Scientists reveal stepwise hydration motifs of sulfur dioxide

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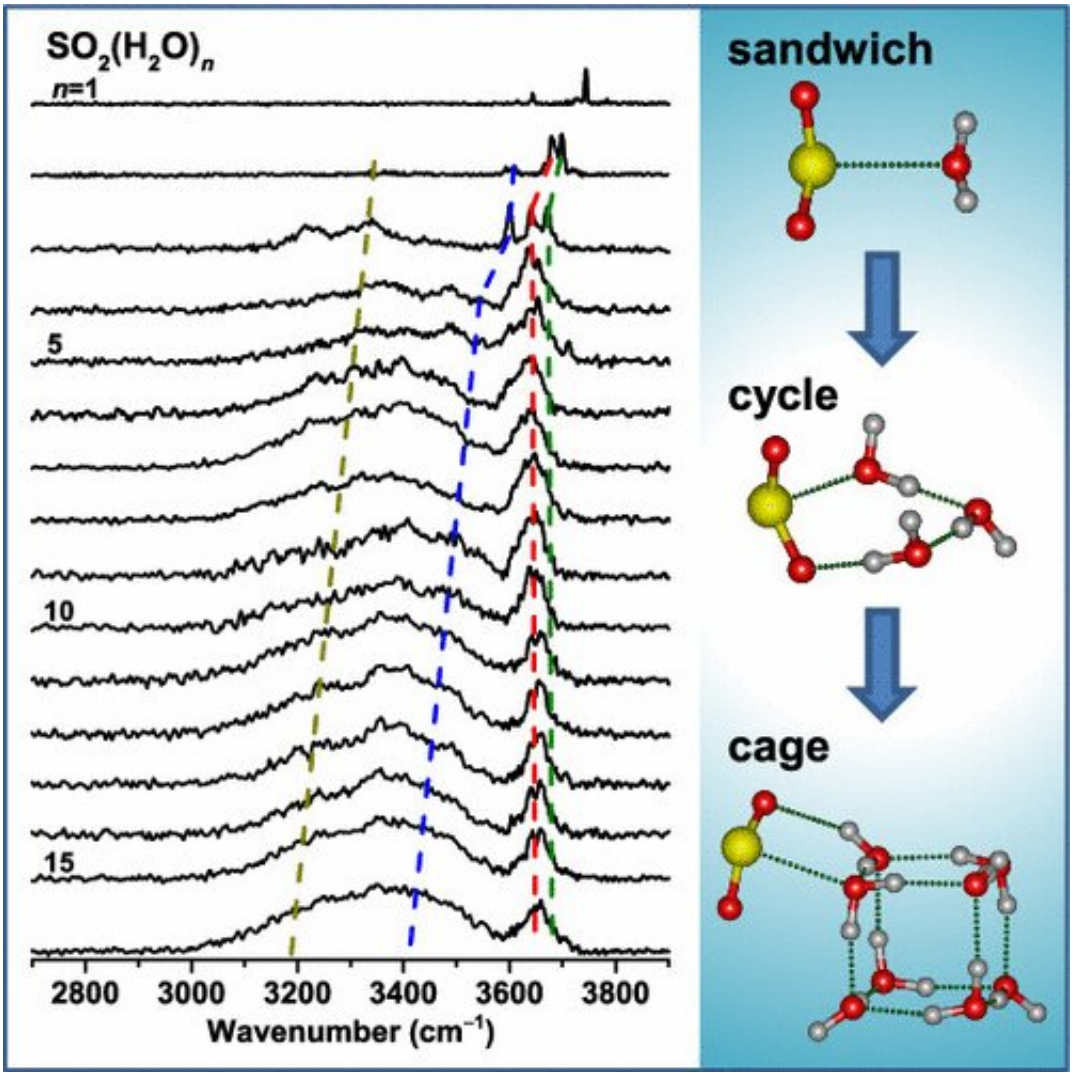

Graphical abstract. Credit: *The Journal of Physical Chemistry Letters* (2022). DOI: 10.1021/acs.jpclett.2c01472

A research team led by Prof. Jiang Ling and Zhang Zhaojun from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS) identified the infrared signature of stepwise hydration motifs of sulfur dioxide (SO_2).

Their findings were published in the *Journal of Physical Chemistry Letters* on June 16.

The researchers revealed the size-dependent development of SO_2 hydrate structure and cluster growth in the $SO_2(H_2O)_n$ (n = 1-16) complexes and highlighted a general model to elucidate the formation mechanism of the SO_2-containing aerosol systems.

SO_2 is an important atmospheric pollutant and is involved in many atmospheric processes such as the formation of cloud condensation nuclei and acid rain. Characterizing the chemical composition, structure and growth of nucleating precursors is essential for understanding the underlying mechanisms of atmospheric new particle formation.

Experimental characterization of microscopic events and behaviors of SO_2-H_2O interactions is challenging due to the difficulty in size selection.

Based on the recently-developed infrared spectroscopy using a tunable vacuum ultraviolet free electron laser (VUV-FEL), the researchers measured infrared spectra for the neutral $SO_2(H_2O)_n$ (n = 1-16) clusters in the 2700-3900 cm^{-1} spectral regions.

They conducted quantum mechanical calculations to identify the low-lying isomers and to assign the experimental spectral features. They found that the sandwich structure initially formed at n = 1 developed into cycle structures with the sulfur and oxygen atoms in a two-dimensional plane (n = 2 and 3) and then into three-dimensional cage

structures ($n \geq 4$) with the binding of SO_2 on the outer side of water clusters.

"Since the structures of hydrated SO_2 could affect the reactive sites and electrophilicity of SO_2, the present cluster perspectives would deepen our understanding of the solvation behaviors of SO_2 on the water nanodroplets and surfaces and have atmospheric implications for studying the SO_2-containing aerosol systems," said Prof. Jiang.

More information: Chong Wang et al, Infrared Spectroscopy of Stepwise Hydration Motifs of Sulfur Dioxide, *The Journal of Physical Chemistry Letters* (2022). DOI: 10.1021/acs.jpclett.2c01472

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