Quantum chemical studies of ion and radical cyclizations of 3,4-bis(indol-3-yl)-, 3-(indol-1-yl)-4-(indol-3-yl)- and 3,4-bis(indol-1-yl)-maleimides

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Earlier we have shown by mean quantum chemical methods that the ion cyclization of **2** and **3** leads to **2'** and **3'**(2-4' and 2-7'directions respectively) with low activation barriers. In the case of **1** (2-4' cyclization) activation energy was high and 2-2'cyclization took place with the consequent destruction of cation **1'** (Figure) [1,2].

Intermolecular 2- 2' cyclizations of 3,4-bis-(indol-3-yl)maleimide **1**, 3-(indo-1-yl)-4-(indol-3-yl)maleimide **2** and 3,4-bis-(indol-1-yl)maleimide **3** under the action of ultraviolet radiation were studied in order to estimate the thermochemical parameters (ΔH, ΔG, $\Delta G^{\#}$) of these reactions. Quantum chemical calculations by the method of density functional UB3LYP in basis 6-31G(d) has shown, that for the cyclization **2** to **2''** the values of ΔH, ΔG, $\Delta G^{\#}$ are higher, then for cyclization **1** to **1''**. For structure **3''** the SPE-minimum was not determined, and it suggests that the reaction **3→3''** is impossible. Indeed, contrary to compound **1,** the photochemical transformation **3→3''** did not occur under UV-irradiation .

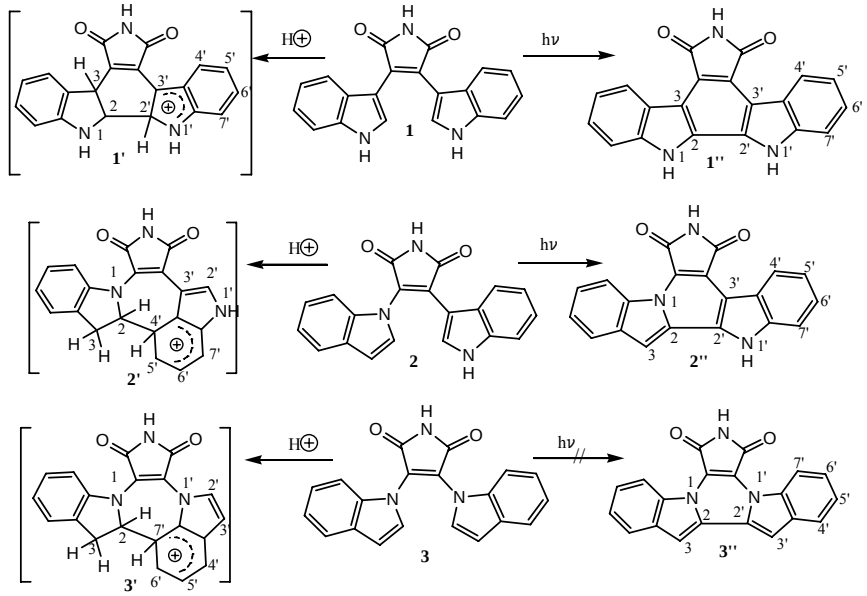

Figure. Radical and ion cyclization of 3,4-bis-indolylmaleimides.

References

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