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Excited state dynamics of protonated dopamine: Hydration and conformation effects

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Supplementary Material

Table S1 Gibbs free energy (180 K) of the ten lowest energy conformers of $DAH^+(H_2O)_3$.

Conf.	ΔG_{180K} / kJmol^{-1}
G1-1	0
G1-2	2.8
G1-3	7.8
G2-1	9.8
G1-4	11.2
G1-5	15.0
G1-6	17.7
G2-2	19.7
G1-7	20.1
G1-8	21.2

Table S2 Gibbs free energy (180 K) of the six lowest energy conformers of $DAH^+(H_2O)$.

Conf.	ΔG_{180K} / kJmol^{-1}
G1-1	0
G1-2	0.4
G2-1	0.5
G2-2	1.5
G2-3	1.5
G1-3	2.1

Table S3 Gibbs free energy (180 K) of the ten lowest energy conformers of $DAH^+(H_2O)_2$.

Conf.	ΔG_{180K} / kJmol^{-1}
G1-1	0
G1-2	2.0
G2-1	2.9
G1-3	3.2
G2-2	4.3
G2-3	4.8
G1-4	5.5
G2-4	7.1
G1-5	7.5
G1-6	8.5

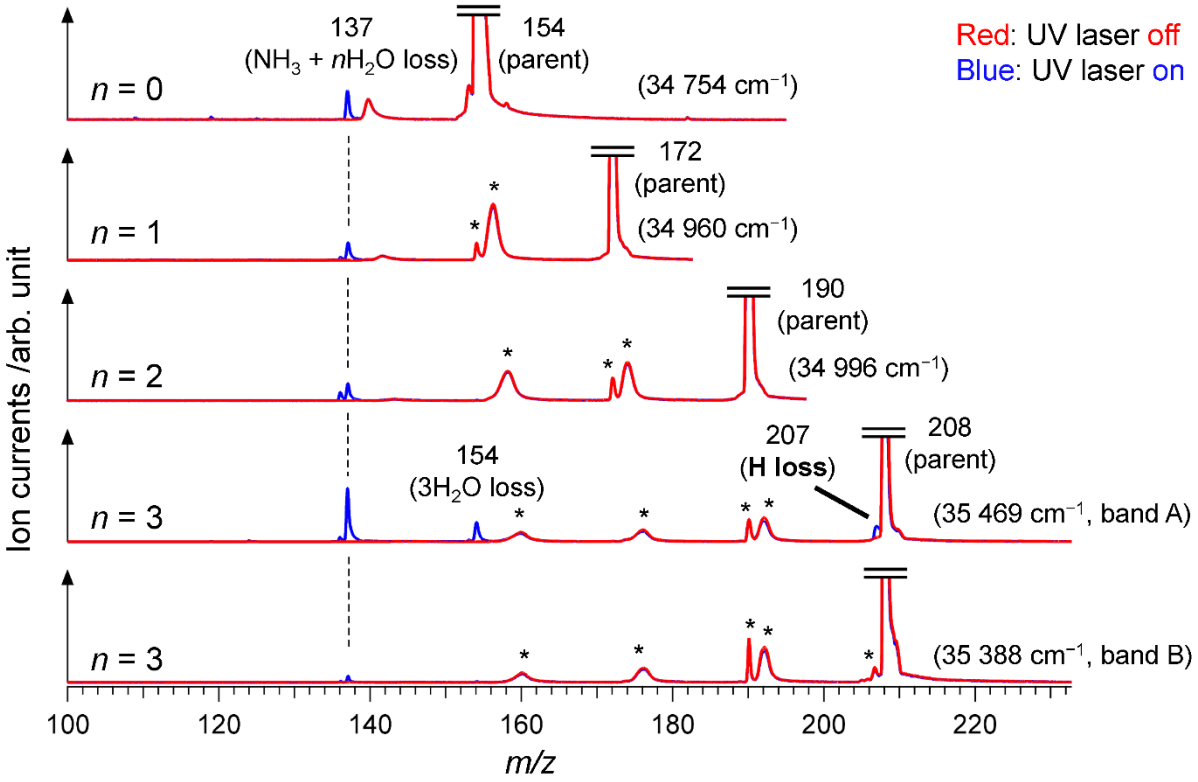

Fig. S1 UV photodissociation mass spectra of $DAH^+(H_2O)_n$ (n = 0 – 3). Blue and red lines correspond to the spectra with UV laser on and off, respectively. The peaks marked by asterisk show fragments caused by collision-induced dissociation. Numbers in parentheses show excitation wavenumber.

