

New aspects of UV photolysis of hydrogen peroxide : nitrogen matrix isolation FTIR and theoretical studies.

Autorzy

Justyna Krupa

Maria Wierzejewska

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Streszczenie

UV photochemistry of H_2O_2 isolated in solid nitrogen at 15 K has been studied experimentally by FTIR matrix isolation technique and theoretically using DFT and MP2 methods. The major photoproducts were identified as (i) nitrous oxide and $\text{N}_2\text{O}\cdots\text{H}_2\text{O}$ complex and (ii) free and complexed to N_2O hydroxyl radicals. Except for the OH radicals all observed species are unique and characteristic for H_2O_2 photolysis in solid nitrogen. The identities of the products have been confirmed by comparison with results of quantum chemical calculations, and reference to the spectral data of related molecules. Differences in the photolysis course upon irradiation at 230 and 212 nm are discussed.

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