SyMath : Data analysis platform on Mathematica
SpectrumFit : Analytical spectrum analysis software
SyMath-Molecule : Analysis and prediction of quantum states and transitions with matrix mechanics

Georg Ch. Mellau[(1)(2)]
(1) Physikalisch-Chemisches-Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 58, D-35392 Giessen, Germany
(2) Mellau Consulting, Anneröder Str. 3 35463 Fernwald, Germany

After many years of development and testing we present a new type of scientific software. The basic idea is to shift the scientific software development from algorithm development to setting up and solving a set of equations. Two general software systems are used to achieve this task: Mathematica [1] and SyMath [2].

SyMath is a data analysis software platform running under Mathmetica ver. 4.1.2. **SyMath** implements a powerful user interface allowing the input of physical symbols, parameters and calculation formulae. These symbols and formulae are converted to executable functions and used for the calculations; also they can be saved in a database file and reloaded at any time in the program. The database set up for an analysis contains not only the numerical values of the parameters, BUT all symbol definitions and formulae.

SpectrumFit is a data analysis program running on the **SyMath** platform for "spectrum" type data as low or high resolution molecular spectra. The program implements spectrum analysis tasks as peak search, background correction or lineshape fit. New in this program is the feature that any function can be used as "lineshape function", the user has only to type the formula of your lineshape function using the LineshapeEditor and start fitting the lineshape parameters to the measured spectrum. EACH parameter for EACH peak can be set to FIT or FIX for the fit, any number of peaks can be fitted together.

SyMath-Molecule program adds analytical matrix mechanics modules to the general SyMath system allowing the prediction and analysis of transitions and states of any quantum system described through the analytical formulas of the matrix elements. Using this program the user can simulate or analyze high resolution rotation-vibration spectra of molecules in gas phase.

(1) http://www.wolfram.com

(2) http://www.symath.com