BCONT, LEVEL and RKR1: PROGRAMS FOR SIMULATING OR FITTING TO BOUND→CONTINUUM OR BOUND↔BOUND DIATOMIC MOLECULE SPECTRA

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We have developed three flexible general purpose computer programs for simulation of and/or fitting to diatomic molecule bound state level patterns, bound↔bound transitions and bound→continuum absorption or emission intensities or predissociation rates. **RKR1** is a first-order RKR inversion procedure code incorporating a number of special features, such as: (i) it tests for, and can use automatic extrapolation to smooth over irregular or unphysical inner wall behaviour; (ii) it allows the use of either Dunham-type or near-dissociation expansion representations of the input $G(v)$ and B_v functions.[a]

Program **LEVEL** solves the radial or one-dimensional Schrödinger equation for bound and quasibound levels of any smooth single or double-minimum potential, and can calculate rotational and centrifugal distortion constants, expectation values, and Franck-Condon factors or other off-diagonal matrix elements, either among levels of a single potential or between levels of two different potentials.[b] The code incorporates a wide range of analytic model potential functions, and can interpolate over and extrapolate beyond a set of input (*ab initio* or RKR) turning points.

Program **BCONT** can simulate bound→continuum absorption or emission intensities, either from particular specified initial levels or from a thermal initial-state population, into the continuum associated with one or several final electronic states.[c,d] It can also perform least-squares fits to experimental total or partial absorption cross sections or branching ratios to determine the repulsive potentials of the final electronic state(s) and the associated distance-dependent transition moment functions. It can also simulate or fit to predissociation data using various types of coupling functions.

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

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[a] R.J. Le Roy, University of Waterloo Chemical Physics Research Report CP-425 (1992).
[b] R.J. Le Roy, University of Waterloo Chemical Physics Research Report CP-642R (2000).
[c] R.J. Le Roy and G.T. Kraemer, University of Waterloo Chemical Physics Research Report CP-650 (2001).
[d] An earlier version of this code was reported by R.J. Le Roy, *Comp. Phys. Comm.* **52**, 383 (1989)