Supplementary Information to: Correlated proton dynamics in entangled hydrogen bonding networks: the benchmark case of 3-hydroxyglutaric acid

Bruno Martínez–Haya[a], Juan Ramón Avilés–Moreno, Francisco Gámez, Jonathan Martens, Jos Oomens, Giel Berden

1. Atomic coordinates of 3-hydroxy glutaric molecular configurations

Files **'atomic-coordinates.zip'**: neutral molecule (Cko.xyz; k=1-4), protonated molecule (Ckp.xyz), deprotonated molecule (Ckm.xyz)

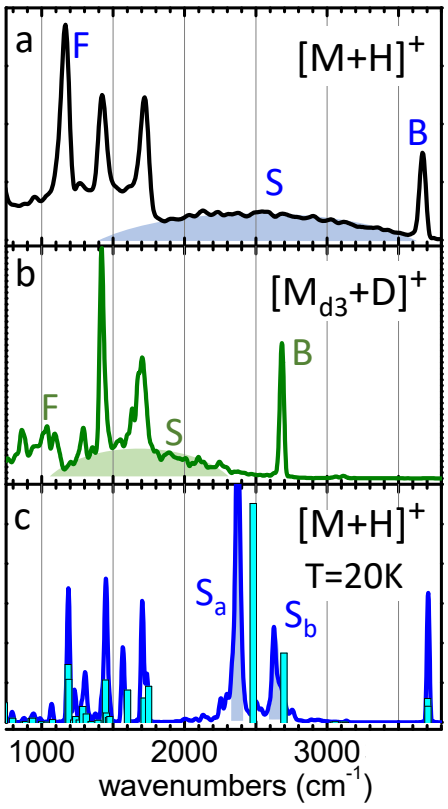
2. Video animations of BOMD trajectories

Files **'p-proton.mp4'** and **'m-proton.mp4'**: Animations of BOMD trajectory for the $[M+H]^+$ and $[M-H]^-$ complexes, respectively, illustrating correlations in proton diffusion along the two H-bonds.

File **'p-angle.mp4'**: Animation of BOMD trajectory for the $[M+H]^+$ complex illustrating a transit from a bent backbone configuration to a linear one.

3. Additional BOMD computations

Fig. S1 a) BOMD IR spectrum of protonated 3-hydroxy glutaric acid at 350 K; b) same spectrum for the four-fold deuterated isotopologue: c) BOMD IR spectrum of protonated 3-hydroxy glutaric acid at 20 K. Shaded areas highlight the bands associated with O-$H^{\delta+}$ stretching in the proton-bonding moiety. Blue bars indicate B3LYP-D3(BJ)/6-311++G(d,p) harmonic transitions. No scaling factor for the vibrational frequencies is introduced in these plots.



[a] author for correspondence: bmarhay@upo.es