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, ΔG°) 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, ΔG° 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
2. E. E. Bykov, S. A. Lakatosh, and M. N. Preobrazhenskaya

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