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Investigating the Difference in Stability of Various Isomeric Hydrogen Bonded Dimers

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Abstract : The structures and energetics of various isomeric hydrogen bonded dimers, such as (FH…OC, FH…CO), (FH…CNH, FH…NCH), (FH…N2O, FH…ON2), and (FH…NHCO, FH…OCNH) have been investigated using DFT B3LYP with aug-cc-pVTZ basis set and by natural bond orbital (NBO) analysis. For each isomeric pair we calculated: H-bond energy (ΔEB…H), charge-transfer (QCT), where B is atom bearing lone-pairs in CO, CNH, NCH, N2O, and NHCO, H-bond distances (RB…H), the elongation of HF bond (ΔRHF) and the red-shift of HF stretching frequency (ΔVHF). We conclude that the principle difference in the relative stability between each isomeric pair is attributed to distinctive interaction of carbon and oxygen lone pairs of CO, carbon and nitrogen lone-pairs of CNH and NCH, and nitrogen and oxygen lone pairs of N2O and NHCO into the unfilled antibond on HF (σ*HF).

Keywords : charge transfer, computational chemistry, isomeric hydrogen bond, natural bond orbital
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