DIRECT-POTENTIAL-FIT ANALYSES OF DIATOMIC DATA ARE BECOMING "ROUTINE": PROGRAM DPOTFIT

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

In recent years it has become increasingly common for diatomic data analyses to be performed using "direct potential fits", in which observed transition energies are compared with eigenvalue differences calculated from an effective radial Hamiltonian based on some parameterized analytic potential energy and (possibly) other radial functions, and the parameters defining those radial functions optimized by a least-squares procedure. However, to date this type of work has been largely restricted to a small handful of laboratories which have each developed their own computer programs, as there are few documented and publicly distributed computer codes for performing such analyses.[a] The object of the present work has been to develop such a code. Program DPOTFIT performs least-squares fits of diatomic molecule spectroscopic data consisting of any combination of microwave, infrared or electronic vibrational bands, fluorescence series, and tunneling predissociation level widths, involving one or more electronic states and one or more isotopologues, to determine the potential energy and other radial functions defining the observed levels of each state. Four main families of analytical potential functions are allowed by the current version of the code: the Expanded Morse Oscillator (EMO), the Morse/Lennard-Jones oscillator (MLJ), the Double Exponential/Long-Range (DELR) potential, and Šurkus' Generalized Potential Energy Function (GPEF), which incorporates a variety of polynomial potential forms. In addition, DPotFit allows the fit to determine atomic-mass-dependent Born-Oppenheimer breakdown, and singlet-state Λ-doubling or $^2\Sigma$ splitting radial strength functions for one or more of the electronic states. The Fortran source code for this program, together with a manual describing its use, may be downloaded freely from the 'computer programs' link on the www site `http://leroy.uwaterloo.ca`. Features of the code and its use will be outlined, and a number of illustrative applications will be described.

[a] A noteworthy exception is Pashov's code for fitting to a spline-pointwise potential: A. Pashov, W. Jastrzębski and P. Kowalczyk, Comp. Phys. Comm. **128**, 622 (2000).