

FULL DIMENSIONAL POTENTIALS, DIPOLE MOMENT SURFACES AND (RO)VIBRATIONAL CALCULATIONS FOR H_5^+ , H_7^+ AND HOCO

JOEL BOWMAN, STUART CARTER, YIMIN WANG, *Department of Chemistry, Emory University, Atlanta, GA, USA.*

I will describe progress in the first-principles calculations of “line-list” ro-vibrational spectra of H_5^+ , D_5^+ and HOCO and low-resolution spectrum of H_7^+ , along with insights into the internal motions of these species. The calculations make use of full-dimensional ab initio potential and dipole moment surfaces and the code “MULTIMODE”.