INVERSION OF SPECTRAL DATA OF DIATOMIC MOLECULES WITH COMPUTATIONAL SPECTROMETRY

J. F. OGILVIE, *Universidad de Costa Rica, Escuela de Quimica, Ciudad Universitaria Rodrigo Facio, San Pedro de Montes de Oca, San Jose 2060, Costa Rica; also, Simon Fraser University, Centre for Experimental and Constructive Mathematics, Department of Mathematics, 8888 University Drive, Burnaby, British Columbia V5A 1S6, Canada*.

Rather than computational spectroscopy that implies a qualitative treatment relying on visual observations of spectra, we apply *computational spectrometry*[a] to achieve a quantitative reproduction of precise data from spectra measured with electronic instruments. For spectra involving pure rotational and vibration-rotational transitions of diatomic molecules, even full isotopic substitution for spectra measured in the absence of applied magnetic fields fails to provide sufficient data to enable a complete evaluation of parameters for all of potential energy, adiabatic, and nonadiabatic rotational and vibrational effects, even omitting nuclear field shifts that might be neglected for light atomic centres. We hence calculate, for internuclear distances over a broad range, the rotational g factor, which measurements of the Zeeman effect on vibration-rotational transitions over a large range of quantum numbers v and J might in principle produce but which has never been accomplished in practice. Applying this information in constrained fits of spectral data, we evaluated the remaining parameters, for instance for H_2[b], HeH^+[c] and NaCl[d]. Combined with an algebraic approach based on the most highly developed effective hamiltonian[e], this procedure yields the most physically meaningful conventional parameters.

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