3000
3200
3400
3600
3800
4000

Figure S16

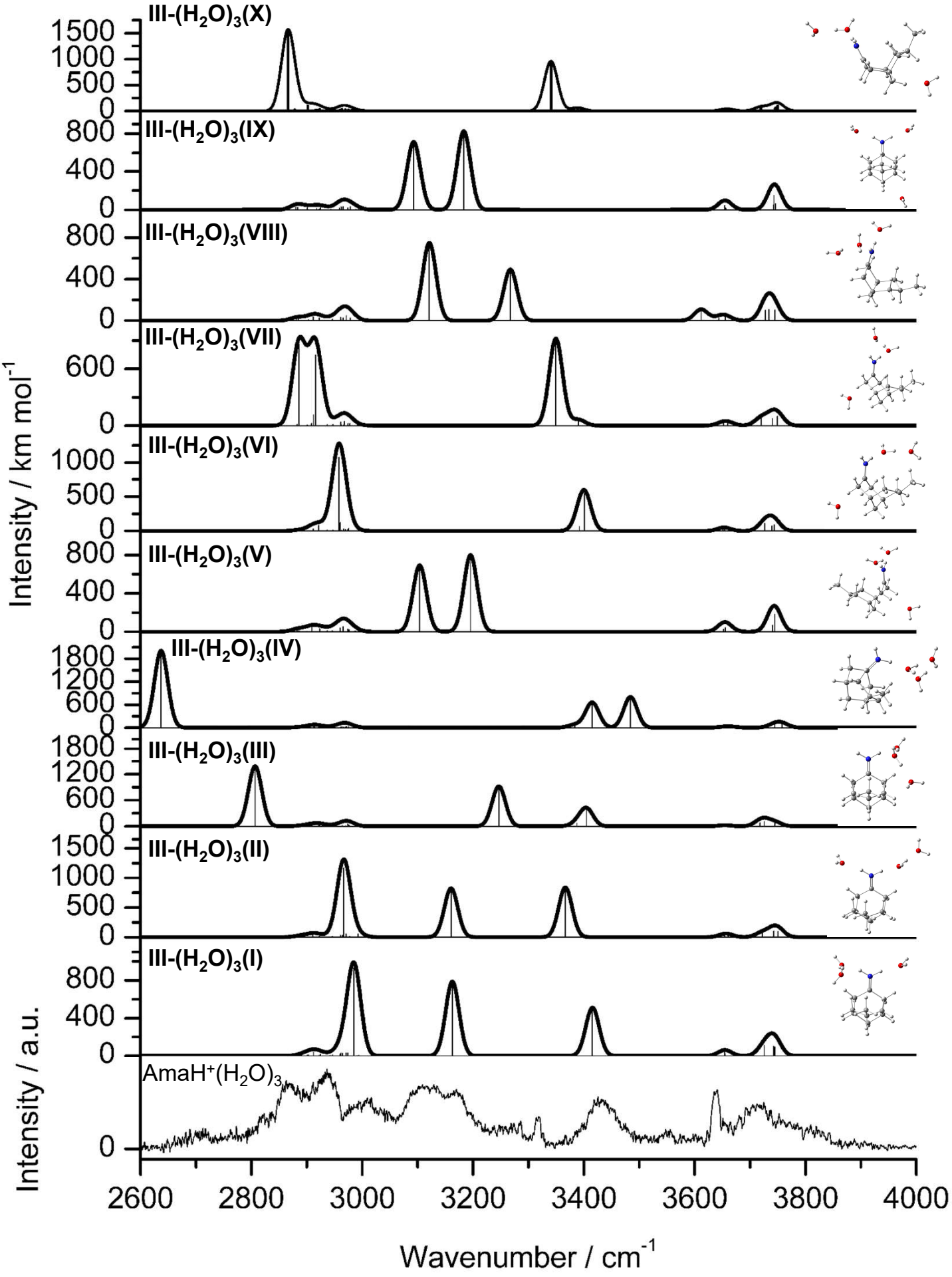

III-(H2O)3(X)
III-(H2O)3(IX)
III-(H2O)3(VIII)
III-(H2O)3(VII)
III-(H2O)3(VI)
III-(H2O)3(V)
III-(H2O)3(IV)
III-(H2O)3(III)
III-(H2O)3(II)
III-(H2O)3(I)
AmaH+(H2O)3
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
2600
2800
3000
3200
3400
3600
3800
4000

Figure S17

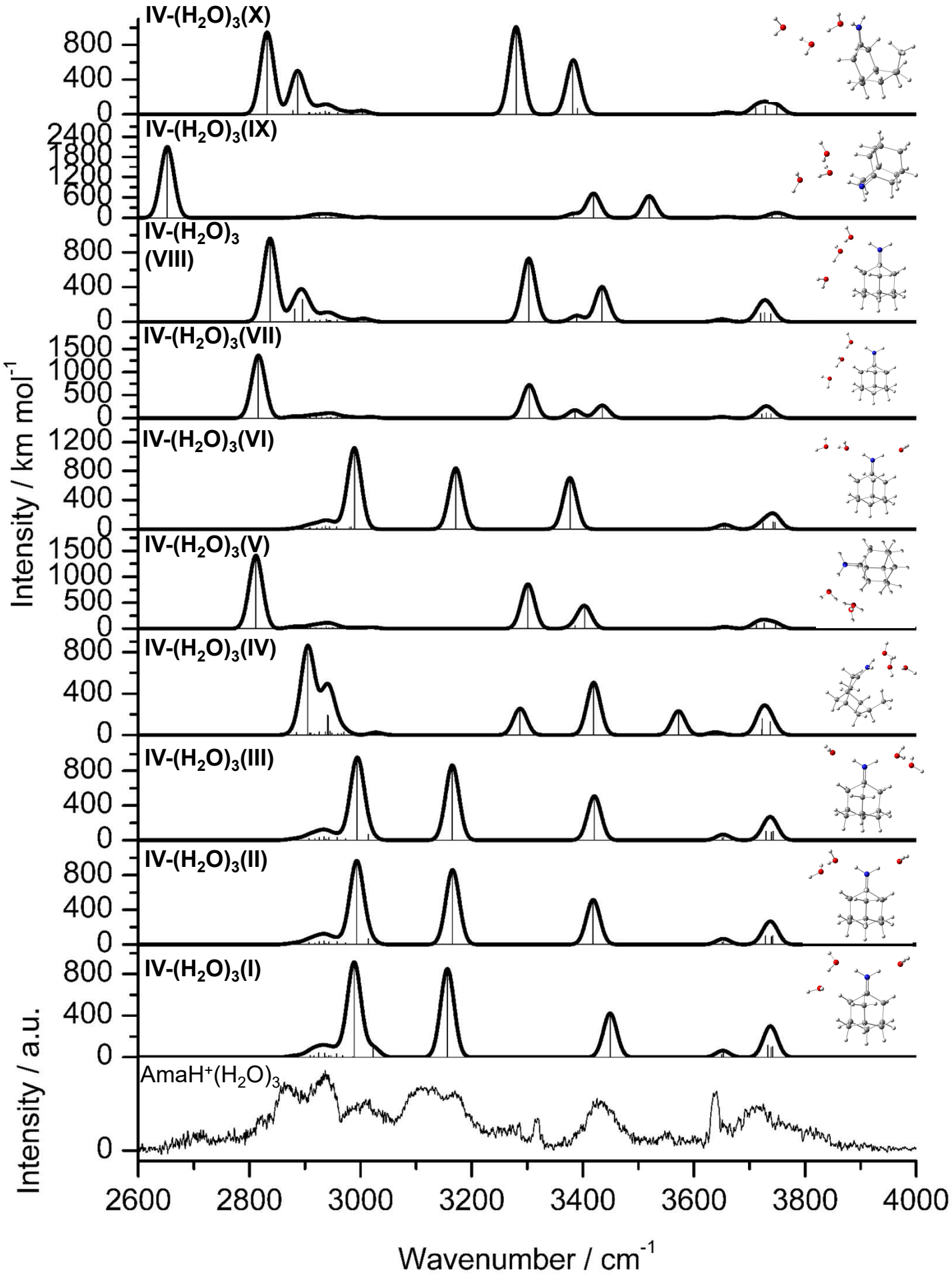

IV-(H2O)3(X)
IV-(H2O)3(IX)
IV-(H2O)3 (VIII)
IV-(H2O)3(VII)
IV-(H2O)3(VI)
IV-(H2O)3(V)
IV-(H2O)3(IV)
IV-(H2O)3(III)
IV-(H2O)3(II)
IV-(H2O)3(I)
AmaH+(H2O)3
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
2600
2800
3000
3200
3400
3600
3800
4000

Figure S18

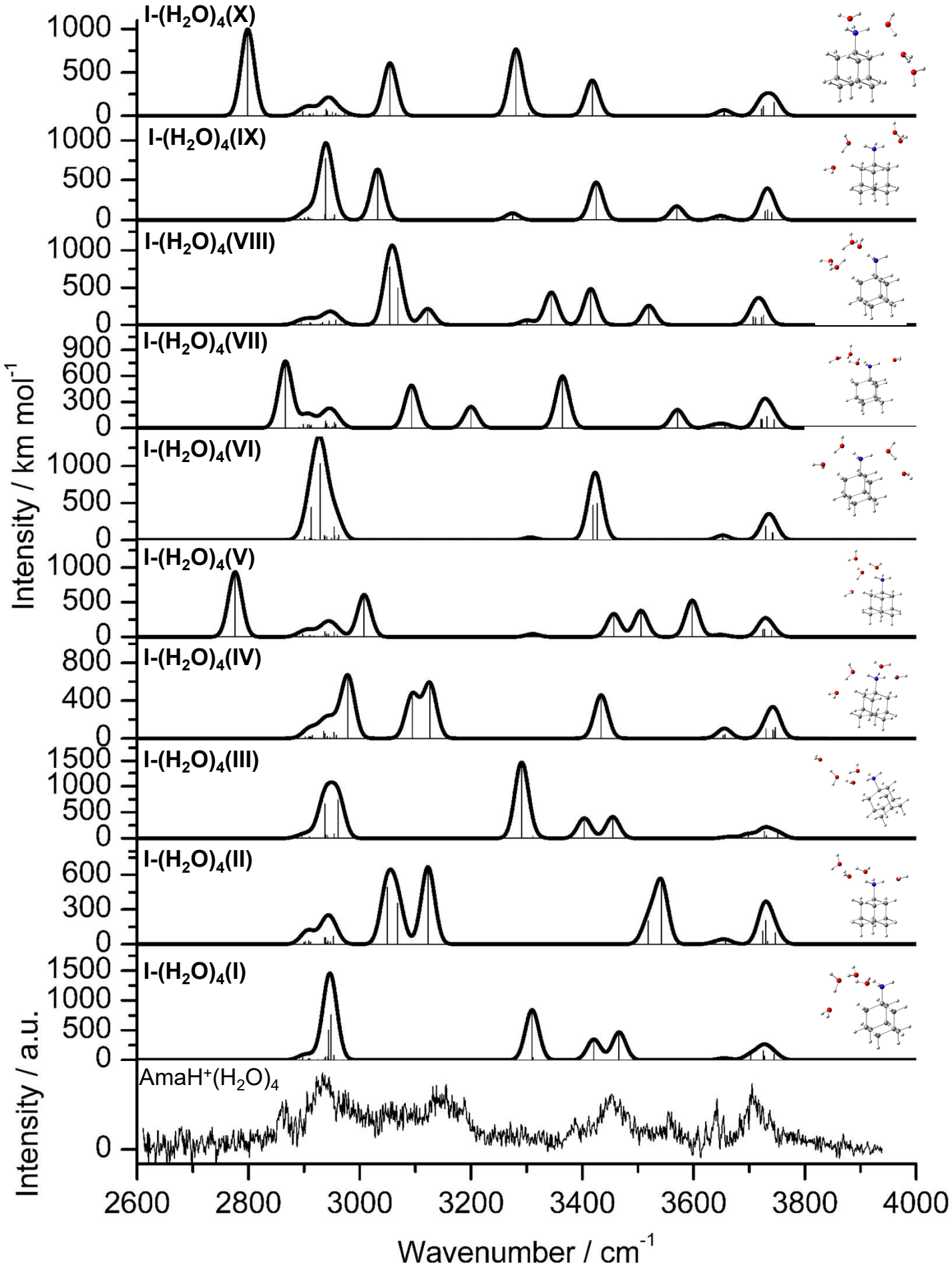

I-(H2O)4(X)
I-(H2O)4(IX)
I-(H2O)4(VIII)
I-(H2O)4(VII)
I-(H2O)4(VI)
I-(H2O)4(V)
I-(H2O)4(IV)
I-(H2O)4(III)
I-(H2O)4(II)
I-(H2O)4(I)
AmaH+(H2O)4
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
2600
2800
3000
3200
3400
3600
3800
4000

Figure S19

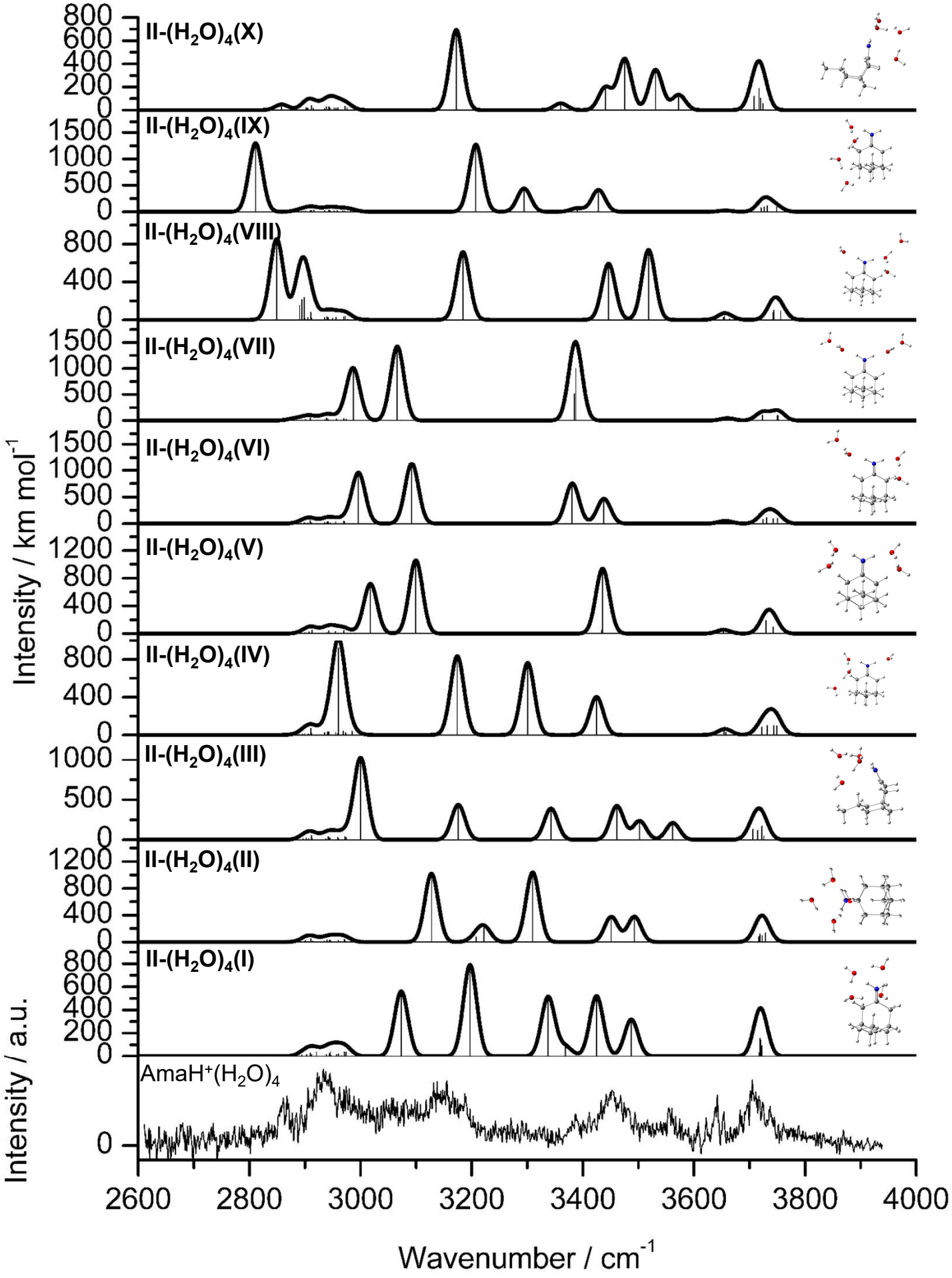

II-(H2O)4(X)
II-(H2O)4(IX)
II-(H2O)4(VIII)
II-(H2O)4(VII)
II-(H2O)4(VI)
II-(H2O)4(V)
II-(H2O)4(IV)
II-(H2O)4(III)
II-(H2O)4(II)
II-(H2O)4(I)
AmaH+(H2O)4
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
2600
2800
3000
3200
3400
3600
3800
4000

