

MISCELLANEOUS IGOR PRO^a AND EXCEL^b ADD-INS FOR SPECTROSCOPIC ANALYSIS

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The charting and tabulating abilities of commonly used programs such as Excel and IGOR Pro are indispensable to scientists for the display and manipulation of data. In addition, the programming languages built into these programs provide an alternative programming environment to traditional Fortran or C command-line utility programs. It is often found that the features provided in the programming languages built in to programs such as Excel and IGOR Pro allow for more rapid development of utility procedures. Routines designed for these programs also tend to be more user-friendly than command-line utilities.

We have developed several packages/add-ins for IGOR Pro and Excel to automate and simplify many of the common tasks performed during spectroscopic data reduction and analysis^d. These packages/add-ins integrate seamlessly with existing documents. The IGOR Pro packages include: a suite of routines that fits data to zeroth, first, and second derivative Gaussian and Lorentzian lineshapes; a routine to export a graph as a large aspect-ratio graphic file, suitable for printing on a banner printer; a sophisticated baseline removal routine; a routine to remove etaloning from laboratory spectra via FFT methods; a set of matrix tools including Jacobi diagonalization; and an interactive Loomis-Wood assignment package (the subject of talk XXXX). The Excel add-in provides: import of FTIR spectra in the binary Giessen format; importing, formatting, and exporting of data from localized versions of the ASYM and ASYMBD7 programs by Arthur Maki; production of stick spectra from peak listings; and tools for manipulating the Microsoft chart engine.

^aIGOR Pro is a commercial product by Wavemetrics, Inc.

^bExcel is a commercial product by Microsoft Corp.

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^dThese packages/add-ins are available at <http://fermi.uchicago.edu/oka/freeware>