THE GROUND STATE FOUR DIMENSIONAL MORPHED POTENTIALS OF HBr AND HI DIMERS

BLAKE A. MCELMURRY, ZHONGCHENG WANG, <u>ROBERT R. LUCCHESE</u>, and JOHN W. BEVAN, *Chemistry Department, Texas A&M University, College Station, TX 77843-3255*; SERGEY P. BELOV, *Institute of Applied Physics of Russia Academy of Sciences, Uljanova Str. 46, Nizhny Novgorod 603950, Russia.*

The assigned rotational-tunneling transitions including quadrupole substructure of H⁷⁹Br-H⁸¹Br are combined with previously recorded rovibrational infrared and microwave data, to provide a basis for optimizing a ground state four-dimensional morphed potential with quantifiable uncertainties. The determined potential minimum has a value $V = -644.0 \text{ cm}^{-1}$ at the geometry R = 4.04 Å, $\theta_1 = 16.9^\circ$, $\theta_2 = 108.3^\circ$, and $\phi = 180.0^\circ$. The peak of the minimum energy path between the two equivalent minima occurs at $V = -571.2 \text{ cm}^{-1}$, leading to a barrier height of 72.8 cm⁻¹. A corresponding investigation for the HI dimer will also be presented.