Figure S20

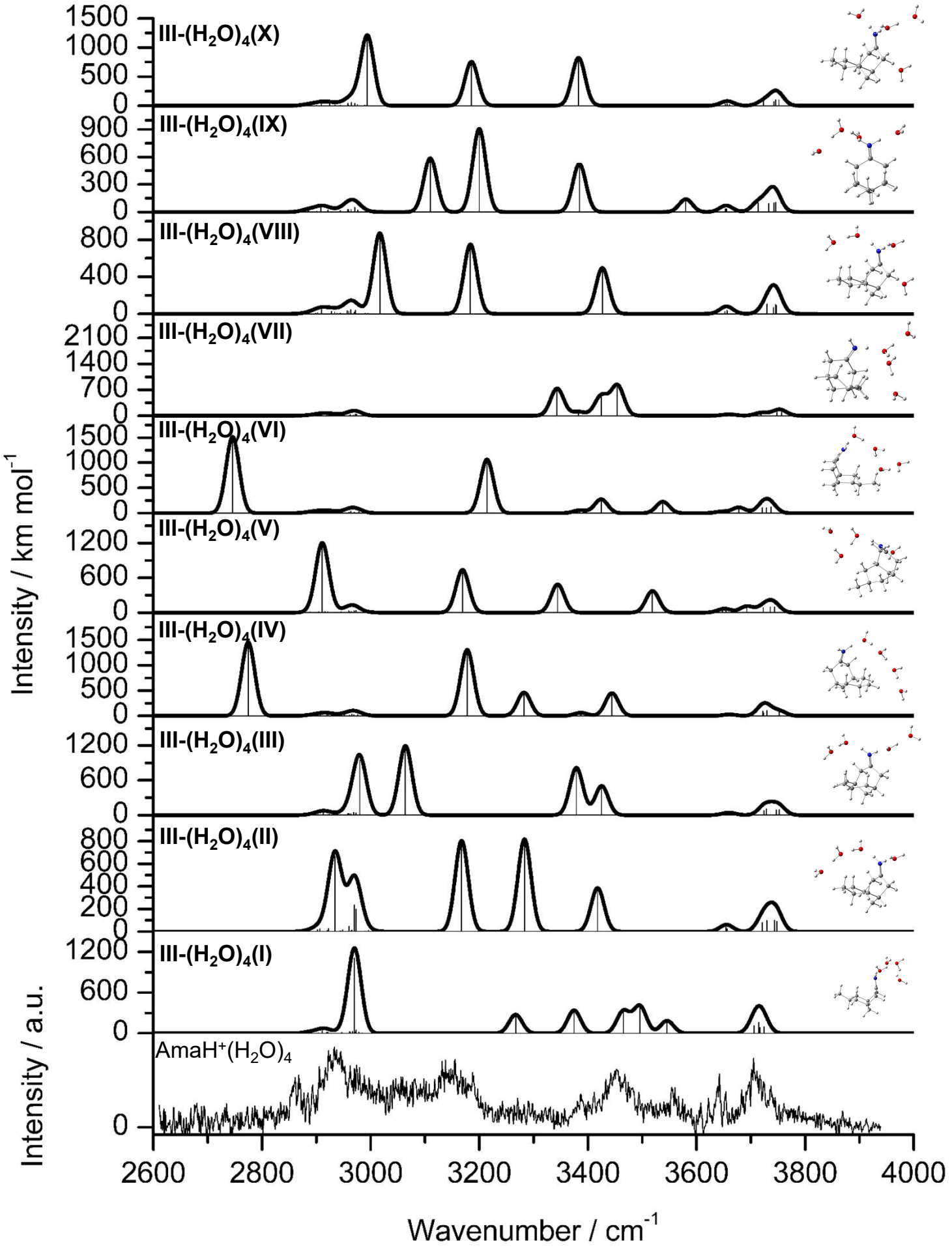

III-(H2O)4(X)
III-(H2O)4(IX)
III-(H2O)4(VIII)
III-(H2O)4(VII)
III-(H2O)4(VI)
III-(H2O)4(V)
III-(H2O)4(IV)
III-(H2O)4(III)
III-(H2O)4(II)
III-(H2O)4(I)
AmaH+(H2O)4
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1

Figure S21

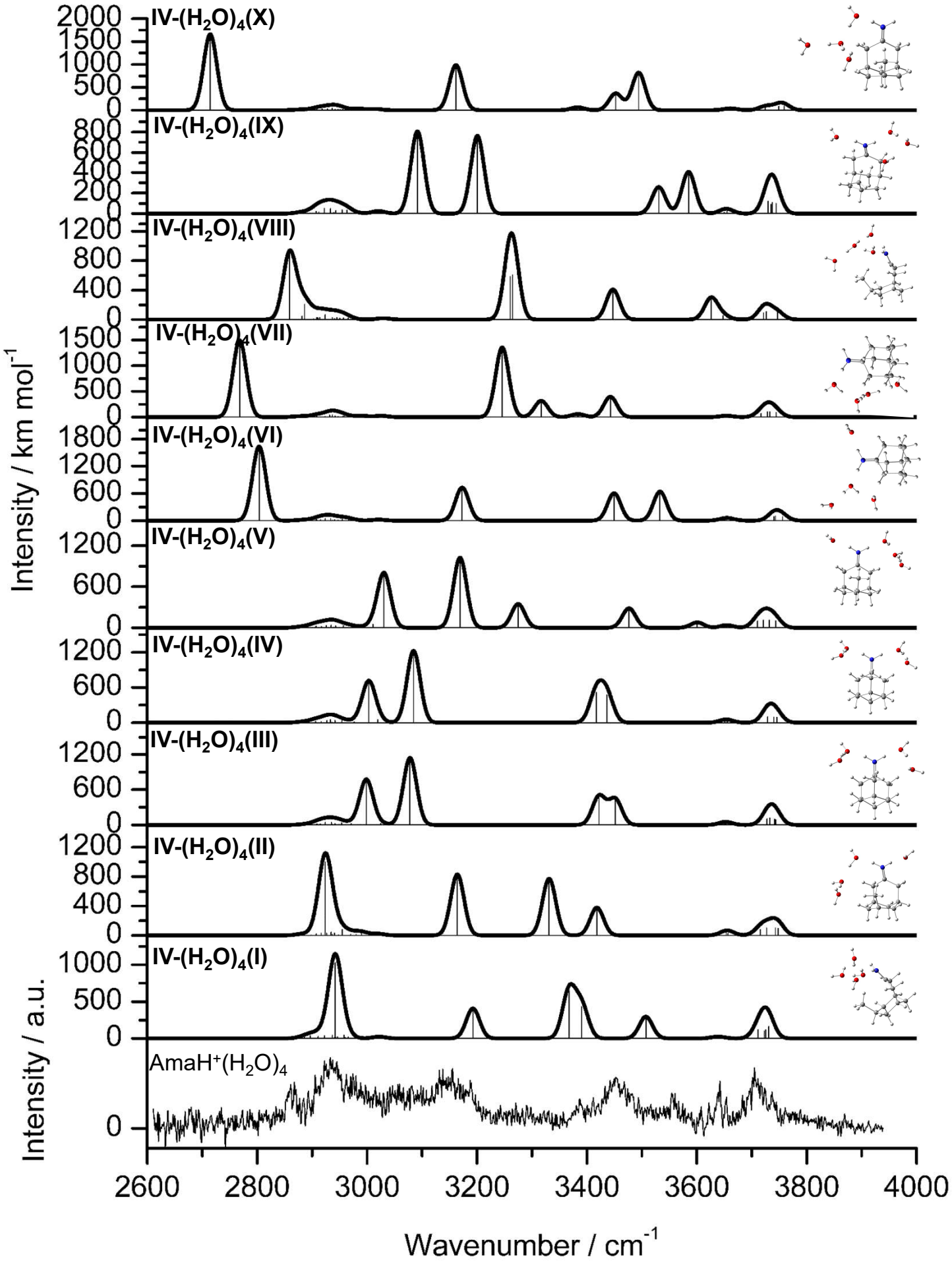
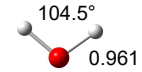
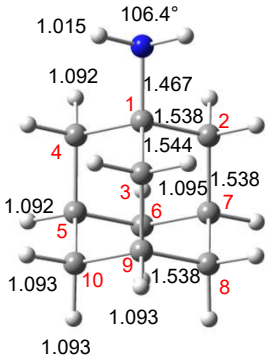

IV-(H2O)4(X)
IV-(H2O)4(IX)
IV-(H2O)4(VIII)
IV-(H2O)4(VII)
IV-(H2O)4(VI)
IV-(H2O)4(V)
IV-(H2O)4(IV)
IV-(H2O)4(III)
IV-(H2O)4(II)
IV-(H2O)4(I)
AmaH+(H2O)4
Intensity / km mol-1
Intensity / a.u.
Wavenumber / cm-1
2600
2800
3000
3200
3400
3600
3800
4000

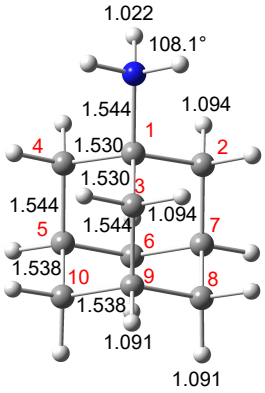
Figure S22



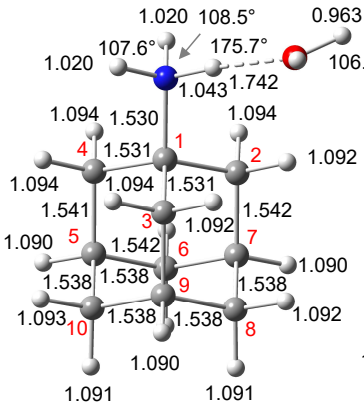
H_2O (C_{2v})



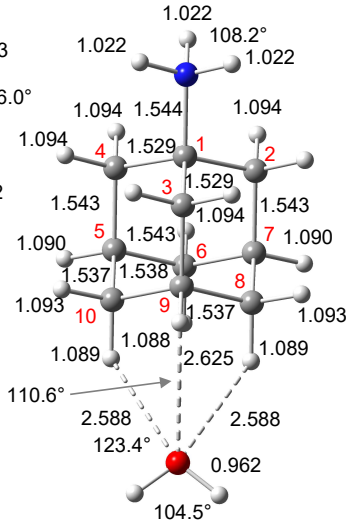
Ama (C_s)



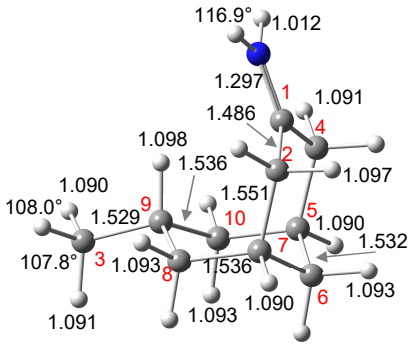
I (C_{3v})



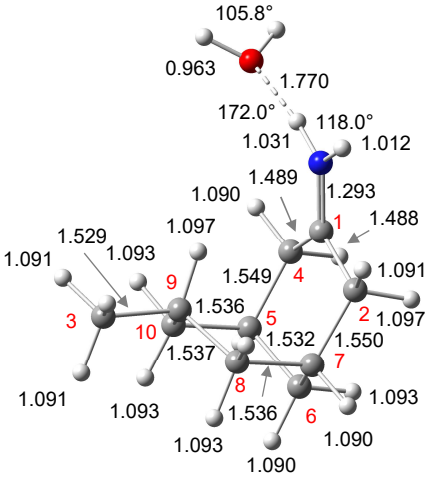
I-H_2O(I)



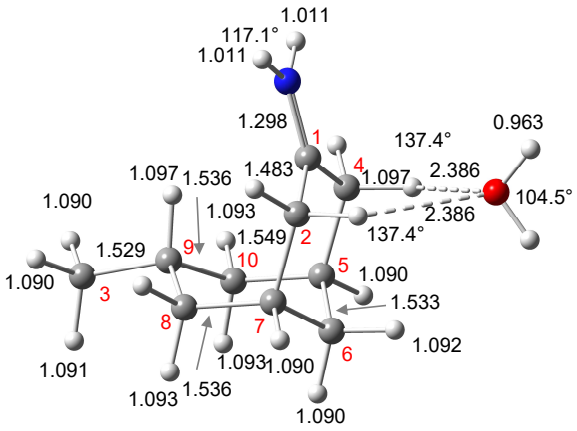
I-H_2O(II)



II (C_s)

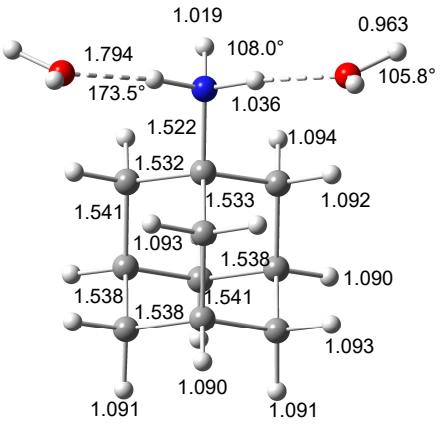


II-H_2O(I)

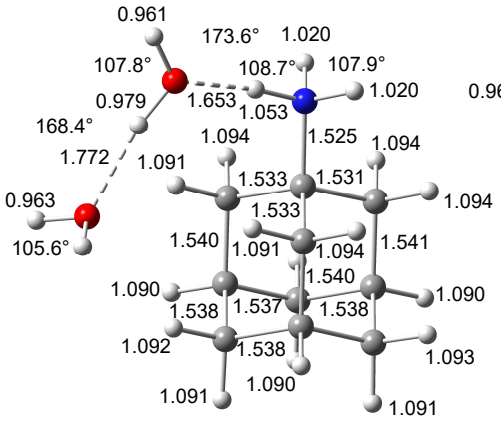


II-H_2O(II)

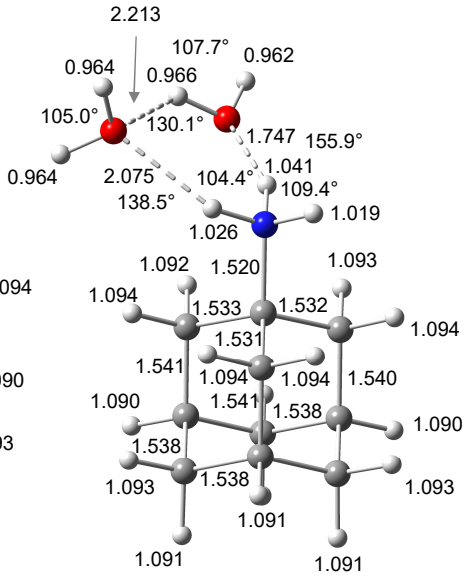
Figure S23



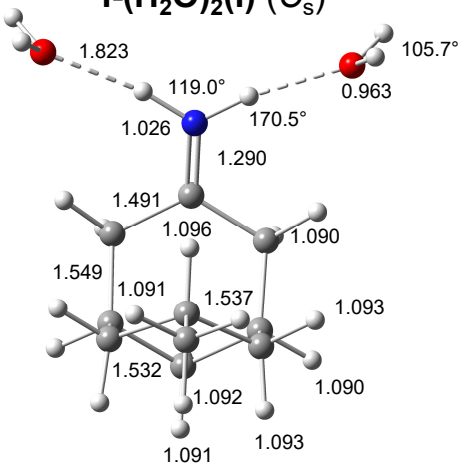
I-$(H_2O)_2$(I) (C_s)



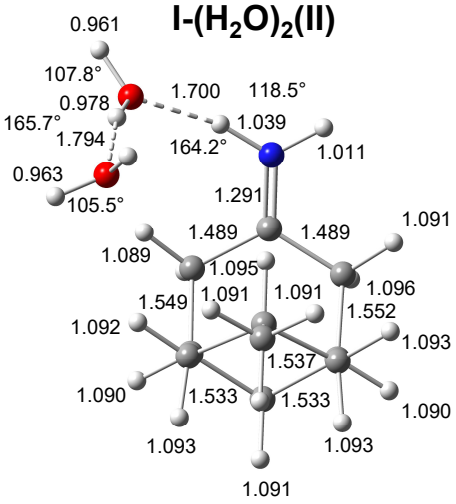
I-$(H_2O)_2$(II)



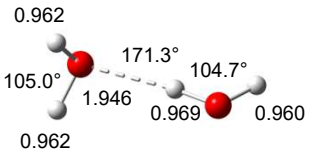
I-$(H_2O)_2$(III)



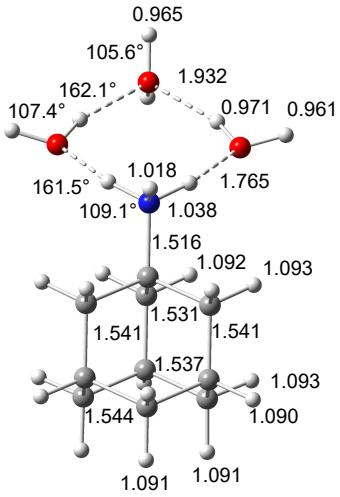
II-$(H_2O)_2$(I) (C_s)



