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**Title:** Water-assisted ground state intra-molecular proton transfer in 2,5-dihydroxy-substituted azobenzenes: experimental and computational studies†

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**Keywords:** Phenomenon  
Ground-state  
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**Abstract:** Herein, the phenomenon of ground-state proton transfer in a series of 2,5-dihydroxy azobenzene derivatives was studied. The mechanism of proton transfer in a dimethylacetamide (DMA)–water mixture was investigated by UV-vis spectroscopy. Time-dependent density functional theory (TD-DFT) calculations were performed to achieve further confirmations. The intramolecular hydrogen bond between the hydrogen atom of the o-hydroxyl group and the azo-group was found to be reinforced during the hydrogen transfer process. The topological properties of the intramolecular interactions were determined by atoms in molecules (AIM) calculations using the AIM2000 package. It was observed that water molecules and substitutions at the ortho-position corresponding to the azo-group facilitated the occurrence of the proton transfer mechanism in the ground state. The effect of the substitutions and water molecules was investigated by the DFT calculations.

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