CRYOGENIC ION SPECTROSCOPY OF TRANSITION METAL-EDTA COMPLEXES: ION-DEPENDENT SPECTRAL AND STRUCTURAL SHIFTS

MADISON M. FOREMAN, J. MATHIAS WEBER, *JILA and Department of Chemistry, University of Colorado, Boulder, CO, USA*.

Ethylenediaminetetraacetic acid (EDTA) is a useful model system for studying the ubiquitous divalent ion-carboxylate interactions in protein binding pockets.[a,b] EDTA can chelate most metal cations by forming up to six bonds with its four carboxyl groups and two nitrogen atoms, resulting in water-soluble complexes that are biologically relevant.

Here, we present cryogenic gas-phase infrared spectra of a series of transition metal-EDTA complexes of the form $[M(II)\cdot EDTA]^{2-}$ and assign spectral features using density functional theory calculations. The vibrational spectra inform us of the structure of and intermolecular forces in each complex, revealing the binding geometry of the metal ion within the EDTA binding pocket and its response to changes in ionic radius and electron configuration. The positions of carboxylate vibrational bands depend on the identity of the bound metal, displaying a clear spectral response to changes in binding properties.

---

[a] S. C. Edington, C. R. Baiz, J. Phys. Chem. A 122 (2018) 6585-6592

[b] Q. Yuan, X. T. Kong, G. L. Hou, L. Jiang, X. B. Wang, Faraday Discuss. 217 (2019) 383