Supplementary Material

High energy conformers of $M^+(APE)(H_2O)_{0-1}Ar_{0-1}$ clusters revealed by combined IR-PD and DFT-MD anharmonic vibrational spectroscopy

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Figure S1: Evolution of the Gibbs free energy difference between the Na^+(APE) (left) and K^+(APE) (right) conformers computed at the MP2/TZVPP level of theory.

Figure S2: VDOS analysis of the AG_1-Na^+(add) (left) and AG_1-K^+(add) (right) dynamical IR spectrum. VDOS relative intensities are scaled in order to be compared with the IR.

Figure S3: Evolution of the Gibbs free energy difference between the Na^+(APE)(H_2O) (left) and K^+(APE)(H_2O) (right) conformers computed at the MP2/TZVPP level of theory.

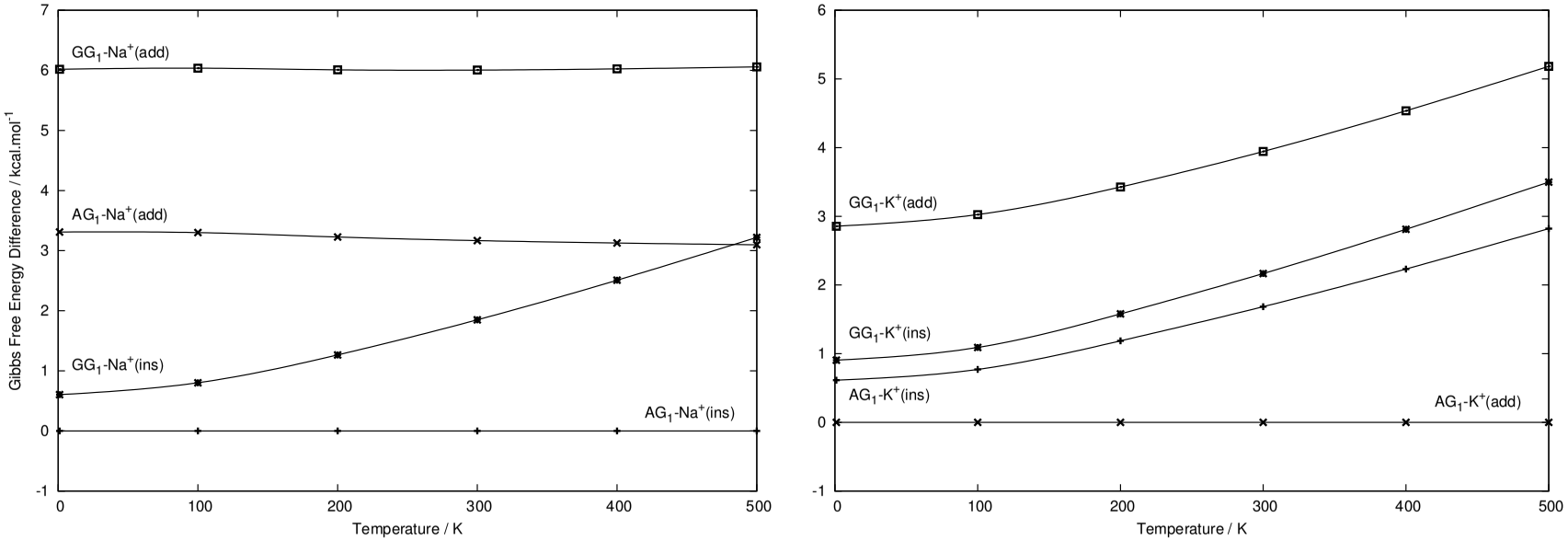
Figure S4: VDOS analysis of the AG_1-$Na^+W(add_2)$ (left) and AG_1-$K^+W(add_2)$ (right) dynamical IR spectrum at 100K. VDOS relative intensities are scaled in order to be compared with the IR.

Figure S5: VDOS analysis of the AG_1-$Na^+W(ins_1)$ (left) at 300 K and AG_1-$K^+W(add_2)$ (right) at 250 K dynamical IR spectrum. VDOS relative intensities are scaled in order to be compared with the IR.