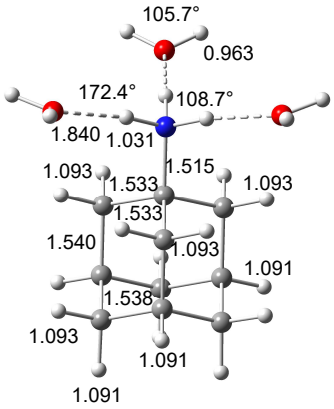
II-$(H_2O)_2$(II)



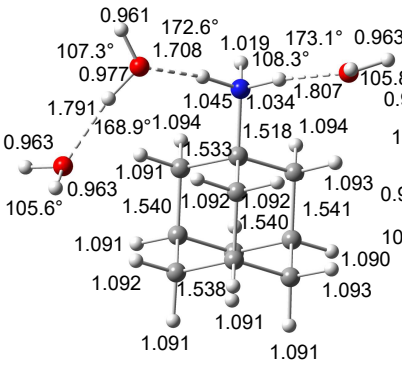
$(H_2O)_2$ (C_s)



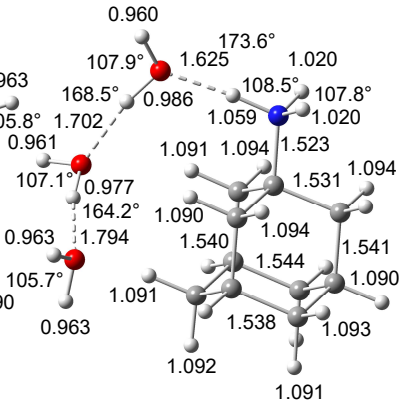
I-(H_2O)$_3$(I) (C_s)



I-(H_2O)$_3$(II) (C_{3v})

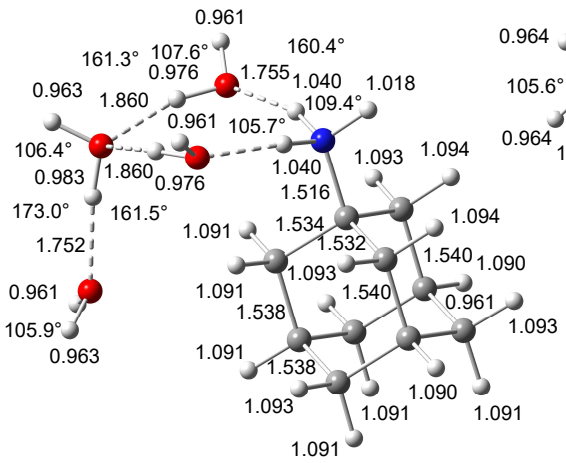


I-(H_2O)$_3$(III)

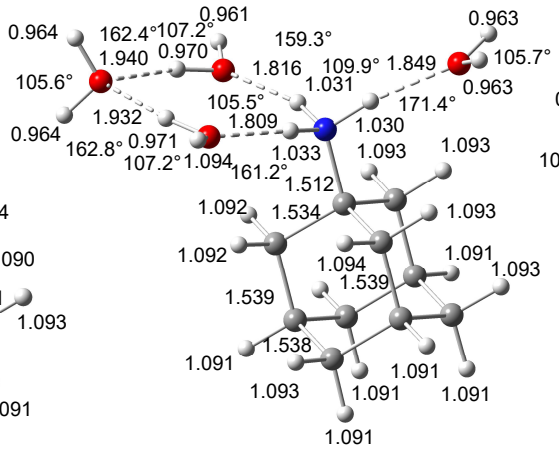


I-(H_2O)$_3$(IV)

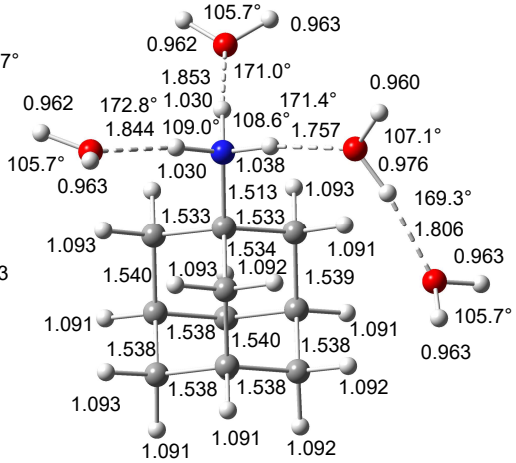
Figure S24



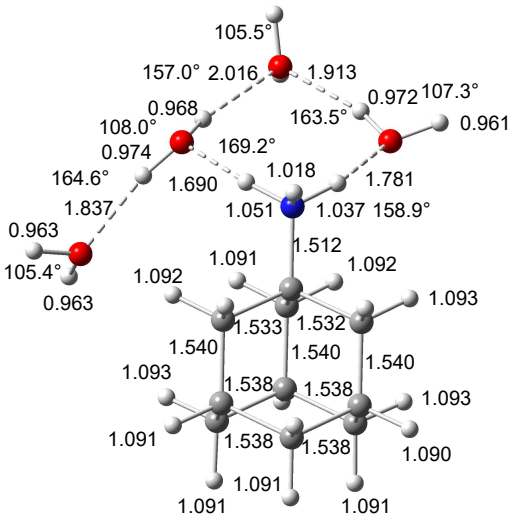
I-(H_2O)$_4$(I)



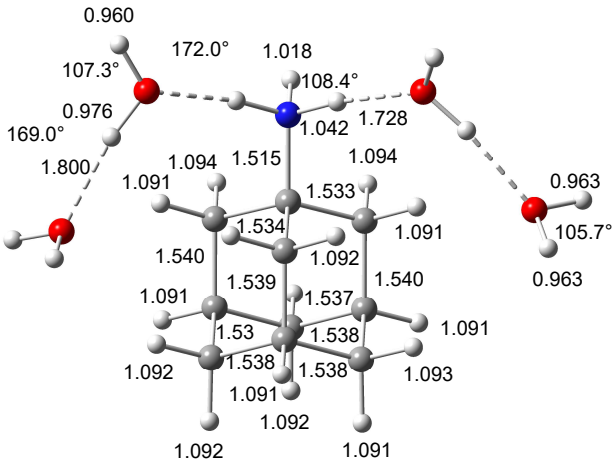
I-(H_2O)$_4$(II)



I-(H_2O)$_4$(IV)



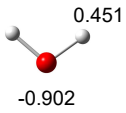
I-(H_2O)$_4$(V)



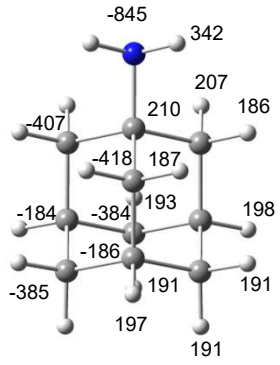
I-(H_2O)$_4$(VI) (C_s)

Figure S25

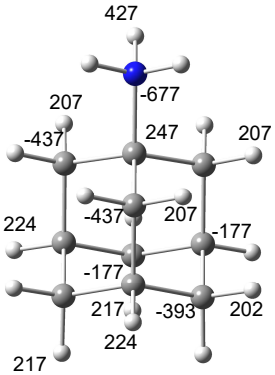
Figure S26



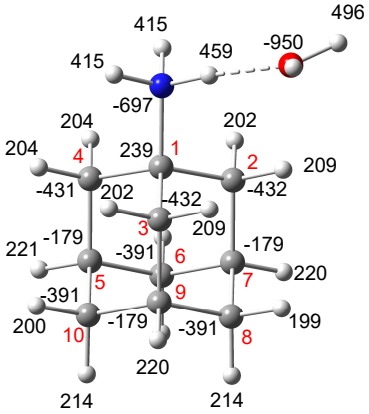
H_2O (C_{2v})



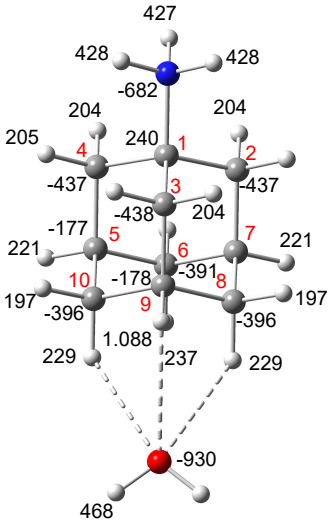
Ama (C_s)



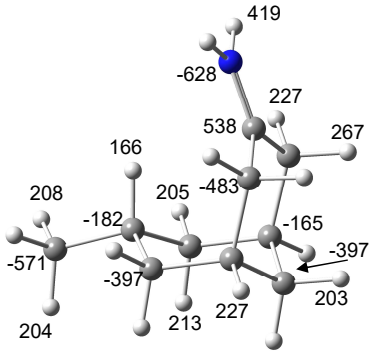
I (C_{3v})



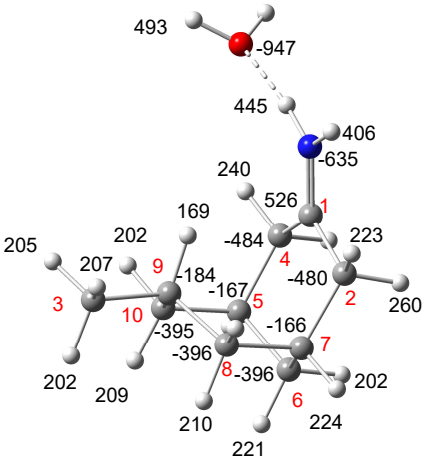
I-H_2O(I)



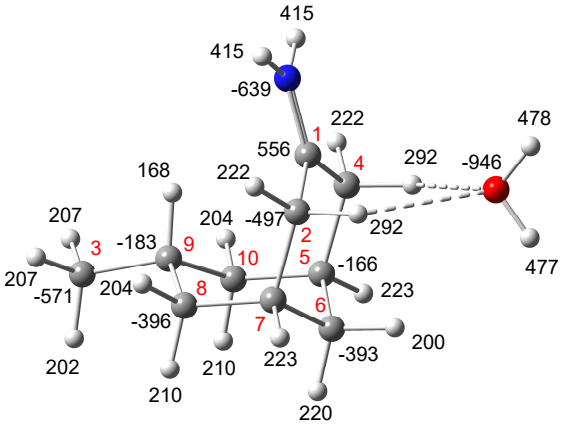
I-H_2O(II)



II (C_s)

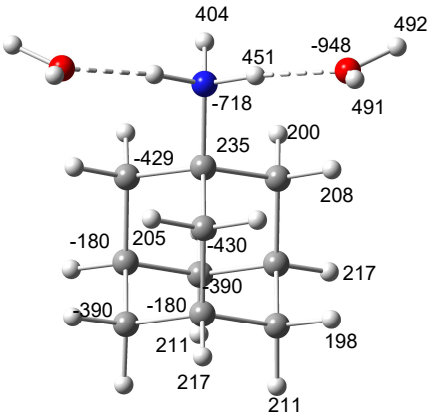


II-H_2O(I)

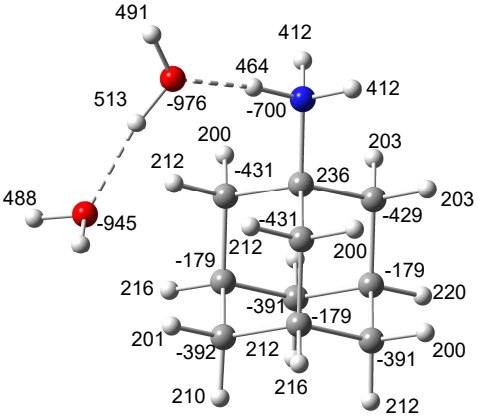


II-H_2O(II)

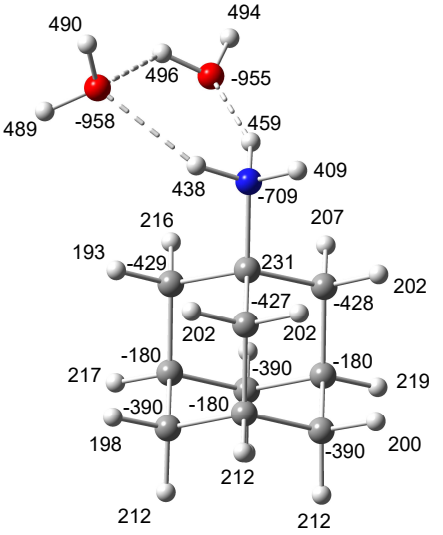
Figure S27



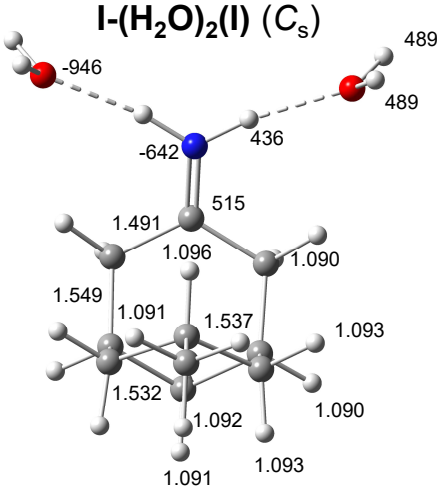
I-$(H_2O)_2$(I) (C_s)



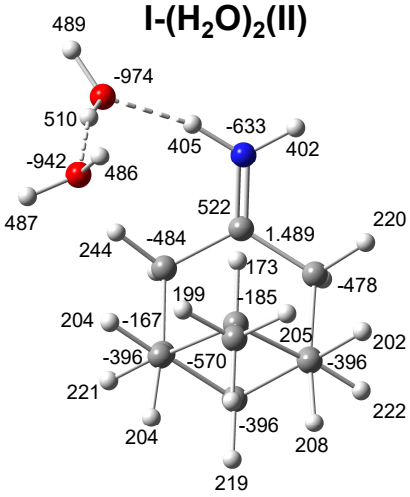
I-$(H_2O)_2$(II)



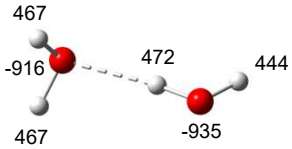
I-$(H_2O)_2$(III)



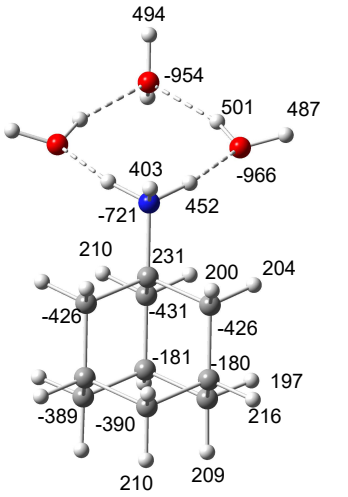
II-$(H_2O)_2$(I) (C_s)



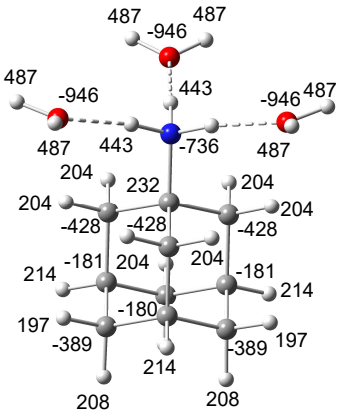
II-$(H_2O)_2$(II)



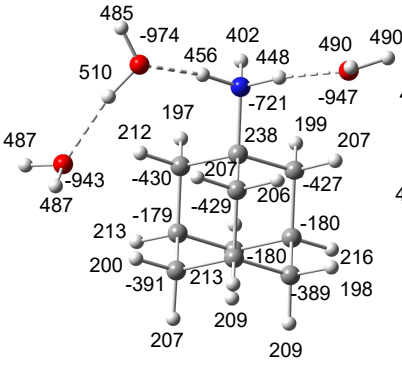
$(H_2O)_2$



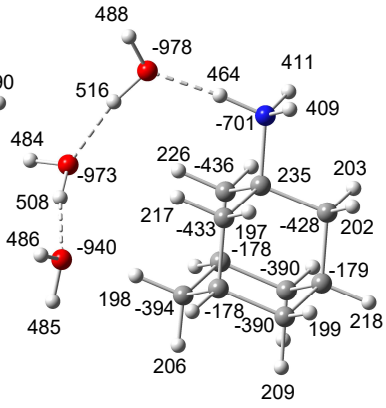
I-(H_2O)$_3$(I) (C_S)



I-(H_2O)$_3$(II) (C_{3v})

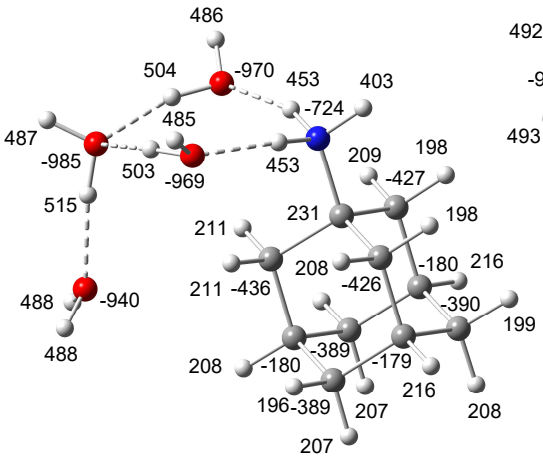


I-(H_2O)$_3$(III)