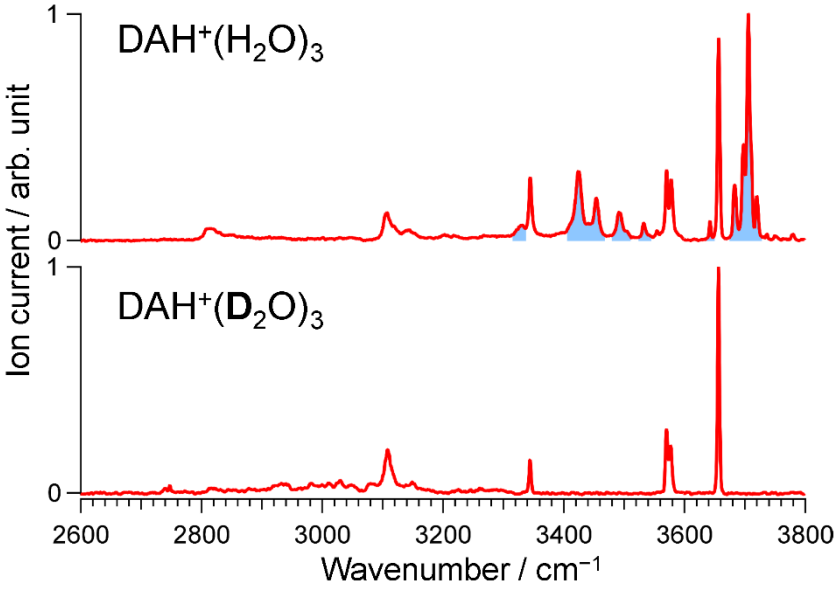

Fig. S2 Comparison between the IRPD spectra of $DAH^+(H_2O)_3$ and $DAH^+(D_2O)_3$. The blue shaded area enlightens the frequencies associated with water that disappear in the heavy water spectrum. The H/D scrambling in the linear ion trap is negligible due to the low temperature (180 K).[1]

