AN INTERACTIVE LOOMIS-WOOD PACKAGE FOR SPECTRAL ASSIGNMENT IN IGOR PRO[a]

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A Loomis-Wood diagram is a two-dimensional peak diagram in which the occurance of a transition is plotted versus frequency, in segments, with successive segments displayed one above another. The lines in a rotational subband of a symmetric top or linear molecule are spaced roughly $2B$ apart. If the length of the segments in a Loomis-Wood diagram matches $2B$, then the subband will appear as a vertical succession of points. Such diagrams were first used by Loomis and Wood in 1928[b]. Because of the time required to manually create a Loomis-Wood diagram, they were not useful in the initial assignment of spectra before the advent of microcomputers. The first computer program to generate a Loomis-Wood plot was written at the Ohio State University in the 1960s[c], and the first interactive Loomis-Wood applications by Winnewisser et al. appeared in the 1980s[d].

Interactive Loomis-Wood assignment programs allow assignment and regression of lines in a subband via a Loomis-Wood diagram. Not only do these programs help assign spectra, but they are also a convenient means of bookkeeping the assignments of spectra with a large number of lines. Loomis-Wood programs are particularly useful for the analysis of congested spectra of symmetric tops, slightly asymmetric tops, and linear molecules. We have developed an interactive Loomis-Wood assignment package[e] has been written for IGOR Pro, a program for the analysis and display of numeric data. IGOR Pro is used in many spectroscopic laboratories. Because this package is implemented in IGOR Pro, the user has access to the features of IGOR Pro, such as user defined functions and enhanced graphical abilities. With this package, Loomis-Wood plots can be seamlessly integrated into existing IGOR Pro experiments. The package will be demonstrated on several molecules.

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[a] IGOR Pro is a commercial product by Wavemetrics, Inc.

[b] F. W. Loomis and R. W. Wood *Phys. Rev.* **32**, 223–236 (1928).

[c] J. F. Scott and K. Narahari Rao *J. Mol. Spectrosc.* **20**, 461–463 (1966).

[d] Brenda P. Winnewisser, Jürgen Reinstädtler, Koichi M. T. Yamada , and Jörg Behrend, *J. Mol. Spectrosc.* **136**, 12–16 (1989).

[e] This package is available at http://fermi.uchicago.edu/oka/freeware