THIOCYTOSINE AS A HOLE TRAP IN A SYSTEM OF STACKED CYTOSINE BASES

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It has been shown that thioguanine and thiocytosine are good hole traps when replacing regular nucleic-acid bases in the DNA model systems. The molecular systems of selected nucleic-acid constituents offer a variety of base arrangements, and make good model systems for studying the mechanism and the migration range of electrons and/or holes. The study at 10 K revealed that in single crystals of cytosine monohydrate the holes induced by gamma irradiation migrate to the distance of 1.0 – 1.5 nm in all directions before they are trapped. The nature of trapped holes in thiocytosine-dopped cytosine crystal are neutral, N1-deprotonated thiocytosine radicals. After precise ENDOR study of the inter- and intra-molecular spin interaction, the Density Functional Theory investigation of the spin interactions for the proposed hole trap has been done. The calculated results are in much better accord with the experimental data if the cytosine molecules surrounding the thiocytosine-centered trapped hole in the lattice are taken into account. The mechanism of hole transfer and trapping is discussed.

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