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Decomposition kinetics of *n*-chloro-alanines in alkaline aqueous solution

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Physiological processes have generated immense interest in the redox reactions of hypochlorous acid with amines, amino acids, peptides and proteins which generate *N*-chlorinated compounds under various conditions. *N*-chloramines have outstanding biological importance because after penetrating into the cells they induce oxidative stress which ultimately leads to the cell death. In addition, N-chloramines exhibit disinfecting activities and sufficiently kill microorganisms, though their efficiency is generally less than that of chlorine or hypochlorous acid. The formation of *N*-chloro-α-alanine (MCA) from HOCl and α-alanine is very fast under alkaline conditions. In spectrophotometric experiments on the decomposition of MCA at 253nm and higher wavelengths simple first-order behavior was observed. The pseudo-first order rate constant for the decomposition, k_{obs}, is identical at each wavelength and independent from the concentration of α-alanine: $k_{obs}=(1.00\pm0.03) \times$ 10-3 s-1. At shorter wavelengths, complex kinetic features were observed confirming that other processes interfere with the decomposition. This work confirms that the stability of the MCA solutions is strongly pH-dependent; they are more stable under neutral conditions than in alkaline solutions. ^{1}H-NMR studies were carried out to obtain detailed information on the products of the decomposition of MCA. Pyruvic acid was confirmed as the main product of the reaction. The spectra are also consistent with the formation of another product which is presumably formed in the acetaldehyde – MCA reaction. Acetaldehyde is postulated as an intermediate in this system. Preliminary results on the formation and decomposition of *N*-chloro-β-alanine and *N*-chloro-phenyl-alanine will also be reported.

Biography

Mária Szabo has received her MSc degree from University of Debrecen in 2015. After graduation, she joined the Homogeneous Catalysis and Reaction Mechanisms Research Group of The Hungarian Academy of Sciences as a research chemist. In September 2016, she started her PhD studies under the supervision of Prof. István Fábián. She is involved in studying the kinetics and mechanisms of complex redox reactions. She is the co-author of two research papers in high level scientific journals and 14 presentations in scientific conferences.

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