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Characteristics of the mechanism of 5-bromo-6-hydroxyl-aminouracyl transformation to 5-amino-6-nitrozo-uracyl

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Abstract

Mechanism of 5-azido-6-hydroxylaminouracil transformation to 5-amino-6-nitrosouracil has been investigated at the B3LYP and MCQDPT2//CASSCF levels of theory. It has been shown that the decomposition of azide group may be activated either photo-chemically or thermally. The dominant reaction channel involves transformation of 5-nitrene-6-hydroxylaminouracil into 5-imino-6-oximouracil which is characterized by low activation barrier (1.4 kJ/mol) and highly exothermic effect (-191.1 kJ/mol). Formation of the final product may proceed *via* a number of alternative pathways, and the most probable are the journey of hydrogen atoms through the solvent molecule bridges or the sequence of tautomeric forms of pyrimidine base.