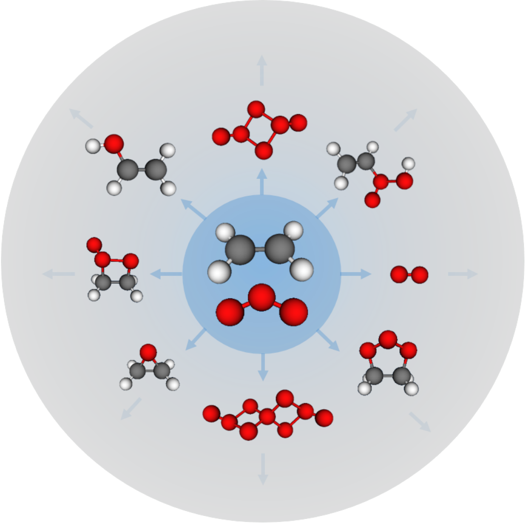
Automated Reaction Network Exploration of Ozonation Processes in Water Treatment

E. Petrus[1,2], J. P. Unsleber[2], T. Weymuth[2], M. Reiher*[2], U. von Gunten[1,3]*, T. B. Hofstetter[1]*

[1]Eawag, Swiss Federal Institute of Aquatic Science and Technology, Dübendorf 8600, Switzerland, [2]Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir-Prelog-Weg 2, 8093 Zürich, Switzerland, [3]School of Architecture, Civil and Environmental Engineering (ENAC), École Polytechnique Fédérale de Lausanne (EPFL), 1015, Lausanne, Switzerland

Ozone has been one of the flagship disinfectants in drinking water and wastewater treatment throughout the past decades, as well as for potable water reuse.[1] However, in many of its applications, the oxidant is scavenged in reactions with dissolved organic matter (DOM). These reactions lead to the formation of potentially toxic oxidation byproducts. Experimental identification of the byproducts is not only very laborious but also inherently incomplete and, thus, alternative strategies have been developed. In this context, quantum chemical (QC) computations have been applied to construct quantitative structure activity relations (QSAR) to ultimately predict rate constants for ozone consumption and byproduct formation routes.[2] Despite the advances of QC in this field, however, there are currently no examples focusing on determining the chemical reaction network, mainly due to the challenging task of finding numerous transition states with electronically complex structures.



Herein, we have addressed this challenge using the automated exploration tool named Chemoton, recently developed in the Reiher group.[3] We have generated a complex reaction network with species that represent the structural moieties of DOM (such as differently substituted olefins) that react with ozone. These explorations will enable us to carry out kinetic simulations which are directly comparable to the experimentally-determined rate constants and product yields.[4] Moreover, a systematic analysis of the network could unveil whether the preferred pathway reproduces the reported Criegee mechanism. Overall, we envision that this work can pave the way for future QC explorations of byproduct formation in disinfection/oxidation processes in aqueous solutions.

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