Proton Transfer by Carbonic Acid: Charge Transfer and Proton Relay

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We have previously proposed that Carbonic Acid H_2CO_3 molecule (CA) is an important protonating agent in both biological and environmental contexts [1,2,3]. In the present talk ---after a brief introduction on the previously published and simpler 'on contact' direct proton transfer (PT) from CA to a base in aqueous solution [1,2] --- we will focus on key molecular level aspects of the more complex ultrafast CA-base PT reaction when the acid and base are initially separated by a water molecule: a proton relay mechanism with important electronic charge transfer involving all three molecules, and appropriate surrounding water solvent rearrangements.

References:

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