

Abstract Submitted
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Infrared spectroscopy of hydrated sulfate dianions JIA ZHOU, GABRIELE SANTAMBROGIO, MATHIAS BRUMMER, DAVID MOORE, LUDGER WOSTE, GERARD MEIJER, DANIEL NEUMARK, KNUT ASMIS, University of California, Berkeley — The first infrared spectra of a multiply-charged anion in the gas phase are presented. The spectra of $\text{SO}_4^{2-} \cdot (\text{H}_2\text{O})_n$, with $n=3$ to 24, show four main bands assigned to two vibrations of the dianionic core, the water bending mode, and solvent libration. The triply degenerate SO_4^{2-} antisymmetric stretch vibration probes the local solvent symmetry, while the solvent librational band is sensitive to the solvent hydrogen bonding network. The spectra and accompanying electronic structure calculations indicate a highly symmetric structure for the $n=6$ cluster and closure of the first solvation shell at $n=12$.

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