Increasing Exposure Risks during Photochemical Transformation of Synthetic Musks: A Modeling Study

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Abstract

Synthetic musks (SMs), have attracted the scientist's attention worldwide recently, due to the widespread occurrence and potential toxicities. They are widely used as fragrance ingredients in various consumer goods. Once released into aquatic environment, SMs may transform into other products. Thus, the aquatic ecosystems and human are exposed to an unknown cocktail of SMs as well as their degradation products. Therefore, it is of great concern to unveil the transformation mechanisms, kinetics and fate of SMs in water environments, as well as the potential toxicity of themselves and their degradation products. In this work, two SMs including polycyclic musk (tonalide) and nitro musk (musk xylene) were chosen as model compounds to investigate the •OH-initiated photochemical transformation processes. The results showed that both SMs can be degraded readily through •OH-addition and H-abstraction pathways, with activation energies of 4.11 and 11.65 kcal mol-1, respectively. The kinetics calculation indicates that H-abstraction pathways occur exclusively for musk xylene, while for tonalide, the •OH-addition pathways were predominance at low temperature (< ˜287 K), whereas H-abstraction were the predominant pathways at high temperature. In assessing the toxicity of SMs and their degradation products using the model calculations, all H-abstraction products were found to be declined aquatic toxicity as compared with the original SMs, while •OH-addition products are more bioaccumulative and harmful to aquatic organisms. Particular for phenolic product of tonalide was found to be critically bioaccumulative. In addition, several transformation products of musk xylene have more potential carcinogenicity. Therefore, particular attentions should be paid to the photochemical products as well as parental SMs. The results will provide the helpful information for environmental protection and policy making for SMs management.

Keywords: polycyclic musk Photochemical Transformationtransformation mechanismExposure Risks

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