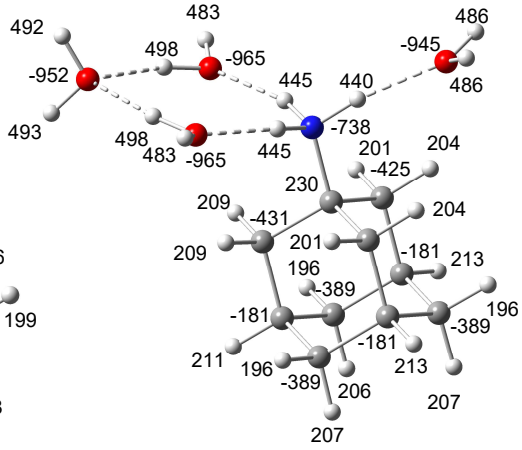


I-(H_2O)$_3$(IV)

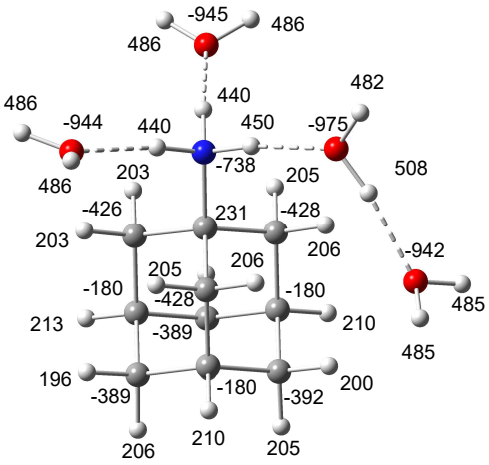
Figure S28



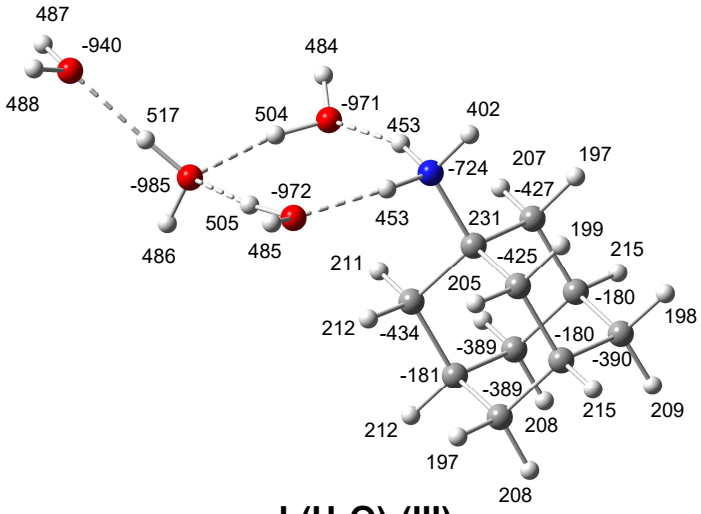
I-(H_2O)$_4$(I)



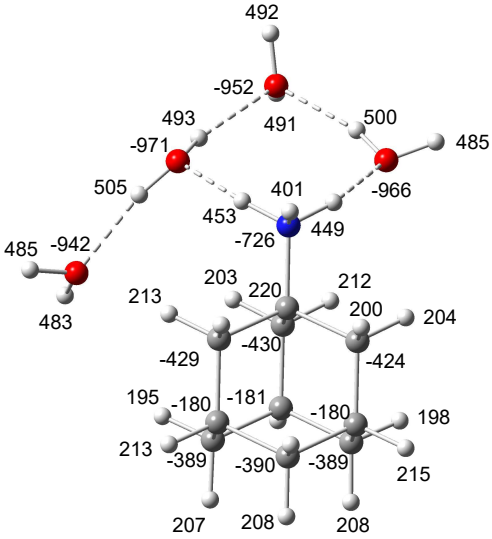
I-(H_2O)$_4$(II)



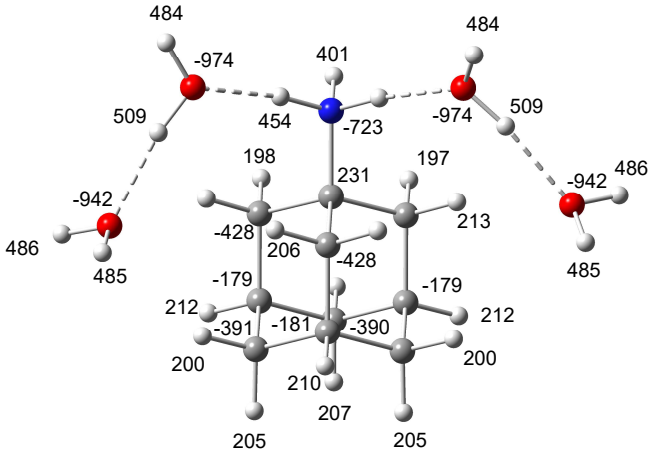
I-(H_2O)$_4$(IV)



I-(H_2O)$_4$(III)

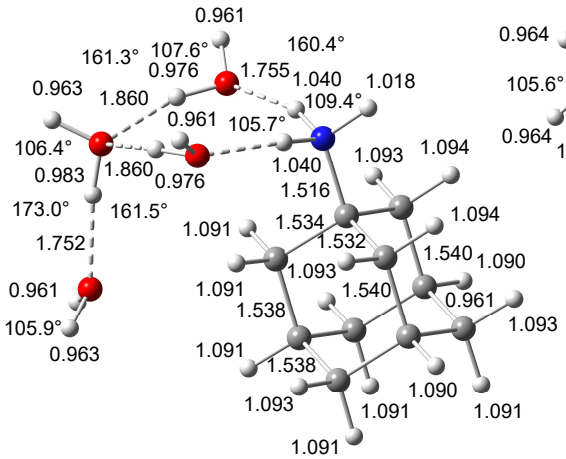


I-(H_2O)$_4$(V)

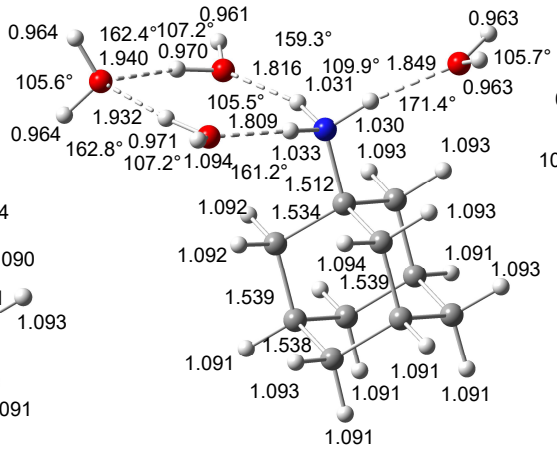


I-(H_2O)$_4$(VI) (C_s)

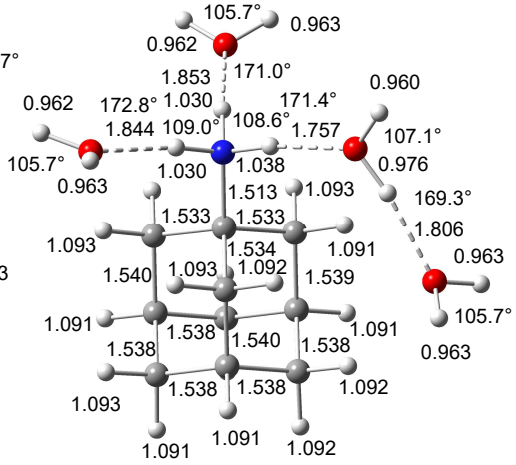
Figure S29



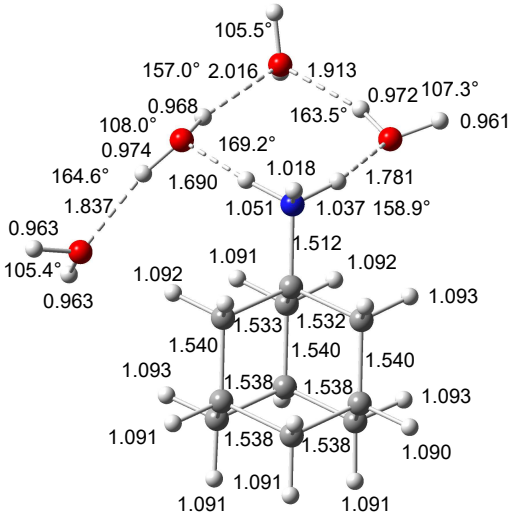
I-(H_2O)$_4$(I)



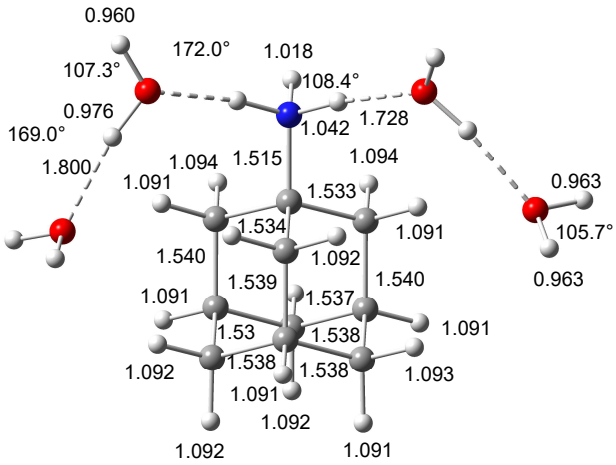
I-(H_2O)$_4$(II)



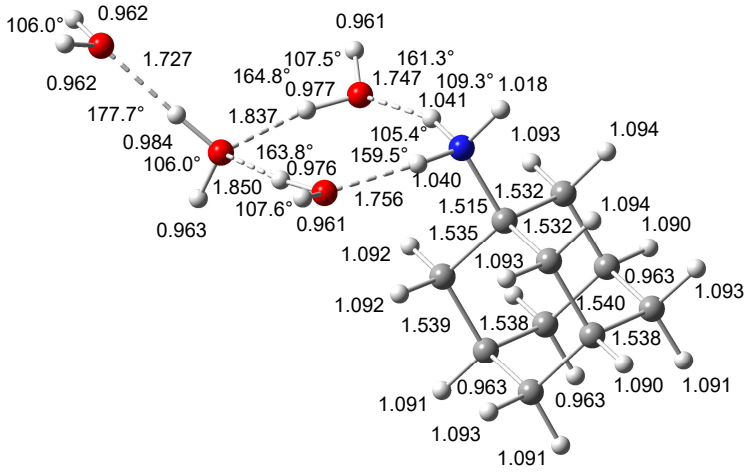
I-(H_2O)$_4$(IV)



I-(H_2O)$_4$(V)



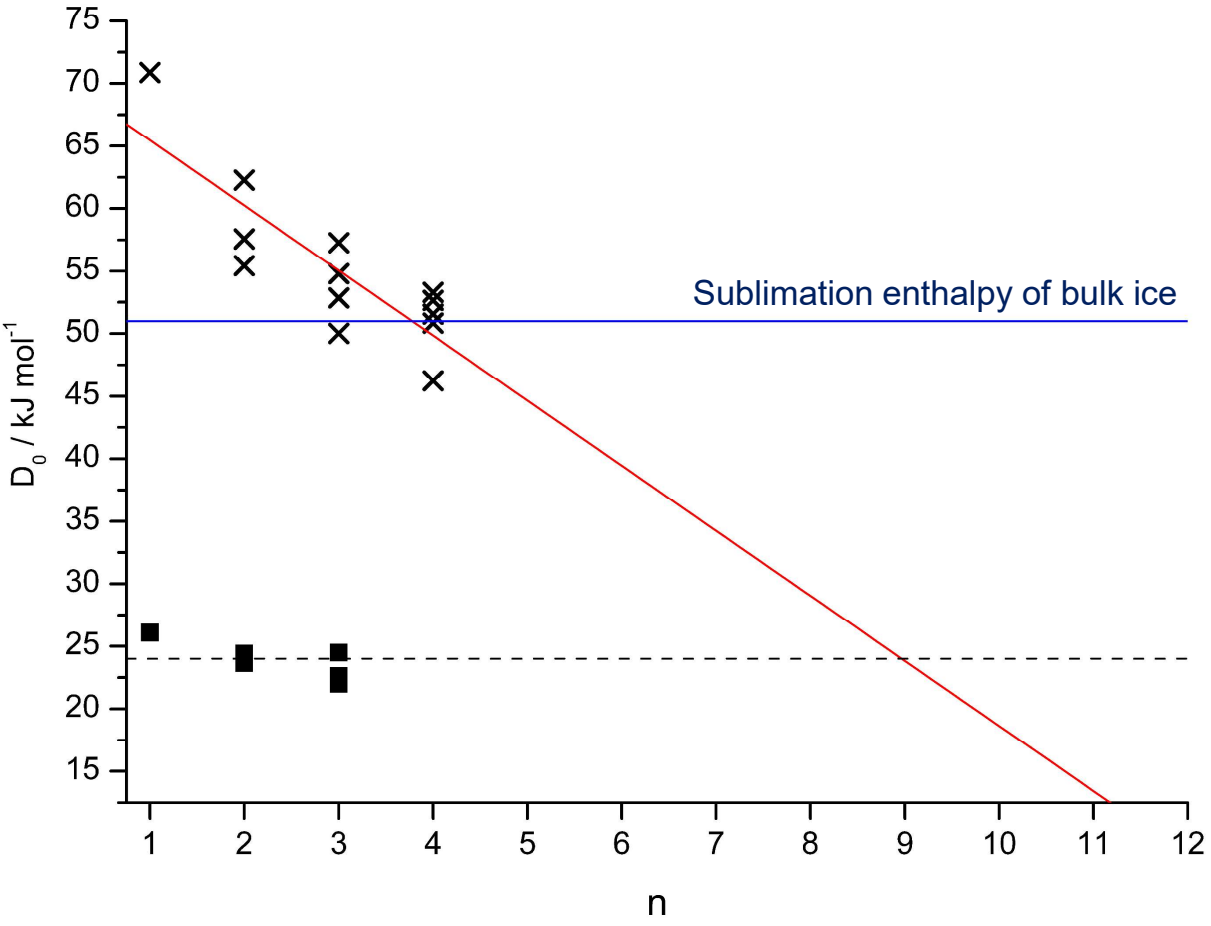
I-(H_2O)$_4$(VI) (C_s)



I-(H_2O)$_4$(III)

Figure S30

Figure S31


Sublimation enthalpy of bulk ice
D_0 / kJ mol^{-1}
n
75
70
65
60
55
50
45
40
35
30
25
20
15
1
2
3
4
5
6
7
8
9
10
11
12

