INVESTIGATION OF BORN-OPPENHEIMER BREAKDOWN IN HCl AND HF BY THRESHOLD ION-PAIR PRODUCTION SPECTROSCOPY

QICHI HU, JOHN W. HEPBURN, *Department of Chemistry, University of British Columbia, Vancouver, BC V6T 1Z1, Canada*.

Threshold Ion-Pair Production Spectroscopy (TIPPS) [a] is applied to two pairs of isotopomers, HCl/DCl and HF/DF. From the high-resolution TIPP spectra, the Ion-Pair dissociation energies of the four molecules have been precisely measured, and from these their bond dissociation energies (D_0 and D_e) can be determined. In this way an experimental estimate of the Born- Oppenheimer breakdown in the long range limit of the ground state potential curve is obtained for HCl and HF. The experimental results about bond dissociation energies from this work are compared to the theoretical studies by Coxon and Hajigeorgiou [b].

[a] J. D. D. Martin, J. W. Hepburn, Phys. Rev. Lett. 79, 3154 (1997)

[b] J. A. Coxon, P. G. Hajigeorgiou, J. Mol. Spec. 203, 49 (2000)