WINDOWS GUI PROGRAM FOR THE ROTATIONAL ANALYSIS OF MOLECULAR SPECTRA

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A graphical-user-interface computer program based on a Windows API platform[a] has been written in the C programming language to aid in the rotational analysis of molecular spectra.[b] Dialog boxes provide a user interface for the calibration, linearization and manipulation of experimental data and for the generation and optimization of the simulated spectra. Resources are provided for the deconvolution of multiple overlapping rotational bands from different conformations and/or isotopomers of a molecule and for the analysis of molecular spectra when internal rotation, centrifugal distortion, nuclear quadrupole coupling interactions and inertial frame reorientation effects are resolved. Specific features of the program will be demonstrated that include resources for importing, manipulating, calibrating and analyzing spectroscopic data. Interactive fitting strategies will be discussed as well as current efforts to implement "automatic" procedures based on Genetic Algorithms[c] and Neural Networks. A WEB site for downloading this software is currently being prepared at NIST.

[a] Registered trademark of Microsoft, Inc.

[b] D. F. Plusquellic, S. R. Davis and F. Jahanmir, J. Chem. Phys. in press; W. A. Majewski, J. F Pfanstiel, D. F. Plusquellic, and D. W. Pratt, "Laser Techniques in Chemistry", edited by A. B. Myers and T. R. Rizzo (Wiley & Sons, New York, 1995).

[c] J. A. Hageman, R. Wehrens, R. de Gelder, W. Leo Meertz, and L. M. C. Buydens. J. Chem. Phys. 113, 7955 (2000).