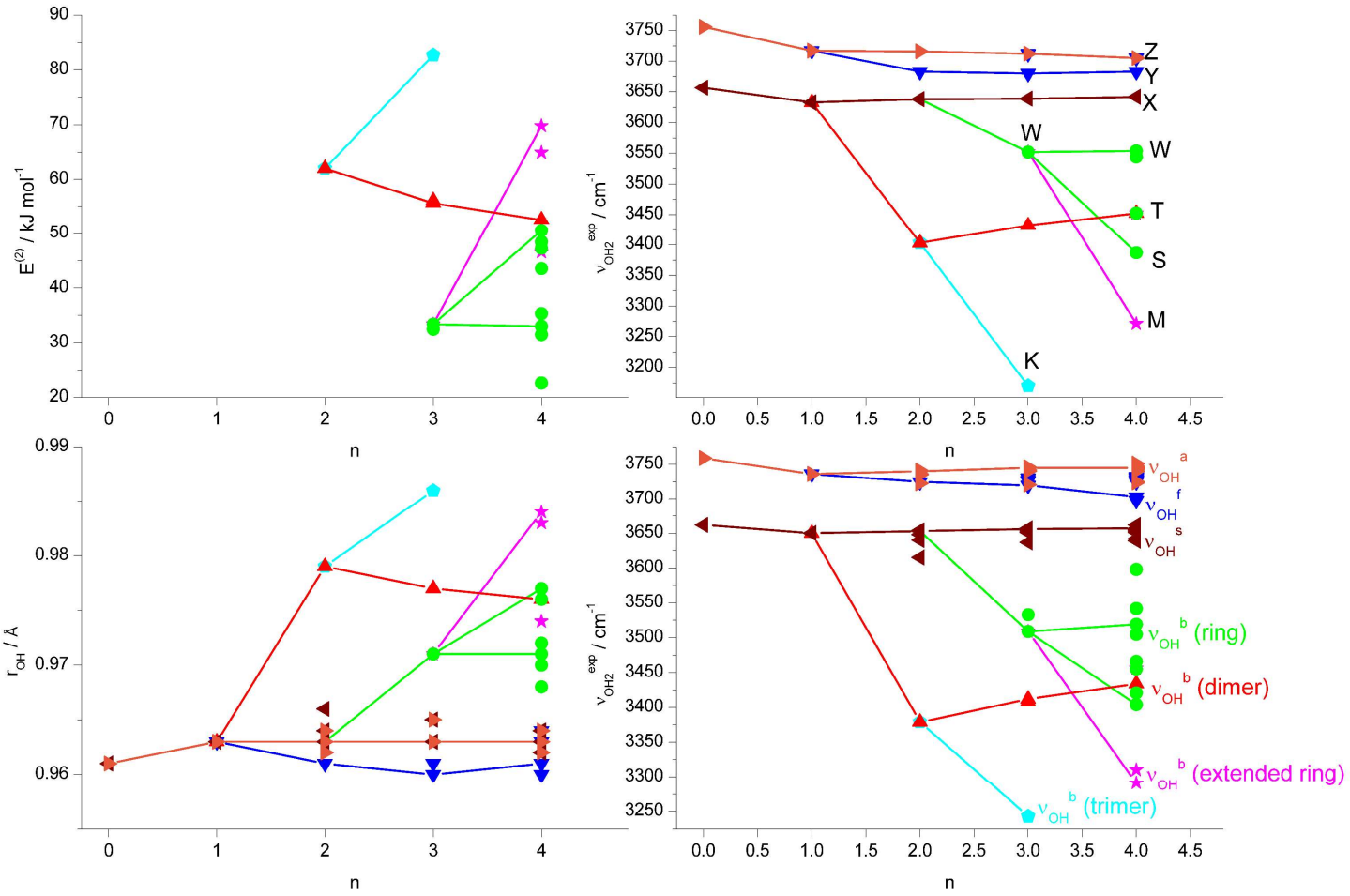
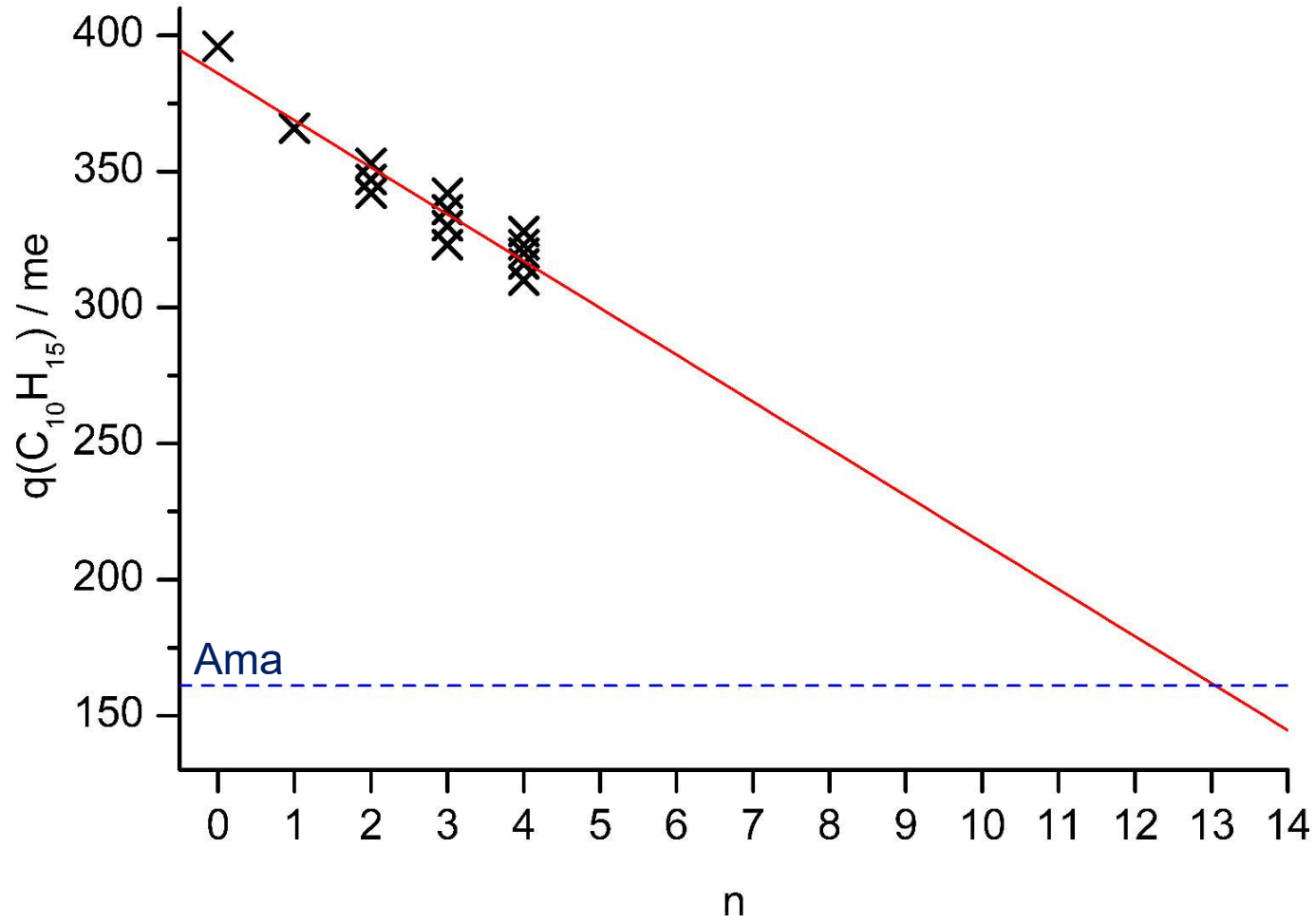
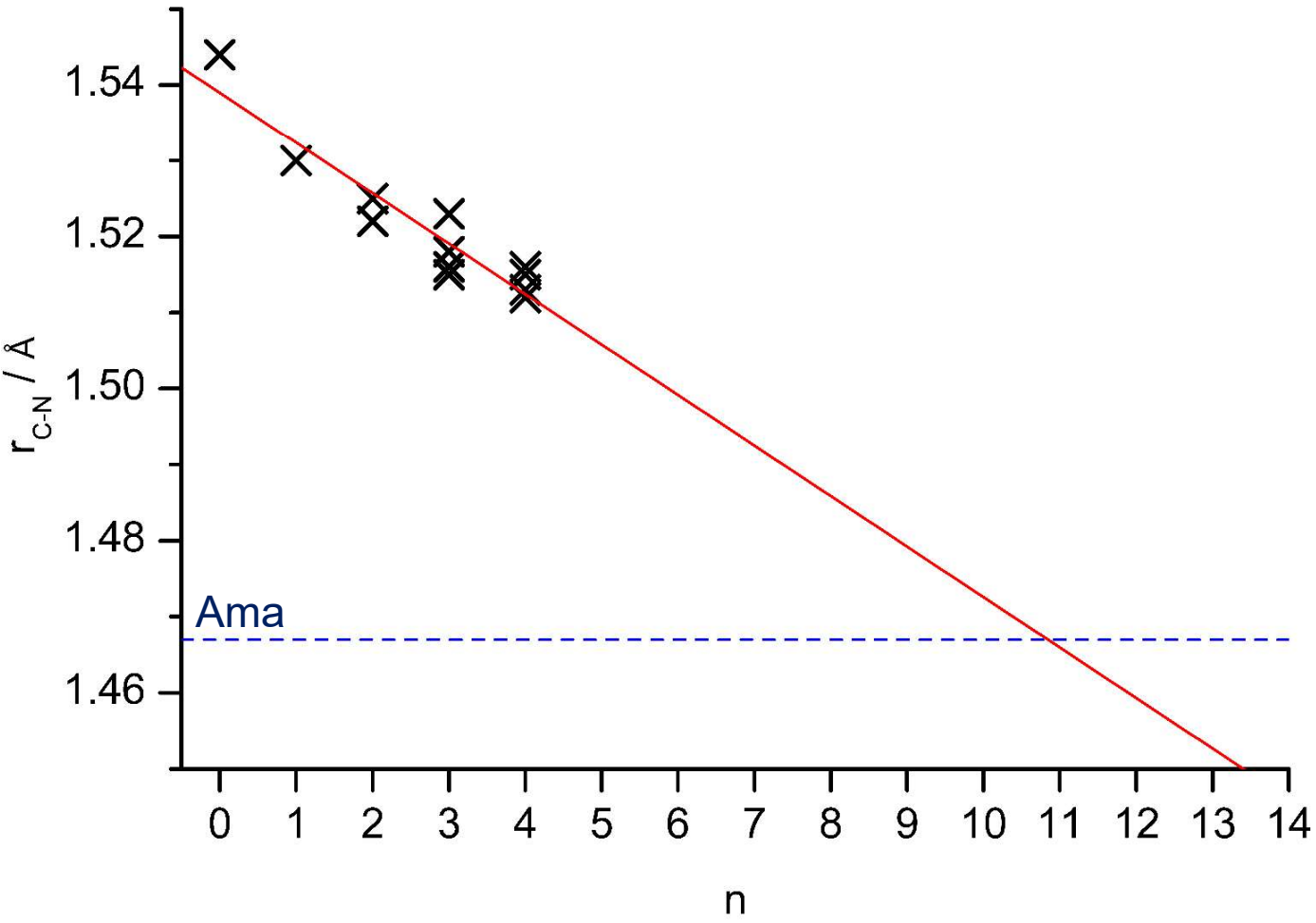

E(2) / kJ mol-1
n
rOH / Å
n
νexp OH2 / cm-1
Z
Y
X
W
W
T
S
M
K
n
νexp OH2 / cm-1
νOH a
νOH f
νOH s
νOH b (ring)
νOH b (dimer)
νOH b (extended ring)
νOH b (trimer)
n

Figure S32

Figure S33


400
350
300
250
200
150
q(C10H15) / me
Ama
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14
n


1.54
1.52
1.50
1.48
1.46
rC-N / Å
Ama
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14
n

Cartesian coordiantes (Å) and energies (hartree) of relevant structures (B3LYP-D3/cc-pVTZ)

Ama

1	6	0	-1.011128	1.127081	1.255703
2	1	0	-0.514261	1.502017	2.154656
3	1	0	-2.038105	1.501352	1.276200
4	6	0	-1.011128	-0.410783	1.256075
5	1	0	-1.521728	-0.777686	2.149414
6	6	0	-0.287239	1.641427	0.000000
7	1	0	-0.281288	2.733996	0.000000
8	6	0	1.158945	1.116612	0.000000
9	1	0	1.696050	1.483603	0.880296
10	1	0	1.696050	1.483603	-0.880296
11	6	0	0.437377	-0.927013	1.249983
12	1	0	0.460778	-2.018647	1.262920
13	1	0	0.962767	-0.582715	2.146909
14	6	0	1.182128	-0.427579	0.000000
15	6	0	0.437377	-0.927013	-1.249983
16	1	0	0.962767	-0.582715	-2.146909
17	1	0	0.460778	-2.018647	-1.262920
18	6	0	-1.736812	-0.921403	0.000000
19	1	0	-2.774040	-0.575535	0.000000
20	1	0	-1.762177	-2.014271	0.000000
21	6	0	-1.011128	1.127081	-1.255703
22	1	0	-2.038105	1.501352	-1.276200
23	1	0	-0.514261	1.502017	-2.154656
24	6	0	-1.011128	-0.410783	-1.256075
25	1	0	-1.521728	-0.777686	-2.149414
26	7	0	2.535235	-0.993222	0.000000
27	1	0	3.048130	-0.666622	-0.812633
28	1	0	3.048130	-0.666622	0.812633

Sum of electronic and zero-point Energies= -445.999992
Sum of electronic and thermal Energies= -445.991746
Sum of electronic and thermal Enthalpies= -445.990802
Sum of electronic and thermal Free Energies= -446.032017

AmaH$^+$(I)

1	7	0	0.000000	0.000000	2.705063
2	1	0	0.000000	-0.955384	3.067886
3	1	0	-0.827387	0.477692	3.067886
4	1	0	0.827387	0.477692	3.067886
5	6	0	0.000000	0.000000	1.161528
6	6	0	0.000000	1.454567	0.688278
7	1	0	-0.884328	1.977269	1.063861
8	1	0	0.884328	1.977269	1.063861
9	6	0	-1.259692	-0.727284	0.688278
10	1	0	-1.270201	-1.754485	1.063861
11	1	0	-2.154529	-0.222784	1.063861
12	6	0	1.259692	-0.727284	0.688278
13	1	0	2.154529	-0.222784	1.063861
14	1	0	1.270201	-1.754485	1.063861
15	6	0	0.000000	1.452026	-0.855237
16	1	0	0.000000	2.485024	-1.201872
17	6	0	-1.257491	-0.726013	-0.855237
18	1	0	-2.152094	-1.242512	-1.201872
19	6	0	1.257491	-0.726013	-0.855237
20	1	0	2.152094	-1.242512	-1.201872
21	6	0	-1.258890	0.726821	-1.359309
22	6	0	1.258890	0.726821	-1.359309
23	6	0	-0.000000	-1.453641	-1.359309
24	1	0	-2.158547	1.246238	-1.021366
25	1	0	-1.278091	0.737906	-2.449633
26	1	0	2.158547	1.246238	-1.021366
27	1	0	1.278091	0.737906	-2.449633
28	1	0	-0.000000	-2.492475	-1.021366
29	1	0	-0.000000	-1.475813	-2.449633

Sum of electronic and zero-point Energies= -446.364241
Sum of electronic and thermal Energies= -446.355795
Sum of electronic and thermal Enthalpies= -446.354850
Sum of electronic and thermal Free Energies= -446.395459

AmaH$^+$(II)

1	6	0	-1.032218	-0.080276	1.248536
2	6	0	-1.920024	-0.103457	0.000000
3	6	0	-1.032218	-0.080276	-1.248536
4	6	0	-0.174398	1.193527	-1.268059
5	6	0	0.671935	1.384485	0.000000
6	6	0	-0.174398	1.193527	1.268059
7	6	0	-0.174398	-1.372459	1.283463
8	6	0	1.378998	2.740017	0.000000
9	6	0	0.523455	-1.643946	0.000000
10	6	0	-0.174398	-1.372459	-1.283463
11	7	0	1.710185	-2.166783	0.000000
12	1	0	-1.651876	-0.102280	2.144793
13	1	0	-2.569775	-0.981990	0.000000
14	1	0	-2.571968	0.770259	0.000000
15	1	0	-1.651876	-0.102280	-2.144793
16	1	0	0.471257	1.202982	-2.149429
17	1	0	-0.848000	2.047625	-1.374939
18	1	0	0.648746	3.551113	0.000000
19	1	0	0.471257	1.202982	2.149429
20	1	0	-0.848000	2.047625	1.374939
21	1	0	0.529042	-1.376449	2.117771
22	1	0	-0.851518	-2.223682	1.429220
23	1	0	2.008692	2.857719	-0.882285
24	1	0	2.008692	2.857719	0.882285
25	1	0	0.529042	-1.376449	-2.117771
26	1	0	-0.851518	-2.223682	-1.429220
27	1	0	2.195815	-2.378022	0.862392
28	1	0	2.195815	-2.378022	-0.862392
29	1	0	1.460851	0.620205	0.000000

Sum of electronic and zero-point Energies= -446.363086
Sum of electronic and thermal Energies= -446.353254
Sum of electronic and thermal Enthalpies= -446.352309
Sum of electronic and thermal Free Energies= -446.397259

AmaH$^+$(III)

1	6	0	0.906969	-0.296697	1.246490
2	6	0	1.667525	-0.757854	0.000000
3	6	0	0.906969	-0.296697	-1.246490
4	6	0	-0.539532	-0.868885	-1.270651
5	6	0	-0.913395	-1.649556	0.000000
6	6	0	-0.539532	-0.868885	1.270651
7	6	0	0.906969	1.267387	1.271436
8	6	0	-2.392481	-2.030142	0.000000
9	6	0	0.344785	1.775760	0.000000
10	6	0	0.906969	1.267387	-1.271436
11	7	0	-0.681722	2.565511	0.000000
12	1	0	1.442834	-0.603444	2.142869
13	1	0	2.684396	-0.359833	0.000000
14	1	0	1.764590	-1.842406	0.000000
15	1	0	1.442834	-0.603444	-2.142869
16	1	0	-1.265617	-0.060210	-1.407496
17	1	0	-0.662583	-1.517986	-2.136895
18	1	0	-0.335073	-2.576938	0.000000
19	1	0	-1.265617	-0.060210	1.407496
20	1	0	-0.662583	-1.517986	2.136895
21	1	0	0.363962	1.650985	2.135132
22	1	0	1.942799	1.612172	1.337199
23	1	0	-2.647755	-2.619608	-0.880911
24	1	0	-2.647755	-2.619608	0.880911
25	1	0	0.363962	1.650985	-2.135132
26	1	0	1.942799	1.612172	-1.337199
27	1	0	-1.097319	2.892752	0.863023
28	1	0	-1.097319	2.892752	-0.863023
29	1	0	-3.025964	-1.139628	0.000000

