

Direct observation of the substitution effects on the hydrogen bridge dynamics in selected Schiff bases—A comparative molecular dynamics study.

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Streszczenie

We have studied substituent effects on the properties of the intramolecular hydrogen bond of some *ortho*-hydroxy Schiff bases using density functional theory (DFT) based first-principle molecular dynamics (FPMD) and path integral molecular dynamics. The studied compounds possess a strong intramolecular hydrogen bond ($r_{(O\cdots N)} \leq 2.6$ Å), which can be tuned by substitution to either (i) enhance the basicity of the acceptor moiety by induction effects or (ii) decrease the hydrogen bond length through steric repulsion. DFT calculations and FPMD were employed to investigate structural and dynamical properties of the selected molecules, while quantum effects on the structural properties were assessed using path integral FPMD. The simulations were performed *in vacuo* and in the solid state to study the influence of the environment on the hydrogen bond and spectroscopic properties. We give computational support to the suggestion that induction effects are less effective to tune the intramolecular hydrogen bond properties of the discussed *ortho*-hydroxy Schiff bases than the steric or the environmental effects.

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