Figure S6: Harmonic spectrum of the Na^+(APE) (left) and K^+(APE) (right) conformers computed at the MP2/TZVPP level of theory.

Figure S7: Harmonic spectrum of the Na^+(APE)(H_2O) (left) and K^+(APE)(H_2O) (right) conformers computed at the MP2/TZVPP level of theory.

Figure S8: MP2/TZVPP optimized structure of the transition state between the Na^+-AG_1 "addition" and "insertion" structures.



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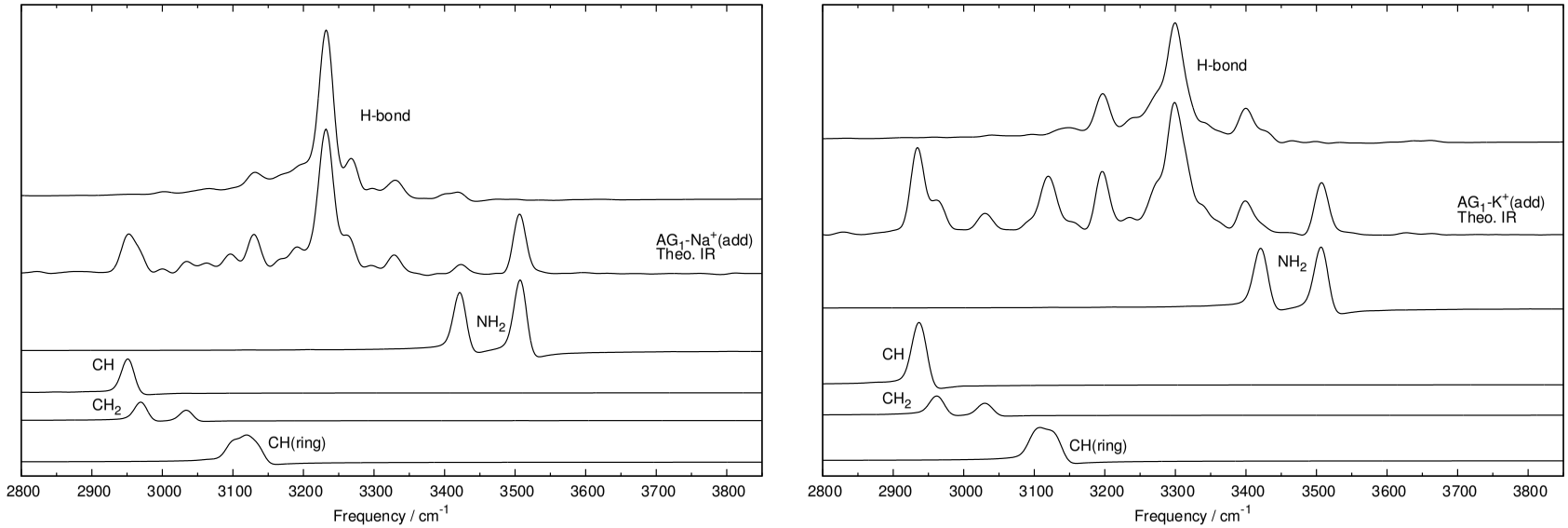
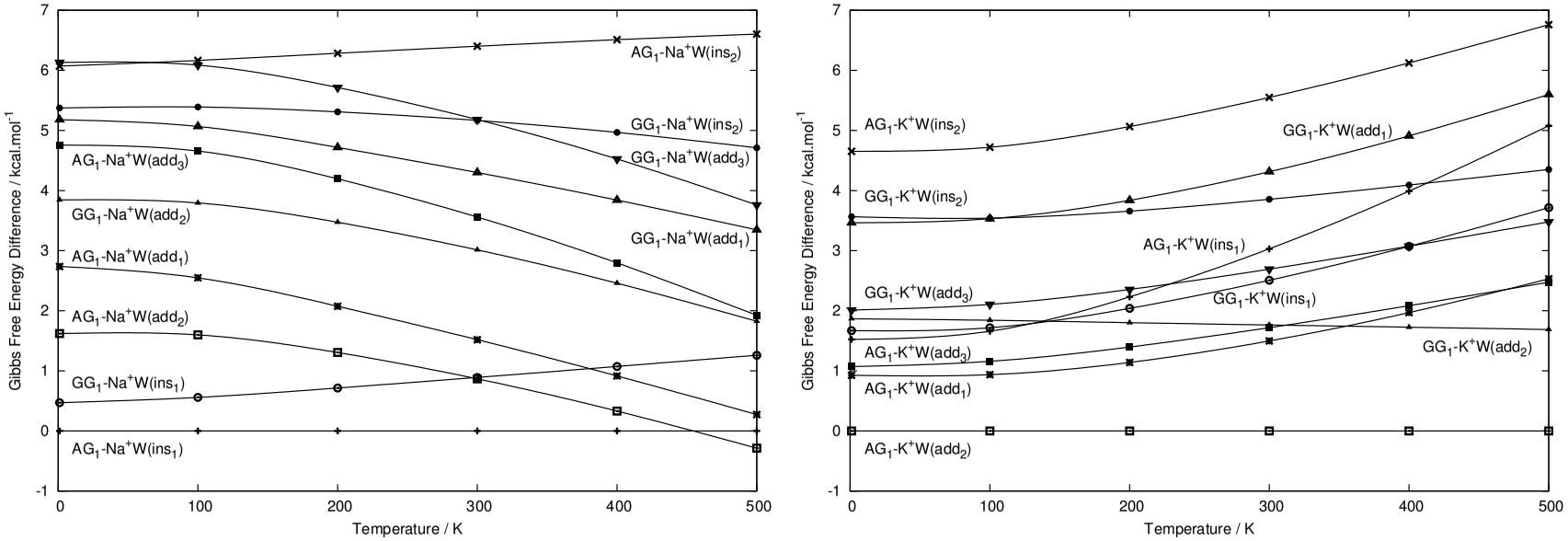


