Accepted Manuscript

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PII: S0304-3894(18)30791-X
DOI: https://doi.org/10.1016/j.jhazmat.2018.09.004
Reference: HAZMAT 19728

To appear in: *Journal of Hazardous Materials*

Received date: 10-4-2018
Revised date: 9-8-2018
Accepted date: 2-9-2018

Please cite this article as: Simon F, Szabó M, Fábián I, pH controlled byproduct formation in aqueous decomposition of *N*-chloro-α-alanine, *Journal of Hazardous Materials* (2018), https://doi.org/10.1016/j.jhazmat.2018.09.004

pH controlled byproduct formation in aqueous decomposition of *N*-chloro-*α*-alanine

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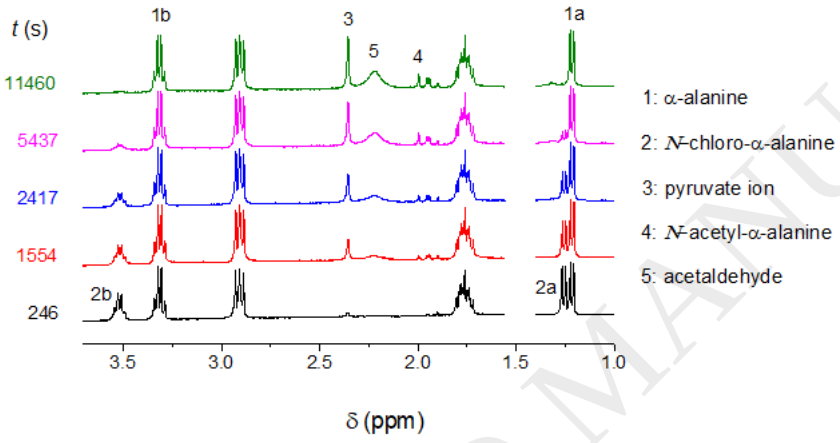
Graphical Abstract



Highlights

- The decomposition of *N*-chloro-*α*-alanine is a multistep process.
- The rate of decomposition increases by increasing the pH.
- The sole product is acetaldehyde under neutral – slightly alkaline conditions.
- In highly alkaline solution, pyruvate ion is the main and *N*-acetyl-*α*-alanine is the secondary product.

Abstract

N-chloro-amino acids are readily formed in chlorination water treatment technologies. These reactions are also important in biological systems where HOCl plays an important role in the defense mechanism against invading pathogens. The intermediates and the products formed are of primary concern because they may have significant biological activities. In order to clarify intimate details and resolve discrepancies in the literature, the decomposition kinetics of *N*-chloro-*α*-alanine (MCA) was studied in the neutral – alkaline pH range by UV-VIS spectrophotometry and ^{1}H NMR method. In contrast to earlier reports, the decomposition reaction proceeds via two distinct reaction paths: $k_{obs1} = k_{OH}[OH^-] + k$, where k_{OH} = (1.38 ±