

Photoinduced double proton transfer in the glyoxal-methanol complex along T1 reaction path – a quantum chemical topological study.

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Streszczenie

The experimentally confirmed double proton transfer (DPT) reaction in glyoxal-methanol complex follows a complicated mechanism triggered by the excitation of the complex to the lowest singlet excited electronic state. The mechanism involves two complementary pathways, the first of which proceeds exclusively in the singlet manifold. The competing one, which is studied here with the use of quantum chemical topological methods, involves the lowest triplet state. Both Atoms-in-Molecules approach and Electron Localizability Indicator based approach demonstrate that protons dressed with some amount of electron density migrate to and from the methanol, which leads to the rearrangement of four covalent bonds. The transition structure nearly coincides with the dissociation of the covalent CH bond in glyoxal. DPT proceeds through a structure formed by the protonated $[\text{MeOH}_2]^{+0.66}$, with H atoms equidistant to O atom, and deprotonated $[\text{C}_2\text{O}_2\text{H}]^{-0.66}$. The key stages of the evolution of the crucial covalent bonds along the intrinsic reaction path have been demonstrated.

Słowa kluczowe

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