

## 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...N<sub>2</sub>O, FH...ON<sub>2</sub>), 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 ( $\Delta E_{B...H}$ ), charge-transfer (QCT), where B is atom bearing lone-pairs in CO, CNH, NCH, N<sub>2</sub>O, and NHCO, H-bond distances (RB...H), the elongation of HF bond ( $\Delta R_{HF}$ ) and the red-shift of HF stretching frequency ( $\Delta \nu_{HF}$ ). 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 N<sub>2</sub>O and NHCO into the unfilled antibond on HF ( $\sigma^*_{HF}$ ).

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

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