UV Photolysis Study of *Para*-Aminobenzoic Acid using Parahydrogen Matrix Isolated Spectroscopy

McKinnon, A.,*[1] Moore, B.,[2] Djuricanin, P.,[2] and Momose, T.[2]

[1] e-mail address: alxmck@chem.ubc.ca, Department of Chemistry, The University of British Columbia, Vancouver BC, V6T 1Z1, CANADA

[2] Department of Chemistry, The University of British Columbia, Vancouver BC, V6T 1Z1, CANADA

Para-aminobenzoic acid (PABA) is one of the original sunscreen chemical agents. As these agents often undergo photodissociation during the process of UV absorption, understanding the photochemical behaviour of sunscreen agents is highly important. In this study, the photolysis of PABA was studied at three different UV ranges (UVA: 355 nm, UVB: >280 nm, and UVC: 266 nm and 213 nm) using parahydrogen (pH$_2$) matrix isolation Fourier-Transform infrared (FTIR) spectroscopy. Parahydrogen has weak cage effects that allow radicals to escape the lattice site and therefore prevent further radical recombination reactions. PABA was found to be stable under UVA irradiation. However, PABA dissociated into 4-aminylbenzoic acid (the PABA radical) through amino hydrogen atom loss under UVB and UVC irradiation.[1] The production of the PABA radical supports a previously proposed mechanism of the formation of the carcinogenic PABA-thymine adduct. The infrared spectrum of the PABA radical was analyzed with quantum chemical calculations. Two conformers of this radical were observed in the pH$_2$ matrix. Both conformers of the PABA radical were stable in solid pH$_2$ for hours after irradiation. This work displays that pH$_2$ matrix isolation spectroscopy is effective for sunscreen agent photochemical studies.

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