

AN INTERACTIVE LOOMIS-WOOD PACKAGE FOR SPECTRAL ASSIGNMENT IN IGOR PRO, VERSION 2.0

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Interactive Loomis-Wood assignment programs allow assignment and regression of subbands in a spectrum 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.

A new version of the Loomis-Wood Package for IGOR Pro previously presented at this conference^a is available online at <http://fermi.uchicago.edu/freeware/>. The latest version of this package does not depend on any externally compiled code and is therefore Macintosh and Windows compatible. In addition, the new version includes more detailed instructions to help new users get started.

^aC. F. Neese, 56th International Symposium on Molecular Spectroscopy, The Ohio State University (2001).