

Subject: ASMS Abstract Submission — Log ID 319488

Your abstract for the ASMS 2024 Anaheim was submitted on 02/02/2024. The log ID for your abstract is 319488.

This abstract may be edited any time BEFORE the submission deadline. To edit, return to the abstract submission site and select 'View my Drafts and Submissions'.

Disinfection By-products from Water Chlorination Reconfirmed by Electrochemistry-MS

Jean-Pierre Chervet¹; Albert T Lebedev²; Martin Eysberg³; Hendrik-Jan Brouwer⁴

¹Antec Scientific, Alphen a/d Rijn, Netherlands; ²Moscow State University, Moscow, Russian Federation; ³Antec Scientific, Boston, MA; ⁴Antec Scientific, Alphen aan den Rijn, Netherlands

Introduction

Among numerous disinfection by-products (DBP) forming during aqueous chlorination nitrogen containing species are of special concern due to their toxicological properties. An interesting reaction involves dealkylation of the substituted amine moiety. In this poster we present the results of the comparative study of one electron oxidation and aqueous chlorination of several aliphatic and aromatic amines. The reaction products were reliably identified with GC-HRMS, HPLC-ESI/HRMS, and electrochemistry-ESI/HRMS). The mechanism of the substituted amines' aqueous chlorination involving one-electron oxidation is proposed and confirmed by the array of the observed reaction.

Methods

Simulation of one-electron oxidation of the studied amines was carried out by the electrochemical method using an EC-ESI/HRMS system, consisting of a Roxy Exceed potentiostat (Antec Scientific, Hoorn, Netherlands) and an Orbitrap ID-X (Thermo Scientific, Waltham, USA) with ESI ion source. An three electrode thin-layer (0.7 μ L internal volume) electrochemical cell with glassy carbon working electrode and HyREF Pd/H₂ reference electrode (Antec Scientific) was used in the potentiostat. The solutions of individual analytes in the mixture of aqueous 20 mM ammonium-formate (pH 7) and acetonitrile (1:1) with the concentration of 10 mg/ L were supplied to the EC-ESI/HRMS system by a syringe pump at a flow rate of 10 μ L/min

Preliminary Data

Study of dealkylation of amines (electrochemically and aqueous chlorination) revealed a one-electron oxidation of alkyl- and arylamines confirming, that both reactions involved the lone pair of electrons at the nitrogen atom at the first stage. For the aliphatic amines the reaction proceeded through formation of imine cation intermediate, which was further hydrolyzed to give a secondary amine and an aldehyde. Chlorination of the secondary amines proceeded faster in full accordance with the literature data. As a result, secondary amines appearing as intermediates transformed further to primary amines and finally nitriles. Several peculiar products were detected in the case of tribenzylamine. Transformation of aromatic amines proceeded similarly.

The single electron transfer mechanism of dealkylation was confirmed. It enables rationalizing the formation of the primary and secondary products. Thus, the schemes of transformation involving all the detected products were proposed.

Novel Aspect

N-dealkylation of amines in aqueous solution using Electrochemistry-MS reveals the formation of similar by-products than in aqueous chlorination

Conflict of Interest Disclosure

The authors declare no competing financial interest.

Poster:

Environmental: General

Submitting Author:

Jean-Pierre Chervet

Antec Scientific

Alphen a/d Rijn,

jp.chervet@antecscientific.com