Sum of electronic and zero-point Energies= -446.353807
Sum of electronic and thermal Energies= -446.343818
Sum of electronic and thermal Enthalpies= -446.342874
Sum of electronic and thermal Free Energies= -446.388567

AmaH$^+$(IV)

1	6	0	-0.573444	-1.316962	1.284082
2	1	0	-1.137686	-0.941170	2.140379
3	1	0	-0.401991	-2.376871	1.482034
4	6	0	0.821153	-0.667853	1.243741
5	1	0	1.355380	-0.986435	2.139060
6	6	0	-1.428799	-1.193903	0.000000
7	1	0	-2.092472	-2.060100	0.000000
8	6	0	-2.371882	0.017165	0.000000
9	1	0	-3.015790	-0.001197	0.879919
10	1	0	-1.865043	0.980393	0.000000
11	6	0	0.821153	0.878044	1.290438
12	1	0	1.846003	1.204899	1.515446
13	1	0	0.189284	1.270896	2.089518
14	6	0	0.497875	1.540261	0.000000
15	6	0	0.821153	0.878044	-1.290438
16	1	0	0.189284	1.270896	-2.089518
17	1	0	1.846003	1.204899	-1.515446
18	6	0	1.584049	-1.129779	0.000000
19	1	0	1.662105	-2.216994	0.000000
20	1	0	2.605267	-0.739745	0.000000
21	6	0	-0.573444	-1.316962	-1.284082
22	1	0	-0.401991	-2.376871	-1.482034
23	1	0	-1.137686	-0.941170	-2.140379
24	6	0	0.821153	-0.667853	-1.243741
25	1	0	1.355380	-0.986435	-2.139060
26	7	0	-0.007701	2.733743	0.000000
27	1	0	-0.220072	3.219394	-0.862291
28	1	0	-0.220072	3.219394	0.862291
29	1	0	-3.015790	-0.001197	-0.879919

Sum of electronic and zero-point Energies= -446.353004
Sum of electronic and thermal Energies= -446.342963
Sum of electronic and thermal Enthalpies= -446.342018
Sum of electronic and thermal Free Energies= -446.387553

Ama$^+$(I)

1	6	0	-1.009933	1.119927	1.260815
2	1	0	-0.519111	1.502470	2.157785
3	1	0	-2.034331	1.491912	1.270028
4	6	0	-1.009933	-0.418569	1.258258
5	1	0	-1.512657	-0.782974	2.154281
6	6	0	-0.292961	1.610622	0.000000
7	1	0	-0.245778	2.709641	0.000000
8	6	0	1.169160	1.189049	0.000000
9	1	0	1.708022	1.497285	0.892533
10	1	0	1.708022	1.497285	-0.892533
11	6	0	0.436294	-0.931980	1.280099
12	1	0	0.450942	-2.023690	1.314481
13	1	0	0.966411	-0.567549	2.163360
14	6	0	1.172297	-0.507942	0.000000
15	6	0	0.436294	-0.931980	-1.280099
16	1	0	0.966411	-0.567549	-2.163360
17	1	0	0.450942	-2.023690	-1.314481
18	6	0	-1.725250	-0.938846	0.000000
19	1	0	-2.762343	-0.601654	0.000000
20	1	0	-1.747492	-2.030538	0.000000
21	6	0	-1.009933	1.119927	-1.260815
22	1	0	-2.034331	1.491912	-1.270028
23	1	0	-0.519111	1.502470	-2.157785
24	6	0	-1.009933	-0.418569	-1.258258
25	1	0	-1.512657	-0.782974	-2.154281
26	7	0	2.515855	-0.841720	0.000000
27	1	0	3.044730	-0.885075	-0.862169
28	1	0	3.044730	-0.885075	0.862169

Sum of electronic and zero-point Energies= -445.710234
Sum of electronic and thermal Energies= -445.701526
Sum of electronic and thermal Enthalpies= -445.700582
Sum of electronic and thermal Free Energies= -445.743151

Ama^{+}(II)

1	6	0	0.878102	-0.318597	1.247668
2	6	0	1.635327	-0.783226	0.000000
3	6	0	0.878102	-0.318597	-1.247668
4	6	0	-0.568901	-0.886083	-1.279077
5	6	0	-0.955442	-1.657448	0.000000
6	6	0	-0.568901	-0.886083	1.279077
7	6	0	0.878102	1.245884	1.270499
8	6	0	-2.392771	-2.036083	0.000000
9	6	0	0.309242	1.748203	0.000000
10	6	0	0.878102	1.245884	-1.270499
11	7	0	-0.730363	2.520450	0.000000
12	1	0	1.416275	-0.624513	2.143007
13	1	0	2.653570	-0.389067	0.000000
14	1	0	1.727499	-1.868303	0.000000
15	1	0	1.416275	-0.624513	-2.143007
16	1	0	-1.294078	-0.080902	-1.429269
17	1	0	-0.686147	-1.547069	-2.136958
18	1	0	-0.364623	-2.585563	0.000000
19	1	0	-1.294078	-0.080902	1.429269
20	1	0	-0.686147	-1.547069	2.136958
21	1	0	0.337490	1.629612	2.135471
22	1	0	1.913834	1.590934	1.332043
23	1	0	-2.899004	-2.268577	-0.926112
24	1	0	-2.899004	-2.268577	0.926112
25	1	0	0.337490	1.629612	-2.135471
26	1	0	1.913834	1.590934	-1.332043
27	1	0	-1.153201	2.838847	0.862911
28	1	0	-1.153201	2.838847	-0.862911

Sum of electronic and zero-point Energies= -445.694426
Sum of electronic and thermal Energies= -445.684131
Sum of electronic and thermal Enthalpies= -445.683187
Sum of electronic and thermal Free Energies= -445.730175

Ama^{+}(III)

1	6	0	0.923219	-0.687401	1.262057
2	6	0	1.637589	-1.195743	0.000000
3	6	0	0.923219	-0.687401	-1.262057
4	6	0	-0.547317	-1.154933	-1.263904
5	6	0	-1.207910	-0.715660	0.000000
6	6	0	-0.547317	-1.154933	1.263904
7	6	0	0.923219	0.854630	1.276496
8	6	0	-2.594709	-0.193357	0.000000
9	6	0	0.358830	1.379799	0.000000
10	6	0	0.923219	0.854630	-1.276496
11	7	0	-0.415579	2.442147	0.000000
12	1	0	1.432506	-1.047956	2.154616
13	1	0	2.679262	-0.869158	0.000000
14	1	0	1.650442	-2.286200	0.000000
15	1	0	1.432506	-1.047956	-2.154616
16	1	0	-1.072493	-0.775868	-2.141394
17	1	0	-0.569959	-2.249855	-1.329234
18	1	0	-1.072493	-0.775868	2.141394
19	1	0	-0.569959	-2.249855	1.329234
20	1	0	0.380399	1.243863	2.139094
21	1	0	1.953469	1.219584	1.347374
22	1	0	0.380399	1.243863	-2.139094
23	1	0	1.953469	1.219584	-1.347374
24	1	0	-0.742050	2.856458	0.860499
25	1	0	-0.742050	2.856458	-0.860499
26	1	0	-2.812381	0.398211	-0.890584
27	1	0	-2.812381	0.398211	0.890584
28	1	0	-3.311898	-1.026340	0.000000

Sum of electronic and zero-point Energies= -445.727708
Sum of electronic and thermal Energies= -445.717586
Sum of electronic and thermal Enthalpies= -445.716642
Sum of electronic and thermal Free Energies= -445.762902

AmaH$^+$(I)H$_2$O(I)

1	6	0	-0.281222	1.206481	-1.453772
2	1	0	-0.063312	0.952367	-2.493764
3	1	0	-0.932166	2.081547	-1.468850
4	6	0	1.016423	1.541694	-0.698125
5	1	0	1.536655	2.360319	-1.194397
6	6	0	-0.995763	0.039851	-0.751465
7	1	0	-1.917684	-0.212444	-1.269585
8	6	0	-0.078385	-1.198531	-0.756574
9	1	0	0.157251	-1.494226	-1.782884
10	1	0	-0.581354	-2.038568	-0.269542
11	6	0	1.940577	0.305460	-0.698527
12	1	0	2.872689	0.531763	-0.172800
13	1	0	2.192878	0.024336	-1.725041
14	6	0	1.200526	-0.835935	0.000717
15	6	0	0.890633	-0.476809	1.454919
16	1	0	0.394239	-1.312706	1.955833
17	1	0	1.815570	-0.259293	1.997180
18	6	0	0.691130	1.927077	0.754859
19	1	0	0.054149	2.812296	0.765475
20	1	0	1.605454	2.187258	1.293210
21	6	0	-1.326269	0.422665	0.699709
22	1	0	-1.997303	1.281717	0.705007
23	1	0	-1.872079	-0.383967	1.189334
24	6	0	-0.030167	0.761844	1.452462
25	1	0	-0.254991	1.026787	2.485258
26	7	0	2.121822	-2.074930	0.002880
27	1	0	1.664527	-2.863678	0.464682
28	1	0	2.355880	-2.356909	-0.950915
29	1	0	2.993083	-1.877610	0.499180
30	8	0	-4.255820	-0.869261	0.080536
31	1	0	-3.958945	-0.836760	-0.831899
32	1	0	-5.035628	-0.306417	0.114865

Sum of electronic and zero-point Energies= -522.829794
Sum of electronic and thermal Energies= -522.817865
Sum of electronic and thermal Enthalpies= -522.816921
Sum of electronic and thermal Free Energies= -522.867188

AmaH$^+$(I)H$_2$O(II)

1	6	0	1.728027	0.942402	0.000000
2	1	0	2.766718	0.603177	0.000000
3	1	0	1.748200	2.032559	0.000000
4	6	0	0.998746	0.439308	1.256970
5	1	0	1.516307	0.784609	2.151781
6	6	0	0.998746	0.439308	-1.256970
7	1	0	1.516307	0.784609	-2.151781
8	6	0	0.998746	-1.104185	-1.258926
9	1	0	2.025340	-1.482314	-1.268392
10	1	0	0.493717	-1.479345	-2.153912
11	6	0	0.998746	-1.104185	1.258926
12	1	0	0.493717	-1.479345	2.153912
13	1	0	2.025340	-1.482314	1.268392
14	6	0	0.270230	-1.576233	0.000000
15	6	0	-1.184023	-1.103016	0.000000
16	1	0	-1.705726	-1.479337	-0.884913
17	1	0	-1.705726	-1.479337	0.884913
18	6	0	-0.452614	0.945396	1.255709
19	1	0	-0.470702	2.034238	1.258081
20	1	0	-0.972101	0.610504	2.157151
21	6	0	-0.452614	0.945396	-1.255709
22	1	0	-0.470702	2.034238	-1.258081
23	1	0	-0.972101	0.610504	-2.157151
24	6	0	-1.179703	0.439577	0.000000
25	1	0	-2.203941	0.805322	0.000000
26	7	0	0.270421	-3.120557	0.000000
27	1	0	-0.207872	-3.481877	-0.827463
28	1	0	1.225705	-3.483309	0.000000
29	1	0	-0.207872	-3.481877	0.827463
30	8	0	-2.249567	3.429971	0.000000
31	1	0	-2.568368	3.925411	-0.760869
32	1	0	-2.568368	3.925411	0.760869

Sum of electronic and zero-point Energies= -522.812610
Sum of electronic and thermal Energies= -522.799930
Sum of electronic and thermal Enthalpies= -522.798986
Sum of electronic and thermal Free Energies= -522.851162

AmaH$^+$(II)H$_2$O(I)

1	6	0	-1.452976	1.350361	-0.472004
2	6	0	-1.363651	1.454300	1.054939
3	6	0	-0.407833	0.375814	1.576074
4	6	0	-0.934239	-1.018832	1.205160
5	6	0	-1.184997	-1.203440	-0.299584
6	6	0	-1.992107	-0.030140	-0.877108
7	6	0	-0.060406	1.650496	-1.081761
8	6	0	-1.866721	-2.541204	-0.588584
9	6	0	1.034595	0.863282	-0.451782
10	6	0	1.013956	0.642069	1.020698
11	7	0	2.019518	0.415659	-1.158972
12	1	0	-2.127534	2.115801	-0.855793
13	1	0	-1.028514	2.449427	1.357125
14	1	0	-2.352964	1.307977	1.489058
15	1	0	-0.330792	0.443575	2.661333
16	1	0	-0.248271	-1.790381	1.563036
17	1	0	-1.875020	-1.174180	1.740158
18	1	0	-2.847086	-2.581773	-0.110697
19	1	0	-2.040821	-0.114413	-1.965472
20	1	0	-3.022650	-0.102603	-0.519217
21	1	0	-0.053616	1.525020	-2.165942
22	1	0	0.178874	2.701350	-0.877833
23	1	0	-1.276474	-3.376180	-0.209366
24	1	0	-2.011152	-2.689215	-1.659294
25	1	0	1.725644	-0.134863	1.299449
26	1	0	1.376551	1.581272	1.457092
27	1	0	2.048175	0.578370	-2.157067
28	1	0	2.786214	-0.128721	-0.735574
29	1	0	-0.212084	-1.230273	-0.806053
30	8	0	3.950482	-1.092935	0.185511
31	1	0	4.790220	-0.758304	0.518494
32	1	0	4.067088	-2.044262	0.088979

Sum of electronic and zero-point Energies= -522.826617
Sum of electronic and thermal Energies= -522.813204
Sum of electronic and thermal Enthalpies= -522.812259
Sum of electronic and thermal Free Energies= -522.865937

AmaH$^+$(II)H$_2$O(II)

1	6	0	-0.479392	-1.012565	-0.628844
2	6	0	-0.608281	-1.212983	0.883064
3	6	0	0.217014	-0.139813	1.601001
4	6	0	1.696038	-0.245050	1.202716
5	6	0	1.934429	-0.189784	-0.314926
6	6	0	0.990345	-1.145720	-1.060119
7	6	0	-1.090426	0.354220	-1.016362
8	6	0	3.397830	-0.473348	-0.657552
9	6	0	-0.610960	1.471415	-0.170657
10	6	0	-0.387108	1.252205	1.281841
11	7	0	-0.440574	2.652861	-0.681352
12	1	0	-1.079051	-1.757834	-1.147148
13	1	0	-1.656845	-1.172555	1.182910
14	1	0	-0.235310	-2.201064	1.153487
15	1	0	0.133355	-0.268009	2.680179
16	1	0	2.280363	0.533638	1.698932
17	1	0	2.074486	-1.197991	1.582708
18	1	0	3.673335	-1.480952	-0.341941
19	1	0	1.084012	-0.994393	-2.138270
20	1	0	1.304987	-2.174899	-0.867090
21	1	0	-0.954915	0.583628	-2.075118
22	1	0	-2.172519	0.281910	-0.834240
23	1	0	4.065156	0.228154	-0.155987
24	1	0	3.574519	-0.399234	-1.730915
25	1	0	0.199548	2.066157	1.711789
26	1	0	-1.384660	1.300703	1.736390
27	1	0	-0.601435	2.830836	-1.664041
28	1	0	-0.134451	3.434995	-0.117531
29	1	0	1.724223	0.832471	-0.656862
30	8	0	-3.813850	-1.040840	-0.200891
31	1	0	-4.053476	-1.860624	-0.641443
32	1	0	-4.603446	-0.779711	0.279814

Sum of electronic and zero-point Energies= -522.818114
Sum of electronic and thermal Energies= -522.804350
Sum of electronic and thermal Enthalpies= -522.803406
Sum of electronic and thermal Free Energies= -522.858143

$AmaH^{+}(I)(H_2O)_2(I)$

1	6	0	1.280617	-1.651785	-1.257888
2	1	0	1.609688	-1.125439	-2.157173
3	1	0	1.748311	-2.637310	-1.278026
4	6	0	-0.250076	-1.800180	-1.257172
5	1	0	-0.571956	-2.334625	-2.151174
6	6	0	1.727253	-0.888394	0.000000
7	1	0	2.811701	-0.775578	0.000000
8	6	0	1.084873	0.512055	0.000000
9	1	0	1.396901	1.072952	-0.884387
10	1	0	1.396901	1.072952	0.884387
11	6	0	-0.892774	-0.399704	-1.258194
12	1	0	-1.983516	-0.486823	-1.269962
13	1	0	-0.591234	0.156696	-2.148671
14	6	0	-0.439202	0.347136	0.000000
15	6	0	-0.892774	-0.399704	1.258194
16	1	0	-0.591234	0.156696	2.148671
17	1	0	-1.983516	-0.486823	1.269962
18	6	0	-0.697863	-2.564045	0.000000
19	1	0	-0.262449	-3.564486	0.000000
20	1	0	-1.783147	-2.690987	0.000000
21	6	0	1.280617	-1.651785	1.257888
22	1	0	1.748311	-2.637310	1.278026
23	1	0	1.609688	-1.125439	2.157173
24	6	0	-0.250076	-1.800180	1.257172
25	1	0	-0.571956	-2.334625	2.151174
26	7	0	-1.069025	1.732333	0.000000
27	1	0	-0.787489	2.260687	0.845485
28	1	0	-0.787489	2.260687	-0.845485
29	1	0	-2.085682	1.657399	0.000000
30	8	0	-0.250076	2.996881	2.390126
31	1	0	-0.758558	3.030090	3.207272
32	1	0	0.488046	3.602139	2.516165
33	8	0	-0.250076	2.996881	-2.390126
34	1	0	0.488046	3.602139	-2.516165
35	1	0	-0.758558	3.030090	-3.207272