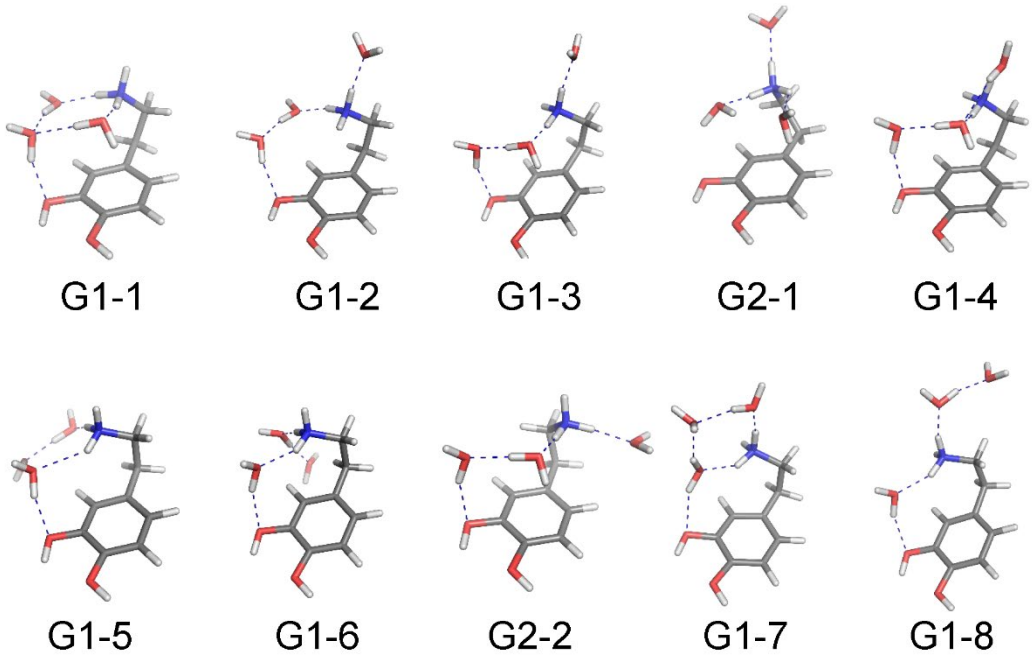

Fig. S3 Structures of the ten lowest energy conformers of $DAH^+(H_2O)_3$. G1 and G2 correspond to the syn and anti rotamer of DAH^+, respectively.

