

MISMATCHED HOST-GUEST PAIRINGS – CRYOGENIC ION SPECTROSCOPY OF OCTAMETHYL-CALIX[4]PYRROLES IN COMPLEXES WITH NITRATE AND FORMATE^a

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

Octamethyl-calix[4]pyrrole (OMC4P) is a prototypical anion receptor, and it has been mainly used to bind halide ions, particularly fluoride and chloride. It is not a good receptor for polyatomic anions without chemical modifications. In the present work, we study the structures of complexes of OMC4P with nitrate and formate, using cryogenic ion vibrational spectroscopy with N₂ messenger tagging. We present the vibrational spectra of these species and obtain structural information by comparison of the experimental spectra with calculated spectra based on density functional theory.

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