CARBONYL BANDS REPORT ON MOLECULAR STRUCTURE IN COMPLEX SPECTRA: CRYOGENIC ION SPECTROSCOPY OF METAL-CYCLAM COMPLEXES[a]

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The feasibility of industrial scale electrocatalytic CO_2 reduction requires the development of catalysts that are both selective and efficient, making it imperative to understand the catalytic structure-function relationship to inform the design of improved catalysts. Nickel cyclam is a high-performing CO_2 reduction catalyst, and its derivatives have demonstrated differing catalytic abilities. Here, we present cryogenic gas-phase infrared spectra of a series of transition metal-cyclam derivative complexes of the form $[M(II)\cdot TEC]^{2+}$ (TEC = cyclam with four ethyl acetate substituents) and interpret spectral features using density functional theory calculations. The size and conformational flexibility of these complexes cause spectral congestion that complicates peak assignment. We address this challenge by utilizing the carbonyl stretching bands as spectroscopic reporters of molecular structure.

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