

Blue or red $\Delta\nu_{\text{XH}}$ complexation shift in $\text{X-H}\cdots\text{CO}_2$ hydrogen-bonded complexes?Autorzy

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The position of the $\nu(\text{XH})$ stretching band for more than 100 proton donors ($\text{X} = \text{O}, \text{N}, \text{C}, \text{S}, \text{Se}, \text{P}, \text{Si}, \text{B}, \text{F}, \text{Cl}, \text{Br}$) complexed with CO_2 was calculated at the MP2/6-311++G(d,p) level. Complexation energies and natural bond orbital characteristics were also determined. These calculations revealed that the direction of the $\nu(\text{XH})$ band shift was related to the charge born by the hydrogen atom of the proton donor. $\text{X-H}\cdots\text{OCO}$ blue-shifting hydrogen bonds were found for compounds characterised by a small charge, while red-shifting was observed for those compounds with a high positive charge on the hydrogen atom.

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