THE USE OF CAAARS (COMPUTER AIDED ASSIGNMENT OF ASYMMETRIC ROTOR SPECTRA) IN THE ANALYSIS OF ROTATIONAL SPECTRA

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The approach presented for the assignment of rovibrational spectra, CAAARS, provides an integrated suite of computer programs to simplify and speed up spectral analysis. CAAARS combines visual, interactive, mouse-assisted line assignment with real-time fitting of the assigned transitions to the spectroscopic constants of an appropriate rovibrational Hamiltonian. The ease of operation and flexibility in the choice of an appropriate theoretical model make it a powerful tool in the hands of a spectroscopist. Its advanced user interface, capable of displaying multiple traces of the experimental spectrum for unambiguous line identification, is a logical extension of the Loomis-Wood approach to line assignment. CAAARS implements user-specified sorting to select subsets of the predicted transitions for transparent assignment and manipulation. The CAAARS software package is implemented on the basis of the Windows version of IGOR Pro (http://wavemetrics.com) and currently uses the SPFIT and SPCAT programs made available by H. M. Pickett (http://spec.jpl.nasa.gov). The current version of CAAARS is available for downloading at http://www.physics.ohio-state.edu/∼medvedev/caaars.htm