SPECVIEW: SIMULATION AND FITTING OF ROTATIONAL STRUCTURE OF ELECTRONIC AND VIBRONIC BANDS

VADIM L. STAKHURSKY, TERRY A. MILLER, *Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus OH 43210*.

A second-generation program called SpecView provides for the simulation and fitting of the rotational structure of electronic and vibronic bands. The application is written in Visual C++ and features MFC classes. A user-friendly environment allows for most spectra manipulation to be done with mouse moves and clicks. SpecView utilizes a DLL library previously created in our lab, which contains a large number of molecular Hamiltonians appropriate for the calculation of the energy levels of various molecules in different electronic states. The program generates spectra for up to 10^6 transitions and has succesfully simulated rotational spectra with J's up to 200. A number of tools allow one to import experimental data, compare data to simulations and provides intelligent assignment of spectral lines. For fitting, a well-known Levenberg-Marquardt's non-linear least square procedure is used. It is noticed that when fitting molecular constants that appear only in non-diagonal matrix elements, using numerical calculations of the derivatives causes the convergence process to be more stable than when analytical derivatives used. The program has an intuitive environment and can be used for educational and demonstrational purposes since all molecular constants can be varied dynamically with spectra changes reflected immediately in application's window.