

# EFFECT OF THE INTRAMOLECULAR HYDROGEN BOND ON THE ELECTRONIC STRUCTURE OF ORGANIC MOLECULES WITH A PLANAR QUASICYCLE

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The electronic structure of the following organic molecules is studied using the HF/6-311G(*d,p*) method: malonic dialdehyde, acetylacetone, thiomalonic aldehyde, 2- $\text{XC}_6\text{H}_4\text{NH}_2$  aniline derivatives, 2- $\text{XC}_6\text{H}_4\text{OH}$  phenol derivatives, 2- $\text{XC}_6\text{H}_4\text{SH}$  thiophenol derivatives ( $\text{X} = \text{CHO}, \text{COOH}, \text{COO}^-, \text{NO}, \text{NO}_2, \text{OH}, \text{OCH}_3, \text{SH}, \text{SCH}_3, \text{F}, \text{Cl}, \text{Br}$ ), 8-hydroxyquinoline, 8-mercaptoquinoline, tropolone. It is found that the intramolecular hydrogen bond (IHB) leads to a local electronic redistribution in the quasi-cycle, and above all to the electron density transfer among the immediate participants of IHB — from the hydrogen atom to the proton-acceptor atom. When the IHB of the  $\text{S}-\text{H}\cdots\text{O}$  type forms, the electron density mainly decreases on sulfhydryl hydrogen atom and increases on sulfur atom.

**Keywords:** intramolecular hydrogen bond, electronic structure, organic molecules with a planar quasi-cycle, *ab initio* quantum chemical study, dipole moment.