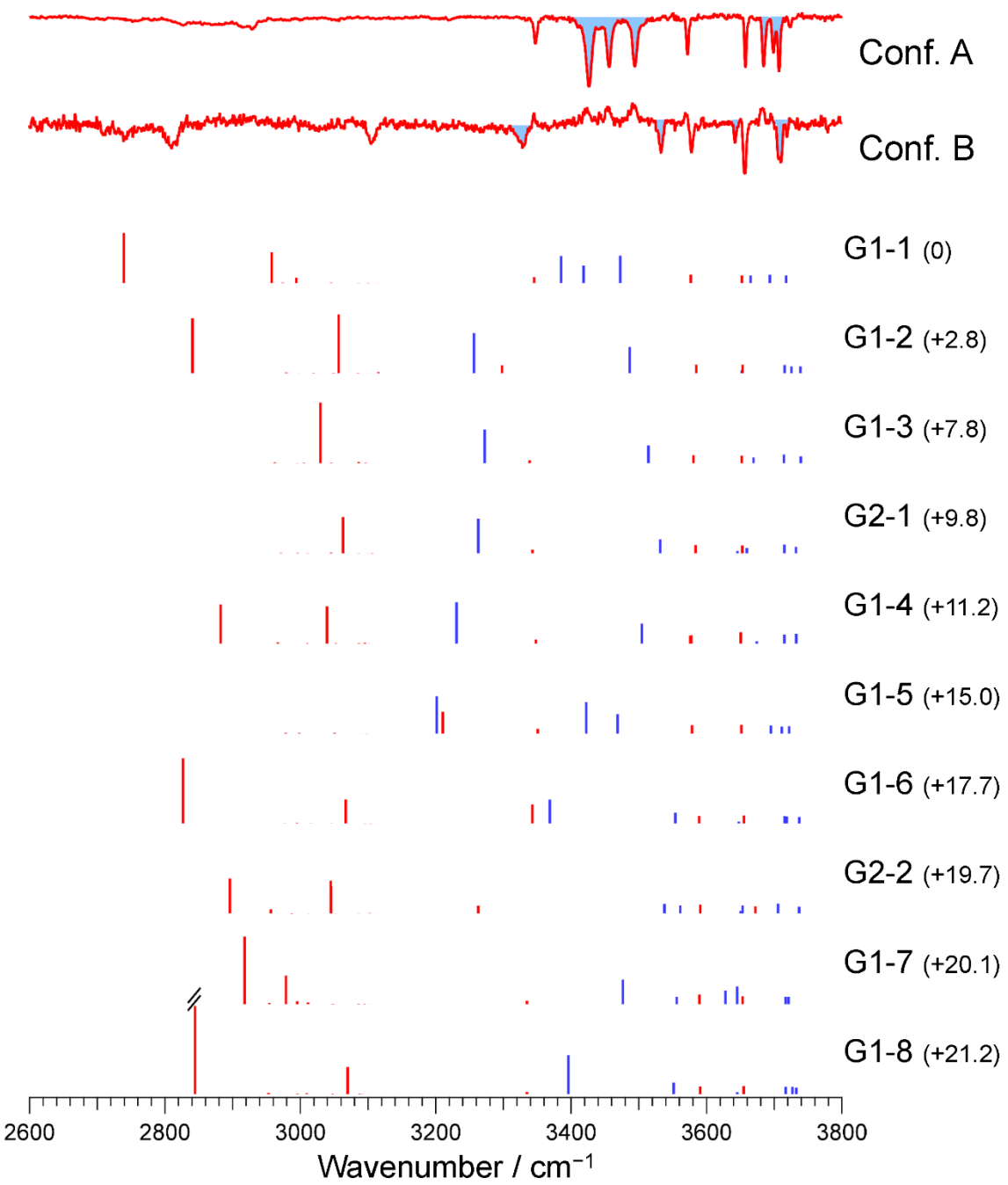

Fig. S4 Calculated IR spectra of the ten lowest energy conformers of $DAH^+(H_2O)_3$. Numbers in parentheses indicate Gibbs free energy at 180 K.

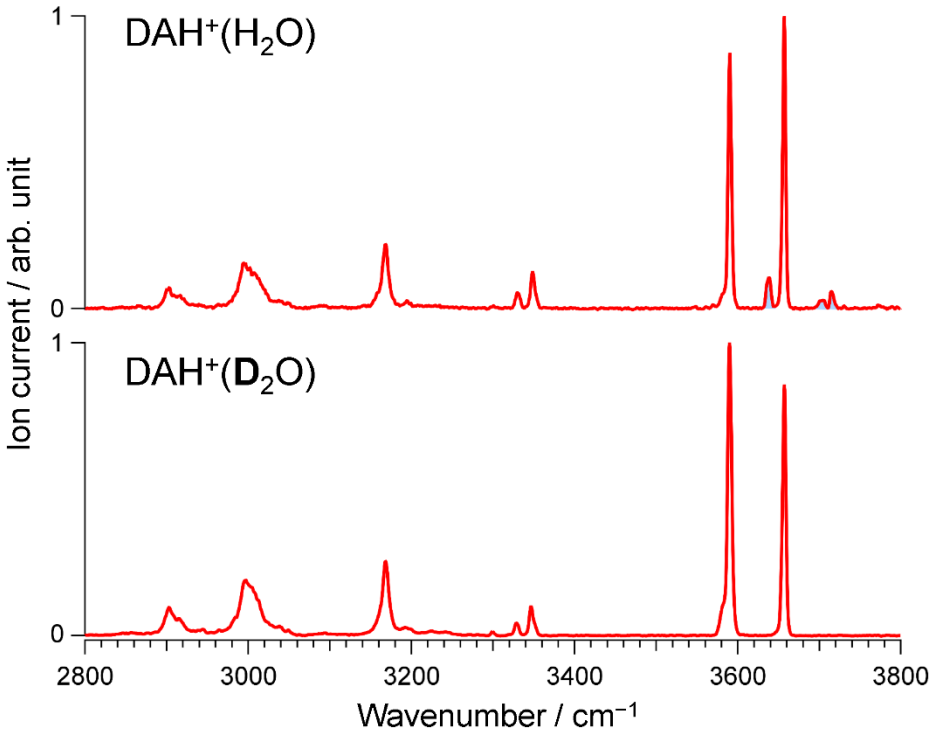

Fig. S5 Comparison between the IRPD spectra of $DAH^+(H_2O)$ and $DAH^+(D_2O)$. The blue shaded area enlightens the frequencies associated with water that disappear in the heavy water spectrum.

