

**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-XC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> aniline derivatives, 2-XC<sub>6</sub>H<sub>4</sub>OH phenol derivatives, 2-XC<sub>6</sub>H<sub>4</sub>SH thiophenol derivatives (X = CHO, COOH, COO<sup>-</sup>, NO, NO<sub>2</sub>, OH, OCH<sub>3</sub>, SH, SCH<sub>3</sub>, F, Cl, Br), 8-hydroxyquinoline, 8-mercaptopquinoline, 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 S—H···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.