Sum of electronic and zero-point Energies= -599.291840
Sum of electronic and thermal Energies= -599.276039
Sum of electronic and thermal Enthalpies= -599.275095
Sum of electronic and thermal Free Energies= -599.335170

$AmaH^{+}(I)(H_2O)_2(II)$

1	6	0	2.640118	-0.568311	1.233865
2	1	0	2.876736	0.066557	2.090976
3	1	0	3.316453	-1.423083	1.276308
4	6	0	2.858388	0.202589	-0.078507
5	1	0	3.888081	0.555023	-0.135711
6	6	0	1.182751	-1.053511	1.313245
7	1	0	1.020102	-1.593661	2.245851
8	6	0	0.238503	0.164858	1.279293
9	1	0	0.438475	0.820283	2.132350
10	1	0	-0.803012	-0.159079	1.340826
11	6	0	1.917063	1.422684	-0.113158
12	1	0	2.069191	1.989481	-1.036380
13	1	0	2.133136	2.088937	0.727171
14	6	0	0.473669	0.919259	-0.032452
15	6	0	0.147490	0.023385	-1.230834
16	1	0	-0.894419	-0.301185	-1.180259
17	1	0	0.282665	0.578141	-2.164247
18	6	0	2.549102	-0.709810	-1.276892
19	1	0	3.224069	-1.566702	-1.271858
20	1	0	2.720677	-0.176093	-2.214653
21	6	0	0.872150	-1.967134	0.115772
22	1	0	1.521817	-2.842868	0.141583
23	1	0	-0.156196	-2.331355	0.173573
24	6	0	1.091799	-1.194914	-1.195952
25	1	0	0.864425	-1.835668	-2.047835
26	7	0	-0.467711	2.124593	-0.066246
27	1	0	-1.464220	1.822945	-0.013234
28	1	0	-0.276334	2.750186	0.716965
29	1	0	-0.335739	2.657696	-0.926358
30	8	0	-3.086512	1.195615	0.080461
31	1	0	-3.685712	1.057720	-0.661089
32	1	0	-3.630513	1.143487	0.873741
33	8	0	-6.916359	-1.008271	-0.038825
34	1	0	-6.048088	-1.417706	-0.047129
35	1	0	-7.590847	-1.688527	0.023761

Sum of electronic and zero-point Energies= -599.290223
Sum of electronic and thermal Energies= -599.275178
Sum of electronic and thermal Enthalpies= -599.274234
Sum of electronic and thermal Free Energies= -599.333450

$AmaH^{+}(I)(H_2O)_2(III)$

1	6	0	2.321940	1.448881	0.384107
2	1	0	1.833455	2.420411	0.492337
3	1	0	3.350948	1.572361	0.724945
4	6	0	2.311367	1.007577	-1.089314
5	1	0	2.807884	1.757271	-1.705497
6	6	0	1.609412	0.392981	1.245578
7	1	0	1.607763	0.705145	2.290196
8	6	0	0.150622	0.249250	0.771406
9	1	0	-0.370960	1.206291	0.868018
10	1	0	-0.384504	-0.484078	1.377721
11	6	0	0.852976	0.862841	-1.565588
12	1	0	0.828971	0.560596	-2.616776
13	1	0	0.331336	1.820745	-1.483449
14	6	0	0.159094	-0.190646	-0.697573
15	6	0	0.857251	-1.546548	-0.842331
16	1	0	0.336979	-2.299329	-0.244546
17	1	0	0.830570	-1.873563	-1.886099
18	6	0	3.027550	-0.346025	-1.231489
19	1	0	4.067007	-0.249129	-0.914930
20	1	0	3.042426	-0.659114	-2.278256
21	6	0	2.324990	-0.961243	1.105193
22	1	0	3.353277	-0.874020	1.459013
23	1	0	1.836530	-1.714022	1.728393
24	6	0	2.315532	-1.401109	-0.368587
25	1	0	2.814994	-2.364502	-0.471616
26	7	0	-1.279856	-0.344792	-1.162297
27	1	0	-1.782345	-1.064669	-0.603496
28	1	0	-1.820944	0.514894	-1.016431
29	1	0	-1.316278	-0.596186	-2.149109
30	8	0	-2.831692	-1.654327	0.662255
31	1	0	-3.448818	-0.931690	0.835893
32	1	0	-3.256154	-2.472677	0.936037
33	8	0	-3.430279	1.163264	0.121613
34	1	0	-4.234361	1.477002	-0.308055
35	1	0	-3.268568	1.788983	0.836969

Sum of electronic and zero-point Energies= -599.289404
Sum of electronic and thermal Energies= -599.274379
Sum of electronic and thermal Enthalpies= -599.273435
Sum of electronic and thermal Free Energies= -599.331419

AmaH$^+$(II)(H_2O)$_2$(I)

1	6	0	0.975220	-1.312306	1.247667
2	6	0	1.670838	-1.866597	0.000000
3	6	0	0.975220	-1.312306	-1.247667
4	6	0	-0.497490	-1.751231	-1.267981
5	6	0	-1.276315	-1.367352	0.000000
6	6	0	-0.497490	-1.751231	1.267981
7	6	0	1.141462	0.226866	1.283983
8	6	0	-2.674397	-1.986210	0.000000
9	6	0	0.767571	0.886573	0.000000
10	6	0	1.141462	0.226866	-1.283983
11	7	0	0.166700	2.027678	0.000000
12	1	0	1.463609	-1.696663	2.143523
13	1	0	2.731851	-1.605084	0.000000
14	1	0	1.613141	-2.955702	0.000000
15	1	0	1.463609	-1.696663	-2.143523
16	1	0	-1.001115	-1.344078	-2.148218
17	1	0	-0.520437	-2.838854	-1.378339
18	1	0	-2.610860	-3.075906	0.000000
19	1	0	-1.001115	-1.344078	2.148218
20	1	0	-0.520437	-2.838854	1.378339
21	1	0	0.606403	0.684228	2.115896
22	1	0	2.206501	0.447310	1.426286
23	1	0	-3.240927	-1.685900	-0.882411
24	1	0	-3.240927	-1.685900	0.882411
25	1	0	0.606403	0.684228	-2.115896
26	1	0	2.206501	0.447310	-1.426286
27	1	0	-0.088645	2.481639	0.884288
28	1	0	-0.088645	2.481639	-0.884288
29	1	0	-1.412512	-0.279660	0.000000
30	8	0	-0.497490	3.017188	-2.577747
31	1	0	0.019986	3.644547	-3.093544
32	1	0	-1.387961	3.052355	-2.942565
33	8	0	-0.497490	3.017188	2.577747
34	1	0	-1.387961	3.052355	2.942565
35	1	0	0.019986	3.644547	3.093544

Sum of electronic and zero-point Energies= -599.286849
Sum of electronic and thermal Energies= -599.269799
Sum of electronic and thermal Enthalpies= -599.268855
Sum of electronic and thermal Free Energies= -599.331236

$AmaH^{+}$(II)$(H_2O)_2$(II)

1	6	0	-2.337906	0.389782	-0.376172
2	6	0	-2.264110	0.421875	1.154514
3	6	0	-0.816586	0.169863	1.590566
4	6	0	-0.353552	-1.212861	1.108835
5	6	0	-0.501046	-1.418650	-0.406247
6	6	0	-1.892132	-0.986096	-0.897652
7	6	0	-1.488206	1.555208	-0.947967
8	6	0	-0.195976	-2.863882	-0.799459
9	6	0	-0.107431	1.579306	-0.391086
10	6	0	0.084363	1.314000	1.061911
11	7	0	0.908883	1.849715	-1.139080
12	1	0	-3.362662	0.569831	-0.701492
13	1	0	-2.625145	1.378581	1.539618
14	1	0	-2.912937	-0.350764	1.568396
15	1	0	-0.748026	0.202197	2.678172
16	1	0	0.685827	-1.385543	1.396251
17	1	0	-0.952038	-1.966815	1.627496
18	1	0	-0.904110	-3.549923	-0.331184
19	1	0	-1.920650	-1.004465	-1.990003
20	1	0	-2.627769	-1.721805	-0.561351
21	1	0	-1.466514	1.543509	-2.038949
22	1	0	-1.957381	2.497057	-0.641755
23	1	0	0.807271	-3.149178	-0.480380
24	1	0	-0.261440	-3.003729	-1.879242
25	1	0	1.137910	1.154669	1.284926
26	1	0	-0.215808	2.241017	1.565590
27	1	0	0.778880	2.040978	-2.123764
28	1	0	1.878546	1.788591	-0.770402
29	1	0	0.250889	-0.797510	-0.904872
30	8	0	3.299538	1.294483	0.020590
31	1	0	4.151761	1.727790	0.117048
32	1	0	3.446726	0.329133	0.072166
33	8	0	3.271341	-1.452886	0.173722
34	1	0	3.551896	-2.010119	-0.560105
35	1	0	3.571045	-1.905548	0.969449

Sum of electronic and zero-point Energies= -599.284990
Sum of electronic and thermal Energies= -599.268675
Sum of electronic and thermal Enthalpies= -599.267731
Sum of electronic and thermal Free Energies= -599.328403

$AmaH^{+}(I)(H_2O)_3(I)$

1	6	0	-2.103850	-1.256649	1.245511
2	1	0	-1.556658	-2.156696	1.536128
3	1	0	-3.053647	-1.275024	1.782508
4	6	0	-2.363607	-1.256626	-0.270285
5	1	0	-2.922177	-2.149746	-0.551492
6	6	0	-1.307786	-0.000025	1.634252
7	1	0	-1.116205	-0.000102	2.707795
8	6	0	0.041644	-0.001609	0.890332
9	1	0	0.627498	-0.884156	1.156536
10	1	0	0.629373	0.879765	1.156256
11	6	0	-1.015037	-1.257927	-1.015344
12	1	0	-1.181633	-1.271207	-2.096768
13	1	0	-0.438831	-2.150454	-0.757423
14	6	0	-0.234521	-0.001509	-0.618606
15	6	0	-1.012208	1.256543	-1.015661
16	1	0	-0.433946	2.147783	-0.757930
17	1	0	-1.178755	1.269938	-2.097090
18	6	0	-3.157125	0.001784	-0.660509
19	1	0	-4.122194	0.002929	-0.151505
20	1	0	-3.363412	0.001876	-1.733552
21	6	0	-2.101026	1.258284	1.245188
22	1	0	-3.050793	1.278878	1.782153
23	1	0	-1.551803	2.157144	1.535621
24	6	0	-2.360752	1.258512	-0.270612
25	1	0	-2.917319	2.152818	-0.552021
26	7	0	1.094324	-0.002910	-1.349018
27	1	0	1.666299	0.823320	-1.087516
28	1	0	1.665754	-0.828942	-1.086124
29	1	0	0.952740	-0.003756	-2.357602
30	8	0	2.842118	1.853483	-0.268356
31	1	0	3.091103	2.776079	-0.370800
32	1	0	3.592626	1.393585	0.141689
33	8	0	2.846291	-1.854100	-0.266205
34	1	0	3.595241	-1.392408	0.144602
35	1	0	3.094046	-2.777914	-0.360136
36	8	0	4.749216	0.002613	0.814810
37	1	0	5.645399	0.001995	0.458216
38	1	0	4.851639	0.004014	1.773985

Sum of electronic and zero-point Energies= -675.752445
Sum of electronic and thermal Energies= -675.734672
Sum of electronic and thermal Enthalpies= -675.733728
Sum of electronic and thermal Free Energies= -675.798234

$AmaH^{+}$(I)$(H_2O)_3$(II)

1	6	0	2.275403	-1.406344	-0.344699
2	1	0	1.937332	-2.415679	-0.591862
3	1	0	3.366511	-1.426525	-0.348764
4	6	0	1.765322	-1.001089	1.048200
5	1	0	2.118120	-1.714438	1.793826
6	6	0	1.767356	-0.402962	-1.393568
7	1	0	2.121219	-0.691269	-2.383999
8	6	0	0.227464	-0.404914	-1.395286
9	1	0	-0.150222	-1.399372	-1.645944
10	1	0	-0.152738	0.298136	-2.140483
11	6	0	0.225864	-1.003055	1.046939
12	1	0	-0.154493	-0.722841	2.032475
13	1	0	-0.153149	-2.000234	0.810254
14	6	0	-0.268582	0.000173	-0.002067
15	6	0	0.223141	1.410682	0.343483
16	1	0	-0.157119	2.122995	-0.393049
17	1	0	-0.158492	1.704067	1.324469
18	6	0	2.270635	0.409248	1.395127
19	1	0	3.361599	0.417609	1.418392
20	1	0	1.927887	0.699357	2.391426
21	6	0	2.272994	1.007877	-1.047827
22	1	0	3.364019	1.025284	-1.062739
23	1	0	1.932463	1.725441	-1.798402
24	6	0	1.762798	1.412455	0.345142
25	1	0	2.113496	2.415287	0.591155
26	7	0	-1.783654	-0.003020	-0.002253
27	1	0	-2.142297	0.661193	-0.705031
28	1	0	-2.137026	-0.945561	-0.226200
29	1	0	-2.140115	0.272908	0.925297
30	8	0	-2.551975	1.891125	-2.009164
31	1	0	-2.780155	2.816641	-1.874850
32	1	0	-2.773837	1.699235	-2.925872
33	8	0	-2.529606	-2.697831	-0.630164
34	1	0	-2.737656	-3.057340	-1.498607
35	1	0	-2.745258	-3.394724	-0.002144
36	8	0	-2.542797	0.793474	2.643444
37	1	0	-2.758499	0.218821	3.385059
38	1	0	-2.755357	1.685577	2.935786

Sum of electronic and zero-point Energies= -675.751499
Sum of electronic and thermal Energies= -675.731540
Sum of electronic and thermal Enthalpies= -675.730596
Sum of electronic and thermal Free Energies= -675.801598

$AmaH^{+}(I)(H_2O)_3(III)$

1	6	0	1.131168	-2.512380	-0.841137
2	1	0	0.325787	-2.964911	-1.424610
3	1	0	2.049980	-3.038728	-1.104887
4	6	0	0.853753	-2.670276	0.663178
5	1	0	0.749389	-3.726493	0.912709
6	6	0	1.265250	-1.020079	-1.187807
7	1	0	1.453909	-0.904179	-2.255739
8	6	0	-0.047210	-0.295547	-0.835978
9	1	0	-0.879769	-0.719125	-1.402706
10	1	0	0.022448	0.764774	-1.085953
11	6	0	-0.458213	-1.944140	1.016279
12	1	0	-0.674808	-2.057256	2.082962
13	1	0	-1.293219	-2.374123	0.458171
14	6	0	-0.308755	-0.460065	0.666320
15	6	0	0.832608	0.164844	1.476046
16	1	0	0.914844	1.227829	1.243284
17	1	0	0.626184	0.070351	2.546434
18	6	0	2.009414	-2.053701	1.469015
19	1	0	2.940438	-2.573956	1.238174
20	1	0	1.832930	-2.178716	2.540175
21	6	0	2.419082	-0.398981	-0.382594
22	1	0	3.358740	-0.889598	-0.642045
23	1	0	2.525323	0.659393	-0.630803
24	6	0	2.143627	-0.561921	1.122020
25	1	0	2.957012	-0.119505	1.698236
26	7	0	-1.600461	0.261095	1.005479
27	1	0	-1.521493	1.275683	0.768771
28	1	0	-2.391368	-0.147725	0.479232
29	1	0	-1.801339	0.178634	2.000857
30	8	0	-1.223218	2.876155	0.252134
31	1	0	-1.734468	3.677156	0.393958
32	1	0	-0.314542	3.149156	0.017748
33	8	0	-3.623850	-0.982984	-0.544667
34	1	0	-3.990402	-0.629490	-1.361782
35	1	0	-4.215565	-1.693816	-0.277169
36	8	0	1.416253	3.309735	-0.412001
37	1	0	1.661176	3.531667	-1.316637
38	1	0	2.032350	3.791963	0.149636

Sum of electronic and zero-point Energies= -675.750760
Sum of electronic and thermal Energies= -675.731975
Sum of electronic and thermal Enthalpies= -675.731031
Sum of electronic and thermal Free Energies= -675.798677