Figure S2: VDOS analysis of the AG_1-Na^+(add) (left) and AG_1-K^+(add) (right) dynamical IR spectrum. VDOS relative intensities are scaled in order to be compared with the IR.



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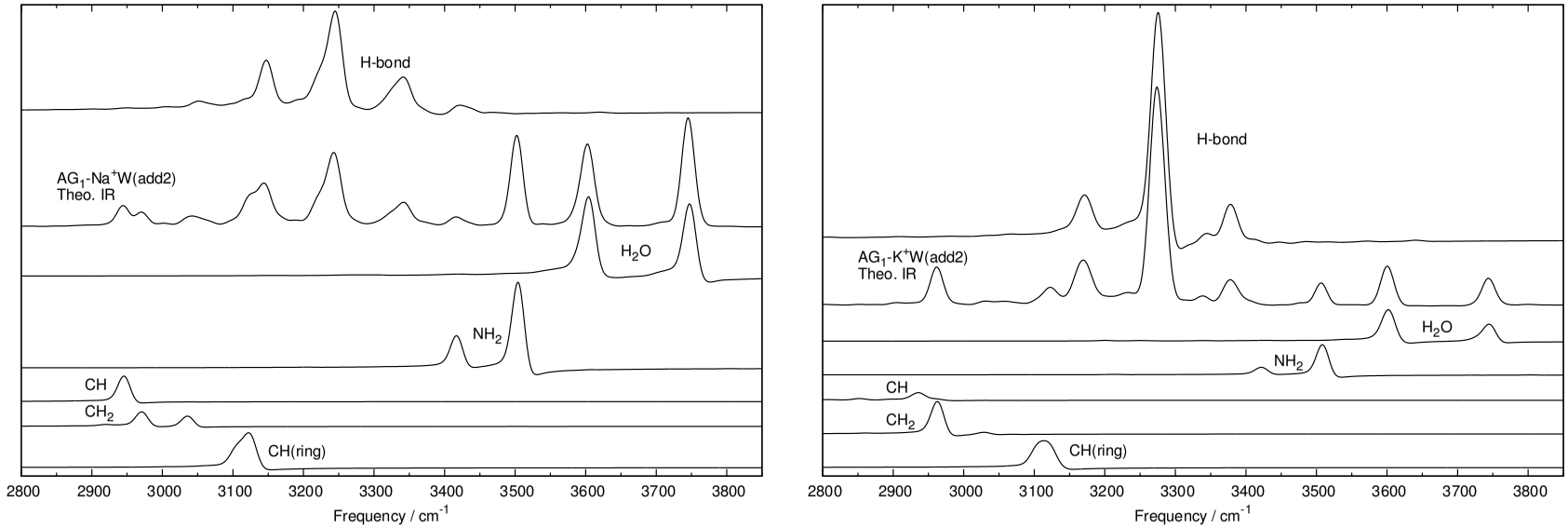

