A realistic DFT potential energy surface of $\text{H}_5^+$ cluster

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The potential energy surface of $\text{H}_5^+$ is characterized using density functional theory. The potential hypersurface is evaluated at selected configurations employing different functionals, and compared with results obtained from *ab initio* CCSD(T) calculations. The lowest ten stationary points (minima and saddle-points) on the surface are located, and the features of the short-, intermediate-, and large-range intermolecular interactions are also investigated. A detailed analysis of the surface's topology, and comparisons with extensive CCSD(T) results, as well as a recent *ab initio* analytical surface, shows that DFT calculations using the B3(H) functional represent very well all aspects studied on the $\text{H}_5^+$ potential; including the tiny energy difference between the minimum at 1-$C_{2v}$ configuration and the 2-$D_{2d}$ one corresponding to the transition state for the proton transfer between the two equivalent $C_{2v}$ minima, as well as the correct asymptotic behavior of the long-range interactions. The calculated binding energy and dissociation enthalpies compare very well with previous benchmark coupled-cluster *ab initio* data, and with experimental data available.

Based on these results the use of such approach to perform first-principles molecular dynamics simulations could provide reliable information regarding the dynamics of protonated hydrogen clusters.

References