$AmaH^{+}(I)(H_2O)_3(IV)$

1	6	0	-2.631788	-1.064310	-0.849576
2	1	0	-2.844667	-0.901782	-1.908847
3	1	0	-3.111168	-2.003508	-0.568955
4	6	0	-3.209909	0.085262	-0.006176
5	1	0	-4.284015	0.165697	-0.173682
6	6	0	-1.114492	-1.161033	-0.619362
7	1	0	-0.693296	-1.965301	-1.222680
8	6	0	-0.449453	0.161456	-1.043230
9	1	0	-0.643029	0.354835	-2.102915
10	1	0	0.630319	0.102582	-0.907910
11	6	0	-2.542686	1.409882	-0.425800
12	1	0	-2.952098	2.239401	0.158117
13	1	0	-2.744234	1.615925	-1.481321
14	6	0	-1.034220	1.292059	-0.190204
15	6	0	-0.740359	1.049884	1.294511
16	1	0	0.335907	0.993726	1.461233
17	1	0	-1.134622	1.877015	1.892409
18	6	0	-2.928569	-0.172901	1.483592
19	1	0	-3.413396	-1.099509	1.795079
20	1	0	-3.352591	0.627838	2.094123
21	6	0	-0.830174	-1.418935	0.870281
22	1	0	-1.280890	-2.365646	1.173803
23	1	0	0.244825	-1.494902	1.042058
24	6	0	-1.411943	-0.271913	1.713850
25	1	0	-1.206539	-0.447040	2.770119
26	7	0	-0.362158	2.595619	-0.601451
27	1	0	0.687029	2.533023	-0.470525
28	1	0	-0.557713	2.805461	-1.579876
29	1	0	-0.712406	3.371622	-0.040220
30	8	0	2.263214	2.310033	-0.144509
31	1	0	3.041164	2.701868	-0.549245
32	1	0	2.530003	1.448990	0.254914
33	8	0	2.656167	-0.094390	0.960079
34	1	0	3.274086	-0.282275	1.672065
35	1	0	2.620789	-0.889348	0.392581
36	8	0	2.245432	-2.227323	-0.741918
37	1	0	1.928273	-3.061427	-0.380085
38	1	0	2.849002	-2.465330	-1.453442

Sum of electronic and zero-point Energies= -675.747897
Sum of electronic and thermal Energies= -675.730084
Sum of electronic and thermal Enthalpies= -675.729140
Sum of electronic and thermal Free Energies= -675.793352

AmaH$^+$(I)(H$_2$O)$_4$(I)

1	6	0	2.496310	1.019368	-1.296213
2	1	0	1.881366	1.154342	-2.189584
3	1	0	3.312274	1.741660	-1.357405
4	6	0	3.067707	-0.408254	-1.257213
5	1	0	3.654233	-0.597108	-2.156768
6	6	0	1.660388	1.273980	-0.030775
7	1	0	1.240240	2.280368	-0.057737
8	6	0	0.502130	0.263797	0.025840
9	1	0	-0.141411	0.373193	-0.848220
10	1	0	-0.108239	0.436471	0.913089
11	6	0	1.907781	-1.419845	-1.200548
12	1	0	2.300397	-2.441187	-1.186309
13	1	0	1.270821	-1.321277	-2.083155
14	6	0	1.086566	-1.154120	0.065644
15	6	0	1.957384	-1.331139	1.313548
16	1	0	1.355042	-1.168278	2.210565
17	1	0	2.349800	-2.351638	1.356097
18	6	0	3.952641	-0.577785	-0.010840
19	1	0	4.789261	0.121663	-0.052827
20	1	0	4.379964	-1.583087	0.015825
21	6	0	2.544086	1.106549	1.216212
22	1	0	3.359123	1.832136	1.196481
23	1	0	1.962789	1.302579	2.120605
24	6	0	3.117262	-0.320311	1.254719
25	1	0	3.739014	-0.445891	2.141539
26	7	0	-0.062650	-2.140233	0.128323
27	1	0	-0.641499	-1.967752	0.975490
28	1	0	-0.703896	-2.012989	-0.681020
29	1	0	0.280992	-3.098447	0.142111
30	8	0	-1.770596	-1.199233	2.078559
31	1	0	-2.203427	-1.499699	2.882074
32	1	0	-2.418525	-0.672819	1.573618
33	8	0	-1.948446	-1.327611	-1.711230
34	1	0	-2.550788	-0.776913	-1.176482
35	1	0	-2.461787	-1.701564	-2.432345
36	8	0	-3.217022	0.287490	0.195773
37	1	0	-4.168263	0.428394	0.238113
38	1	0	-2.806557	1.178031	0.126804
39	8	0	-1.887140	2.662503	-0.018958
40	1	0	-1.837569	3.308210	0.693445
41	1	0	-1.876504	3.170551	-0.836708

Sum of electronic and zero-point Energies= -752.211300
Sum of electronic and thermal Energies= -752.190979
Sum of electronic and thermal Enthalpies= -752.190035
Sum of electronic and thermal Free Energies= -752.259796

$AmaH^{+}$(I)$(H_2O)_4$(II)

1	6	0	2.614344	-1.823826	-0.888866
2	1	0	2.110389	-2.137521	-1.806436
3	1	0	3.522277	-2.423392	-0.802467
4	6	0	1.705590	-2.069894	0.327334
5	1	0	1.440218	-3.126539	0.381964
6	6	0	2.978810	-0.331713	-0.966639
7	1	0	3.617368	-0.150651	-1.832001
8	6	0	1.691079	0.499150	-1.115389
9	1	0	1.161496	0.218867	-2.030048
10	1	0	1.931287	1.563269	-1.180638
11	6	0	0.417824	-1.240243	0.178884
12	1	0	-0.245946	-1.404957	1.030646
13	1	0	-0.124737	-1.527264	-0.724661
14	6	0	0.794373	0.245332	0.102327
15	6	0	1.514918	0.673546	1.385542
16	1	0	1.753766	1.738651	1.336059
17	1	0	0.859615	0.515740	2.246277
18	6	0	2.436535	-1.649376	1.612993
19	1	0	3.340860	-2.247291	1.739057
20	1	0	1.804762	-1.837718	2.484617
21	6	0	3.709385	0.090629	0.318750
22	1	0	4.634426	-0.479202	0.422777
23	1	0	3.989037	1.145655	0.264947
24	6	0	2.802065	-0.157586	1.535407
25	1	0	3.315404	0.146343	2.448358
26	7	0	-0.467776	1.065435	-0.037789
27	1	0	-0.241327	2.067705	-0.103188
28	1	0	-1.007542	0.771963	-0.868022
29	1	0	-1.093115	0.903305	0.768821
30	8	0	0.424710	3.792155	-0.159544
31	1	0	0.473490	4.408114	0.578490
32	1	0	0.586532	4.318051	-0.949283
33	8	0	-2.209209	-0.142103	-1.876395
34	1	0	-2.448567	-0.145235	-2.806888
35	1	0	-2.946719	-0.542889	-1.389562
36	8	0	-2.338530	0.154170	1.846655
37	1	0	-3.051156	-0.317694	1.386872
38	1	0	-2.641322	0.323489	2.742673
39	8	0	-4.113938	-1.179778	0.022741
40	1	0	-4.144718	-2.140333	0.103025
41	1	0	-5.033013	-0.894219	-0.037056

Sum of electronic and zero-point Energies= -752.211061
Sum of electronic and thermal Energies= -752.189248
Sum of electronic and thermal Enthalpies= -752.188304
Sum of electronic and thermal Free Energies= -752.262467

$AmaH^{+}(I)(H_2O)_4(III)$

1	6	0	-3.427192	1.035004	-1.200940
2	1	0	-2.910825	1.928839	-1.559486
3	1	0	-4.351141	0.948249	-1.775228
4	6	0	-3.754488	1.175255	0.295292
5	1	0	-4.367735	2.061643	0.459877
6	6	0	-2.552291	-0.210096	-1.423343
7	1	0	-2.312886	-0.308821	-2.482855
8	6	0	-1.241017	-0.062080	-0.631164
9	1	0	-0.686132	0.817324	-0.964381
10	1	0	-0.603260	-0.936208	-0.778367
11	6	0	-2.442446	1.325489	1.088218
12	1	0	-2.659204	1.439907	2.154816
13	1	0	-1.900194	2.216649	0.761961
14	6	0	-1.582775	0.077935	0.858426
15	6	0	-2.317961	-1.173038	1.350811
16	1	0	-1.685451	-2.052711	1.209188
17	1	0	-2.533240	-1.085134	2.420087
18	6	0	-4.502727	-0.076752	0.782126
19	1	0	-5.443229	-0.180195	0.238349
20	1	0	-4.756664	0.021299	1.840454
21	6	0	-3.300935	-1.462747	-0.938920
22	1	0	-4.222310	-1.589655	-1.509715
23	1	0	-2.693497	-2.354939	-1.109233
24	6	0	-3.628892	-1.321940	0.557077
25	1	0	-4.153406	-2.211377	0.907330
26	7	0	-0.288773	0.216816	1.634152
27	1	0	0.306816	-0.626474	1.501186
28	1	0	0.278668	1.013528	1.281823
29	1	0	-0.473758	0.345860	2.626887
30	8	0	1.402581	-1.782233	0.783922
31	1	0	1.792951	-2.592982	1.120468
32	1	0	2.074024	-1.341307	0.228126
33	8	0	1.441112	1.903133	0.311778
34	1	0	2.113618	1.328194	-0.100303
35	1	0	1.807563	2.789689	0.360405
36	8	0	3.039139	-0.131193	-0.761920
37	1	0	4.009545	-0.169492	-0.602552
38	1	0	2.922660	-0.233562	-1.712315
39	8	0	5.700617	-0.282416	-0.272496
40	1	0	6.316662	0.456235	-0.299531
41	1	0	6.230150	-1.075116	-0.403312

Sum of electronic and zero-point Energies= -752.210637
Sum of electronic and thermal Energies= -752.189959
Sum of electronic and thermal Enthalpies= -752.189015
Sum of electronic and thermal Free Energies= -752.260907

$AmaH^{+}(I)(H_2O)_4(IV)$

1	6	0	-2.668478	0.935254	-1.277359
2	1	0	-2.828167	0.222854	-2.090453
3	1	0	-3.422176	1.717203	-1.385873
4	6	0	-1.261303	1.547874	-1.374872
5	1	0	-1.138154	2.038261	-2.341556
6	6	0	-2.833155	0.236163	0.082775
7	1	0	-3.827051	-0.207449	0.152717
8	6	0	-1.779447	-0.879463	0.212481
9	1	0	-1.908694	-1.619443	-0.581526
10	1	0	-1.887476	-1.393042	1.171129
11	6	0	-0.208977	0.431386	-1.245750
12	1	0	0.797874	0.845885	-1.324382
13	1	0	-0.332037	-0.303157	-2.045405
14	6	0	-0.382152	-0.255668	0.115021
15	6	0	-0.177555	0.755207	1.249611
16	1	0	-0.277837	0.249053	2.212603
17	1	0	0.829058	1.173175	1.193814
18	6	0	-1.060593	2.568843	-0.242307
19	1	0	-1.788825	3.376297	-0.338823
20	1	0	-0.066494	3.015555	-0.313112
21	6	0	-2.636184	1.256916	1.215812
22	1	0	-3.391469	2.041398	1.142413
23	1	0	-2.770588	0.774213	2.186904
24	6	0	-1.229743	1.871038	1.118096
25	1	0	-1.084254	2.591442	1.924322
26	7	0	0.657567	-1.346258	0.249042
27	1	0	0.559098	-1.817774	1.159415
28	1	0	0.548784	-2.042136	-0.502685
29	1	0	1.608947	-0.935714	0.189478
30	8	0	0.212980	-2.439773	2.870408
31	1	0	0.728921	-2.208484	3.649433
32	1	0	-0.321384	-3.197832	3.127597
33	8	0	0.215005	-3.133155	-1.951665
34	1	0	-0.317903	-3.934239	-1.975278
35	1	0	0.731501	-3.139309	-2.763880
36	8	0	3.097011	-0.007582	0.079537
37	1	0	4.021465	-0.263096	0.129273
38	1	0	3.072484	0.959361	-0.049556
39	8	0	2.692454	2.709088	-0.284893
40	1	0	2.884891	3.150465	-1.118751
41	1	0	2.880617	3.357182	0.401930

Sum of electronic and zero-point Energies= -752.209427
Sum of electronic and thermal Energies= -752.186249
Sum of electronic and thermal Enthalpies= -752.185304
Sum of electronic and thermal Free Energies= -752.264813

$AmaH^{+}(I)(H_2O)_4(V)$

1	6	0	2.680092	-1.117811	-0.684350
2	1	0	2.052887	-2.003035	-0.815248
3	1	0	3.640749	-1.329398	-1.157019
4	6	0	2.885293	-0.837411	0.813988
5	1	0	3.345866	-1.702051	1.293144
6	6	0	2.024495	0.102103	-1.353181
7	1	0	1.874154	-0.093771	-2.415769
8	6	0	0.656489	0.367353	-0.698698
9	1	0	0.002391	-0.497924	-0.819872
10	1	0	0.164469	1.224986	-1.162330
11	6	0	1.515702	-0.576461	1.468138
12	1	0	1.639312	-0.389802	2.539253
13	1	0	0.868704	-1.448525	1.350645
14	6	0	0.872852	0.641858	0.795732
15	6	0	1.755574	1.880359	0.980392
16	1	0	1.275325	2.749585	0.523427
17	1	0	1.882978	2.094301	2.045893
18	6	0	3.781746	0.398998	0.993546
19	1	0	4.760494	0.215412	0.546892
20	1	0	3.948626	0.594486	2.055558
21	6	0	2.921953	1.338007	-1.174456
22	1	0	3.888518	1.168249	-1.651854
23	1	0	2.472067	2.205192	-1.663819
24	6	0	3.123818	1.617460	0.324220
25	1	0	3.753393	2.497816	0.456162
26	7	0	-0.475321	0.894586	1.432752
27	1	0	-0.948125	1.707720	0.997060
28	1	0	-1.119197	0.080096	1.271280
29	1	0	-0.380458	1.057792	2.433097
30	8	0	-2.002352	2.619584	-0.111893
31	1	0	-2.241094	3.548522	-0.171930
32	1	0	-2.763689	2.104853	-0.428123
33	8	0	-2.236869	-1.074249	0.746743
34	1	0	-2.852722	-0.717773	0.091033
35	1	0	-1.831119	-1.877532	0.373219
36	8	0	-3.971263	0.678556	-0.838008
37	1	0	-4.832259	0.721581	-0.405512
38	1	0	-4.159920	0.562247	-1.776273
39	8	0	-0.668279	-3.219403	-0.096336
40	1	0	-0.583161	-3.566794	-0.990181
41	1	0	-0.649039	-3.990276	0.481017

Sum of electronic and zero-point Energies= -752.208613
Sum of electronic and thermal Energies= -752.187740
Sum of electronic and thermal Enthalpies= -752.186796
Sum of electronic and thermal Free Energies= -752.258663

AmaH$^+$(I)(H$_2$O)$_4$(VI)

1	6	0	-1.872334	0.938630	1.258775
2	1	0	-1.360193	1.292360	2.156296
3	1	0	-2.885681	1.343443	1.280881
4	6	0	-1.923878	-0.598706	1.256010
5	1	0	-2.437646	-0.953918	2.150103
6	6	0	-1.138513	1.431648	0.000000
7	1	0	-1.096666	2.521861	0.000000
8	6	0	0.298193	0.880357	0.000000
9	1	0	0.842047	1.225621	0.881374
10	1	0	0.842047	1.225621	-0.881374
11	6	0	-0.486205	-1.151838	1.256867
12	1	0	-0.503559	-2.245840	1.266400
13	1	0	0.045634	-0.818380	2.149168
14	6	0	0.235408	-0.652525	0.000000
15	6	0	-0.486205	-1.151838	-1.256867
16	1	0	0.045634	-0.818380	-2.149168
17	1	0	-0.503559	-2.245840	-1.266400
18	6	0	-2.660811	-1.091328	0.000000
19	1	0	-3.685912	-0.716289	0.000000
20	1	0	-2.721618	-2.182376	0.000000
21	6	0	-1.872334	0.938630	-1.258775
22	1	0	-2.885681	1.343443	-1.280881
23	1	0	-1.360193	1.292360	-2.156296
24	6	0	-1.923878	-0.598706	-1.256010
25	1	0	-2.437646	-0.953918	-2.150103
26	7	0	1.655414	-1.180184	0.000000
27	1	0	2.159110	-0.850627	-0.850033
28	1	0	2.159110	-0.850627	0.850033
29	1	0	1.656478	-2.198595	0.000000
30	8	0	2.780733	-0.226611	-2.336265
31	1	0	3.682686	-0.139243	-2.654662
32	1	0	2.204958	0.256705	-2.959166
33	8	0	2.780733	-0.226611	2.336265
34	1	0	3.682686	-0.139243	2.654662
35	1	0	2.204958	0.256705	2.959166
36	8	0	0.893194	1.071654	-3.884716
37	1	0	0.902375	2.024330	-4.024359
38	1	0	0.580438	0.690575	-4.712059
39	8	0	0.893194	1.071654	3.884716
40	1	0	0.580438	0.690575	4.712059
41	1	0	0.902375	2.024330	4.024359

Sum of electronic and zero-point Energies= -752.208946
Sum of electronic and thermal Energies= -752.186818
Sum of electronic and thermal Enthalpies= -752.185873
Sum of electronic and thermal Free Energies= -752.263028