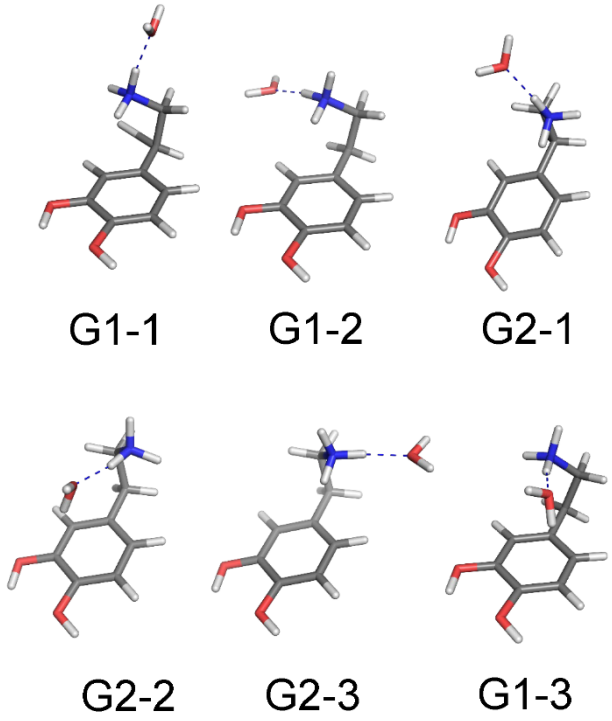

Fig. S6 Structures of the six lowest energy conformers of $DAH^+(H_2O)$.

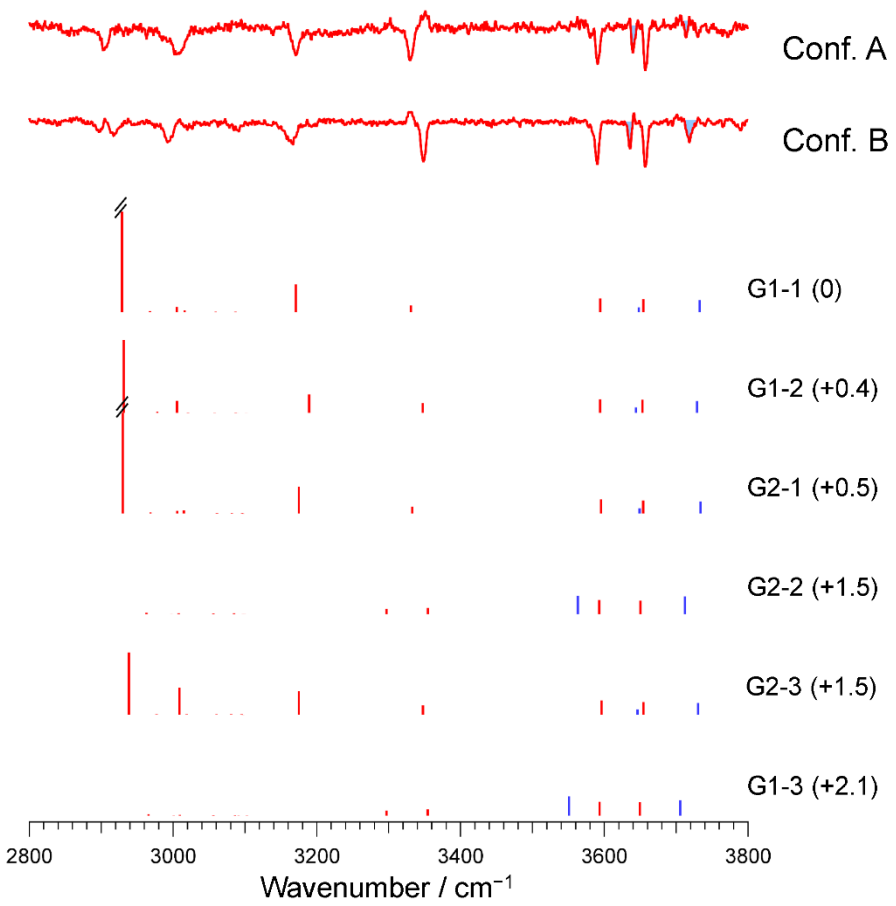

Fig. S7 Calculated IR spectra of the six lowest energy conformers of $DAH^+(H_2O)$. Numbers in parentheses indicate Gibbs free energy at 180 K.