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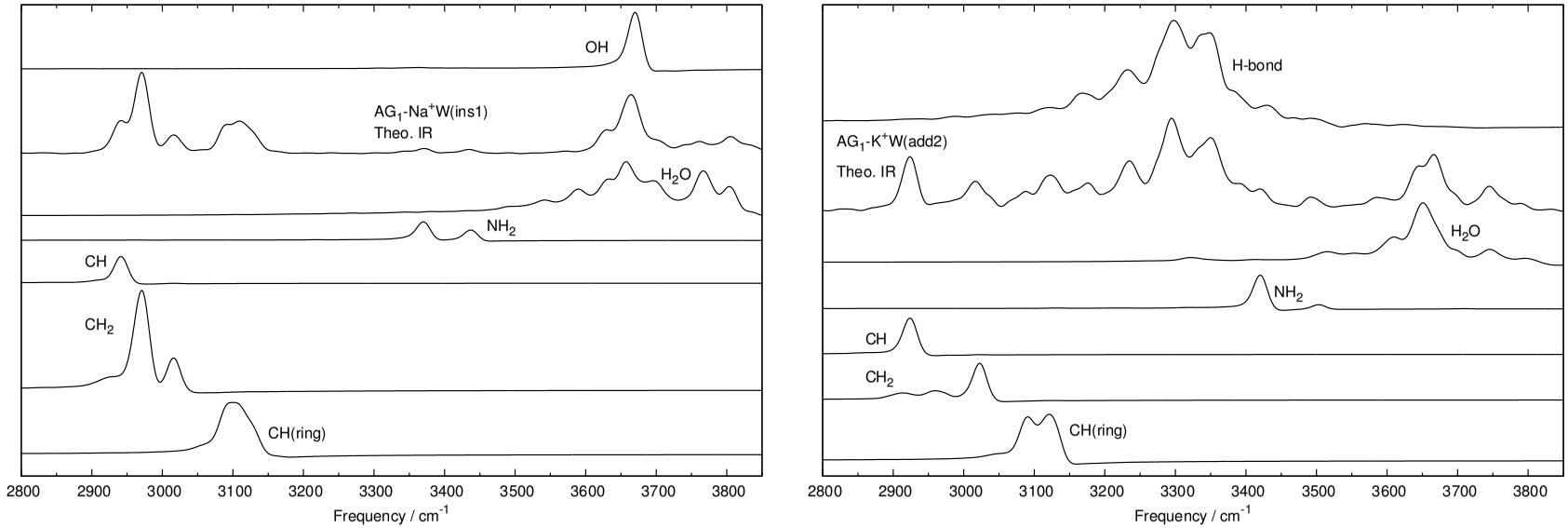

