

An Explanation of the Unusual Strength of the Hydrogen-Bond in Small Water Clusters

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Abstract

We seek to explain why the hydrogen bond possesses unusual strength in small water clusters that account for many of the complex behaviors of water. We have investigated and visualized the donation of covalent character from covalent (σ) to hydrogen-bonds, by calculating the eigenvector coupling properties of QTAIM, stress tensor $\sigma(r)$ and Ehrenfest Force $F(r)$ on the $F(r)$ molecular graph. The next generation 3-D bond-path framework sets are presented and only the $F(r)$ bond-path framework sets reproduce the earlier finding on the coupling between covalent (σ) and hydrogen-bonds that possess a degree of covalent character. The directional character of the covalent (σ) and hydrogen-bonds 3-D bond-path framework sets for the $F(r)$ explains differences found in the earlier results from QTAIM and the stress tensor $\sigma(r)$.

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