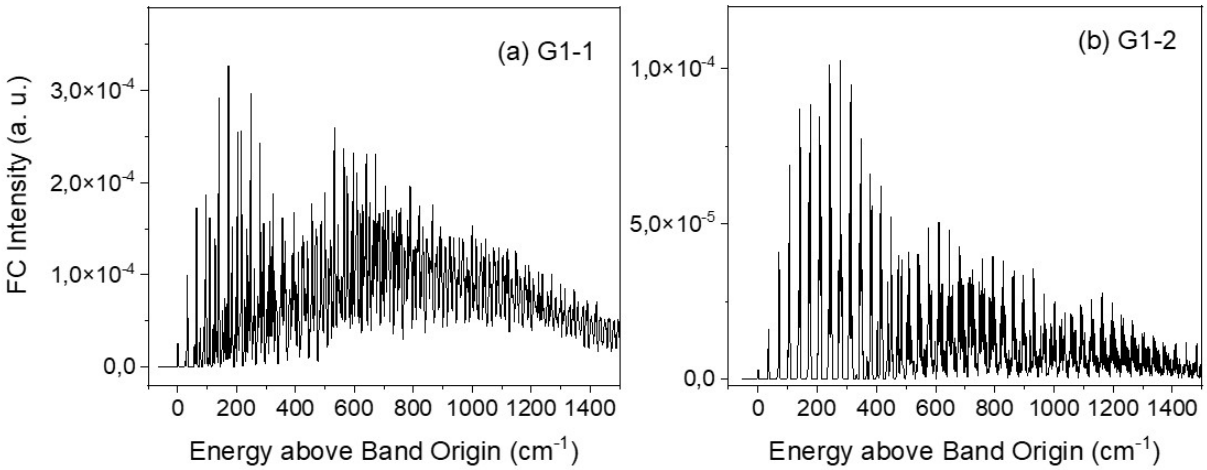

Fig. S8 Calculated Franck-Condon factors of the two conformers (a) G1-1 and (b) G1-2 of DAH^+-(H_2O).

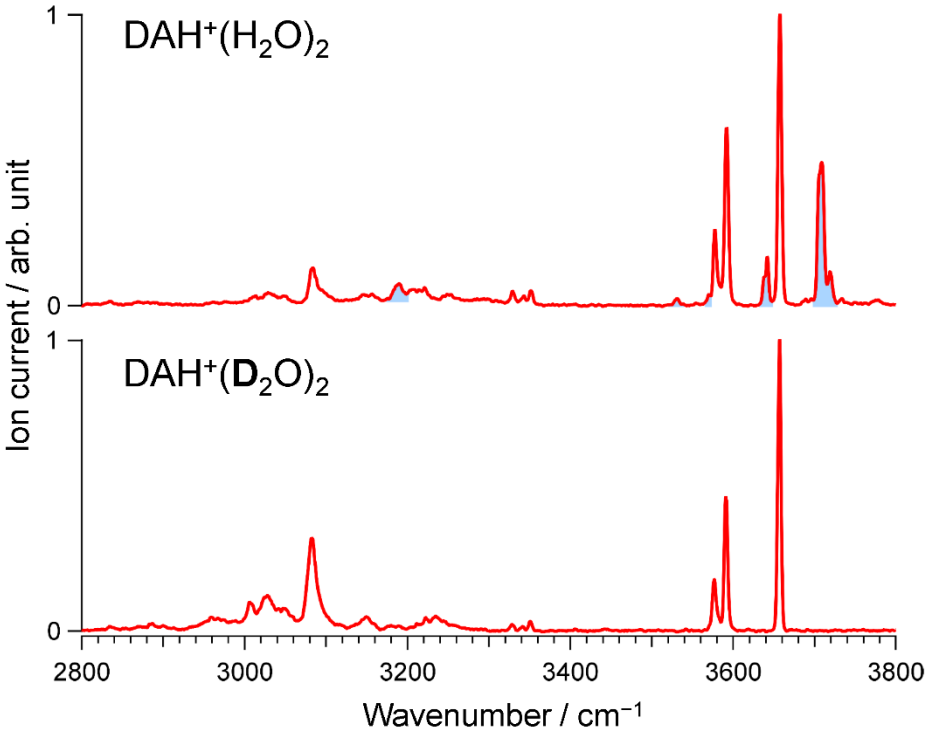

Fig. S9 Comparison between the IR spectra of $DAH^+(H_2O)_2$ and $DAH^+(D_2O)_2$. The blue shaded area enlightens the frequencies associated with water that disappear in the heavy water spectrum.

