ALGEBRAIC vs. NUMERICAL METHODS FOR DIATOMIC DATA ANALYSIS: END TO A DISPUTE

ROBERT J. LE ROY, *Guelph-Waterloo Centre for Graduate Work in Chemistry and Biochemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada*.

The past decade has seen a persistent dispute in the literature and at this meeting concerning the validity and physical significance of two different approaches for the reduction of sets of multi-isotopomer diatomic molecule data to a compact set of parameters defining a potential energy curve and Born-Oppenheimer breakdown (BOB) radial functions. It is shown here that the apparent discrepancies between the algebraic method championed by J.F. Ogilvie and a numerical method pioneered by J.A. Coxon are due to an *ad hoc* truncation convention applied in Ogilvie's algebraic RADIATOM data analysis code. This truncation rule is not essential to the algebraic method, and when it is relaxed, the two approaches yield essentially identical results. Tests reported here also support Watson's [*J. Mol. Spectrosc.* **217**, 157 (2003)] assertion that electric dipole moments and rotational g–factors cannot be determined from transition energy data alone.