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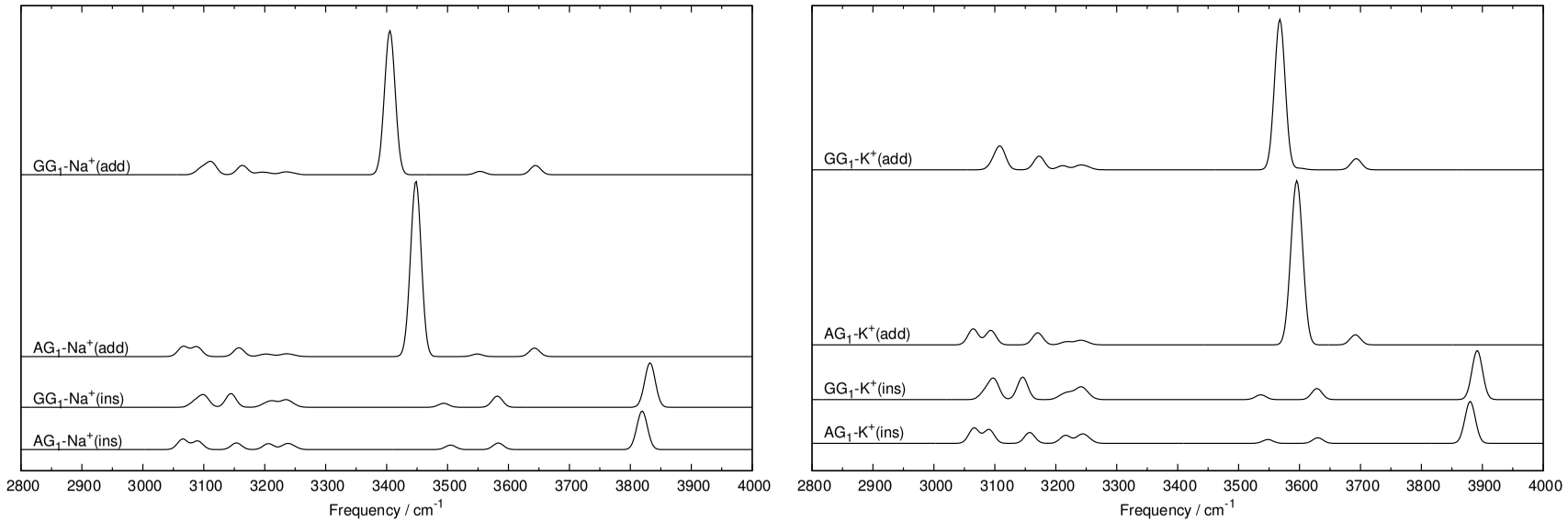

