CARBOXYLATE STRETCHING MODES ARE STRUCTURAL PROBES FOR ION-DEPENDENT BINDING PROPERTIES IN ALKALI EARTH METAL-EDTA COMPLEXES

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Ethylenediaminetetraacetic acid (EDTA) can be used as a chelating agent for binding metal ions in solution. In addition, its binding pocket is a model for the interactions between carboxylate groups and the divalent ions they often bind in some biological systems.[abc] With its four carboxyl groups and two nitrogen atoms, EDTA can chelate nearly any metal cation to form water-soluble complexes, making it a robust model system for studying biologically relevant divalent ion-carboxylate interactions.

Here, we present cryogenic gas-phase infrared spectra of a series of alkaline earth metal-EDTA complexes of the form $[M(II)\cdot EDTA]^{2-}$ and assign spectral features using density functional theory calculations. The vibrational spectra encode structural and electrostatic information, reflecting the geometry of each metal ion within the EDTA binding pocket and its relation to ionic radius.

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