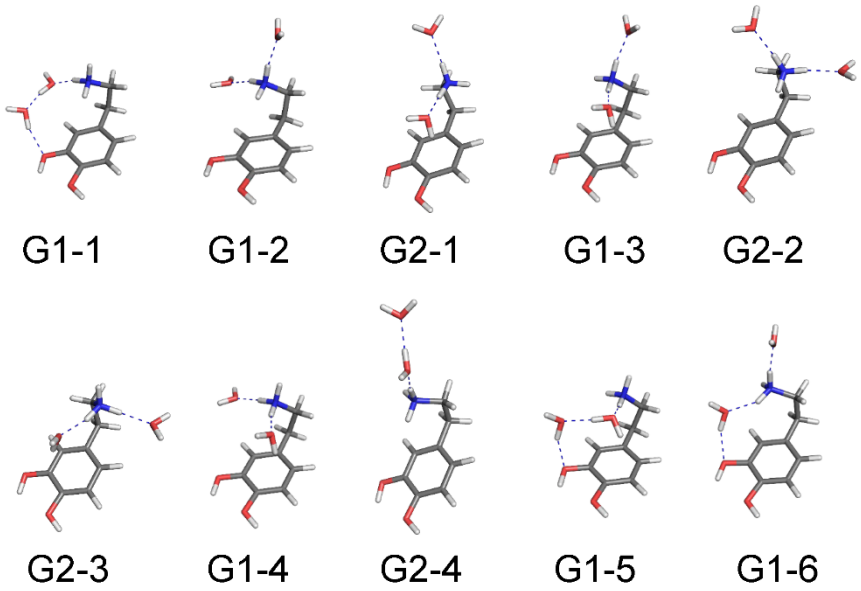

Fig. S10 Structures of the ten lowest energy conformers of $DAH^+(H_2O)_2$.

