DSParFit and DSPotFit: GENERAL PURPOSE PARAMETER– AND POTENTIAL–FITTING PROGRAMS FOR DIATOMIC DATA ANALYSIS

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We have developed two general purpose codes for fitting diatomic spectral data consisting of any combination of microwave, infrared, electronic and fluorescence series measurements, for one or multiple isotopomers, and involving one or several different electronic states, in a unified, combined-isopotopomer analysis. Both programs can determine atomic mass dependent Born-Oppenheimer and JWKB breakdown corrections. Λ–doubling correction parameter expansions (in the parameter-fit program) or radial correction functions (in the potential fit) program may also be determined.

For each electronic state involved in the data set, program **DSParFit** (for "Diatomic Singlet Parameter Fitting") allows the observed level energies to be represented in three ways: (i) by "band constants", a set of $\{G_v, B_v, D_v, H_v, ...\}$ and Λ–doubling parameters $\{q_B(v), q_D(v), ...\}$ for each vibrational level of each isotopomer; (ii) by Dunham-type double power series expansions in $(v + \frac{1}{2})$ and $[J(J+1) - \Omega^2]$, and (iii) by "near-dissociation expansions" for the vibrational energies and rotational constants, which incorporate their theoretically-known limiting near-dissociation behaviour. The two latter choices implicitly incorporate standard first-order mass scaling for multiple isotopomers, while atomic mass dependent Born-Oppenheimer breakdown corrections are included as additive correction terms.

Program **DSPotFit** (for "Diatomic Singlet Potential Fitting") allows a choice of several different flexible analytic functions to represent the potential energy curve for each electronic state involved in the data set. Born-Oppenheimer breakdown "adiabatic" potential correction functions and "non-adiabatic" centrifugal correction functions, as well as radial functions to repesent Λ–doubling perturbation corrections may also be determined. The fitting procedure for this case involves exact (numerical) solution of the radial Schrödinger equation for the upper and lower level of each state involved in each transition included in the data set, for each iteration of the fit which optimizes the parameters defining the potential.

The Fortran source code for these two programs, together with manuals describing their use, may be downloaded freely through the "Computer Programs" link on the www page: http://leroy.uwaterloo.ca.