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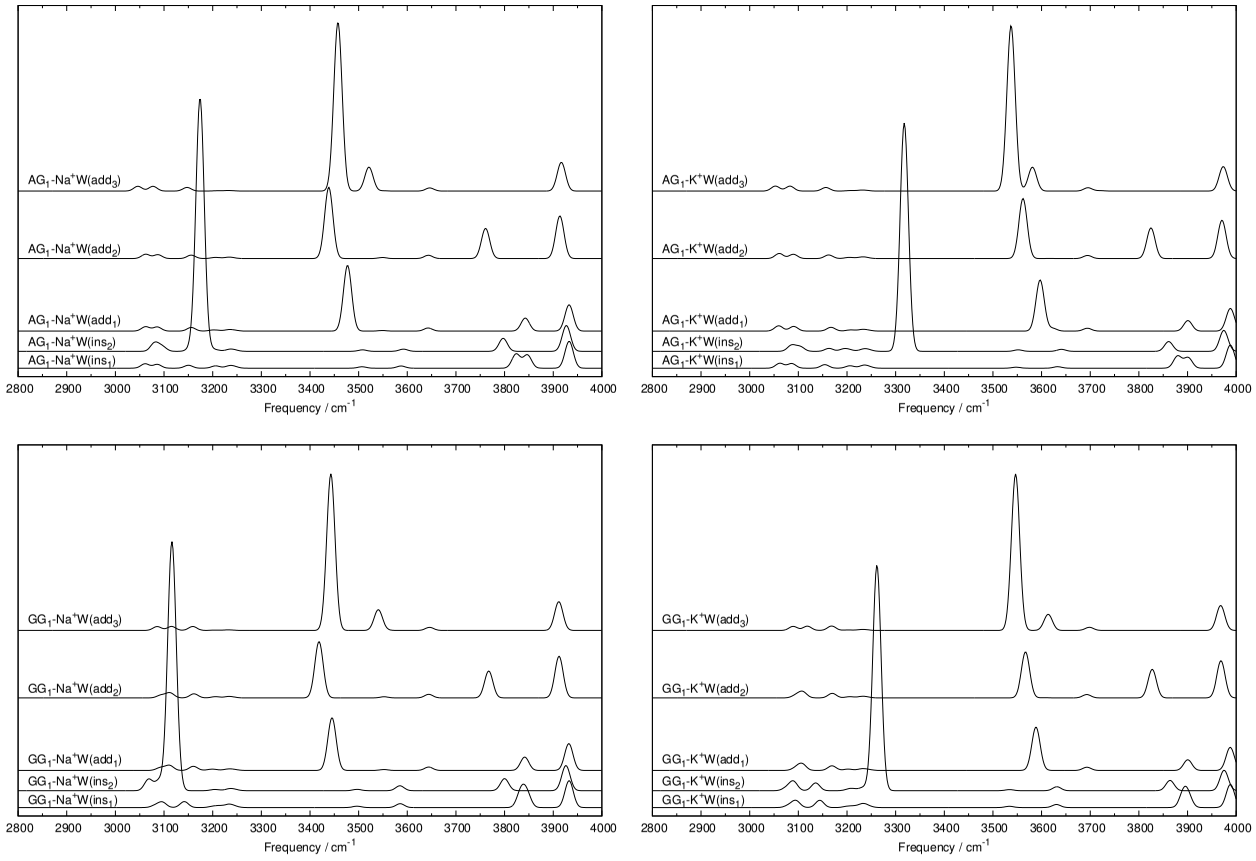
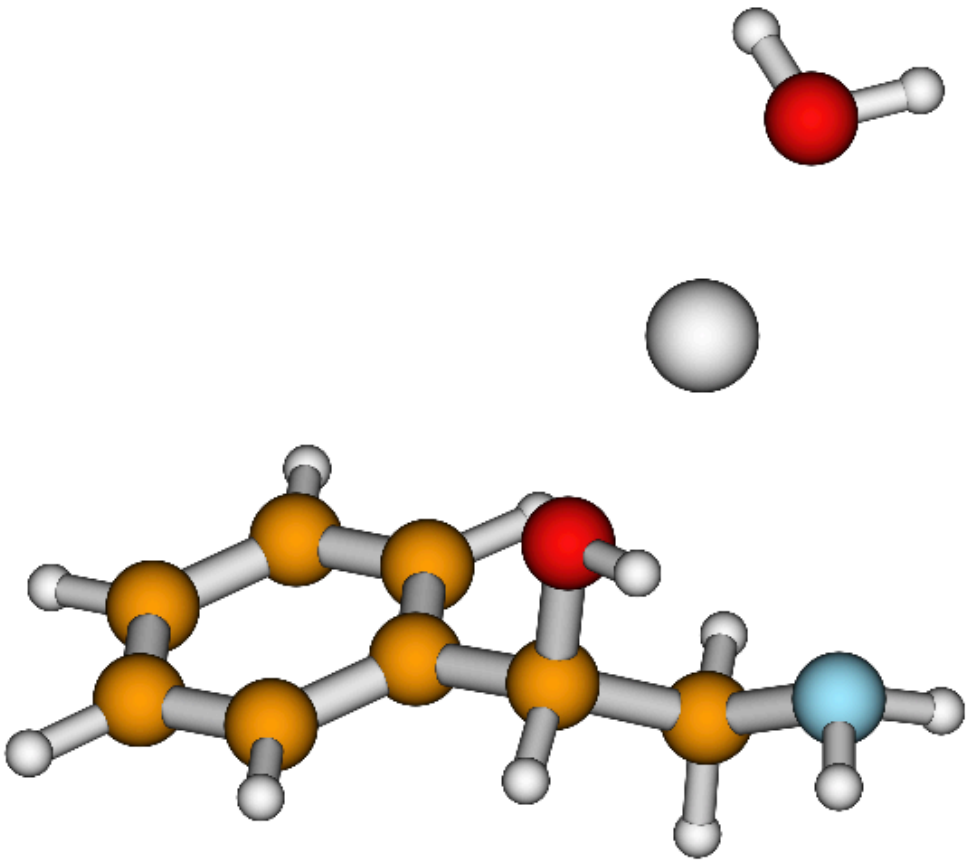


Figure S7: Harmonic spectrum of the $Na^+(APE)(H_2O)$ (left) and $K^+(APE)(H_2O)$ (right) conformers computed at the MP2/TZVPP level of theory.



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