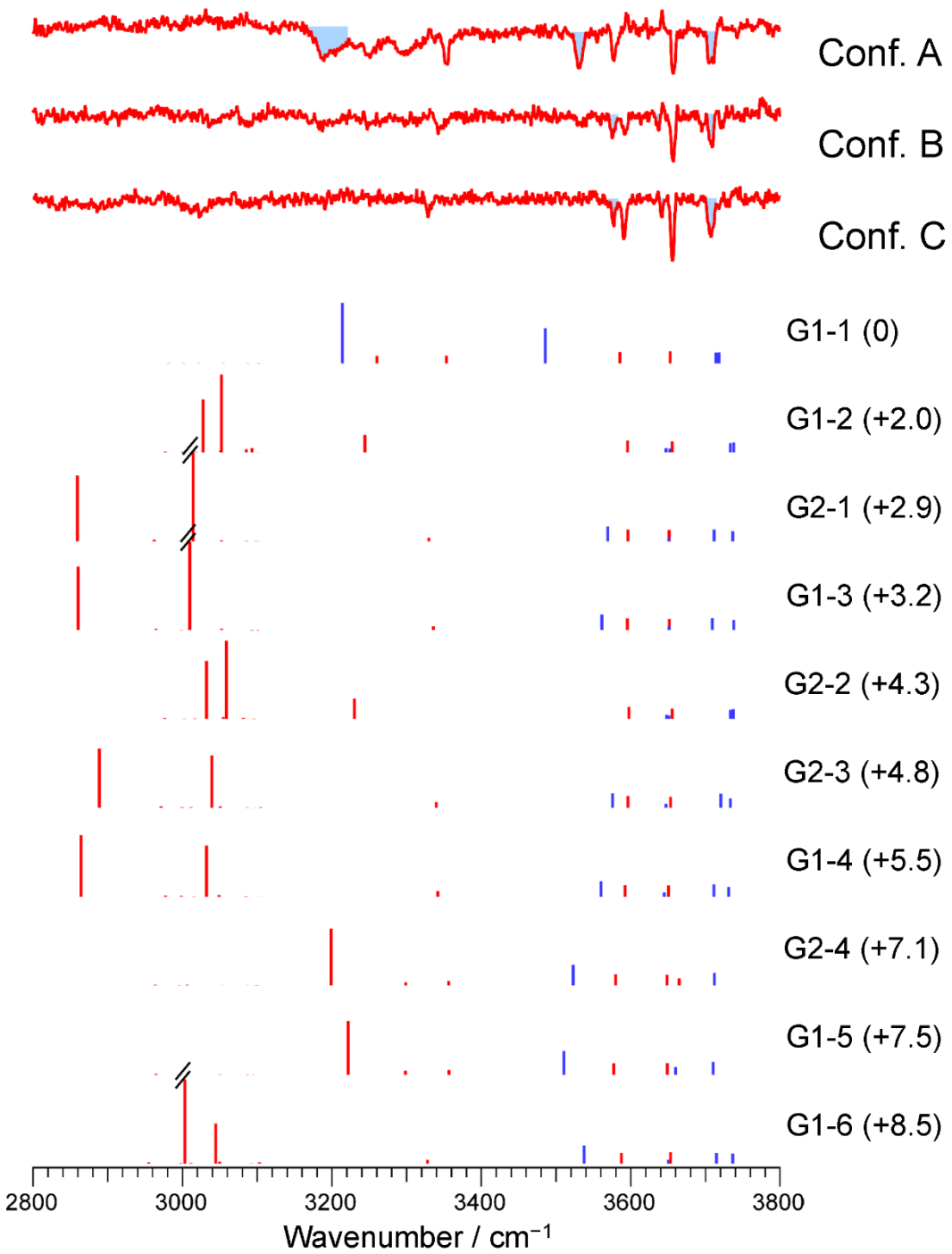

Fig. S11 Calculated IR spectra of the ten lowest energy conformers of $DAH^+(H_2O)_2$. Numbers in parentheses indicate Gibbs free energy at 180 K.

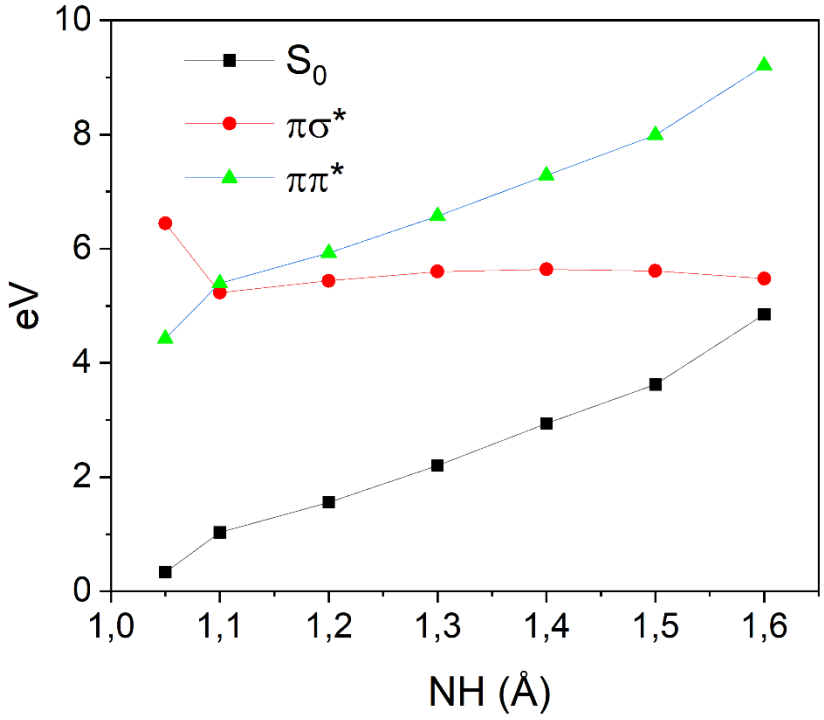

Fig. S12 Minimum Energy Path (MEP) for the G1-1 DAH^{+}-$(H_2O)_3$ conformer along the N-H stretch not involved in H-bond (free N-H).

Reference

1. J. M. Voss, K. C. Fischer and E. Garand, *J. Phys. Chem. Lett.*, 2018, **9**, 2246-2250.