INTERACTIVE COMPUTER PROGRAM FOR COMPUTER-ASSISTED ASSIGNMENT OF MOLECULAR SPECTRA[a]

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While molecular spectra in textbooks are usually regular, many important spectra are irregular, displaying no obvious pattern. Assigning the quantum numbers of an irregular spectrum can be a vexing problem in pattern recognition, which can be computer-assisted by a program to display the stick spectrum. An interactive plotting program for the Windows platform has been written in Visual BASIC. Input parameters include the molecular constants, the selection rules, and the temperature. The program computes and displays a stick spectrum (including intensities) on the computer monitor, and stores the line list with intensities and quantum numbers in an ACCESS database. The program presently handles vibrational-rotational spectra, but could easily handle electronic spectra as well. The program is particularly useful for irregular spectra, such as asymmetric rotors, and for displaying the effect of variation of the molecular constants on the spectrum. The program is highly interactive: the molecular constants can be changed and the spectrum recomputed and displayed in seconds.

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