Structure of Acetone at the air-water interface

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Acetone plays an important role in atmospheric chemistry. It serves as a significant source of hydrogen oxide radicals through photolysis. [1] This oxygenated volatile organic compound is ubiquitous in the atmosphere and impacts atmospheric composition and contributes to aerosol aging and growth. [2]

The air-water interface, particularly at the surface of oceans and water aerosols, represents a unique chemical environment that can significantly influence acetone's behavior and reactivity. Sum-frequency generation (SFG) spectroscopy has emerged as a powerful technique for investigating molecular-level details of such interfaces, allowing direct observation of adsorption processes and providing insights into the arrangement of surface molecules. [1]

In this work, we employed SFG to study acetone at the air-water interface. It was observed that the methyl signal saturates at 10% acetone mole fraction, while the carbonyl signal saturates at a much lower concentration of 1.2%. Notably, we observed a change in the orientation of surface water molecules at 1.2% mole fraction. The study aims to provide a comprehensive understanding of how acetone interacts and behaves at the air-water interface, highlighting the distinct responses of different molecular groups within the acetone molecule.

1. Cyran et al., Angew. Chem. Int. Ed. 58, 3620–3624 (2019).
2. Saak et al., J. Phys. Chem. Lett. 15, 4546–4559 (2024)