A GRAPHICAL-USER-INTERFACE FOR THE ASSIGNMENT OF ROTATIONALLY RESOLVED SPECTRA

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The program *krot* for the simulation, assignment and fitting of rotationally resolved spectra is presented. A graphical user interface has been developed based on the KDE[a] libraries. It displays several experimental and simulated spectra simultaneously and allows one to make assignments using a mouse-driven interface.
Currently the program uses a single engine for the calculation and least-squares-fitting of spectra, but provisions are made to call any program or set of routines to do the actual calculations. The current calculation program *arnirot*[b] allows the calculation of microwave and vibrational/vibronic spectra of asymmetric rotors, including centrifugal distortion terms in Watson's A- or S-reduction. Moreover linear terms for the description of axis reorientation or coupling to internal motions are included.
A link to the download page is given at http://www-public.rz.uni-duesseldorf.de/~mschmitt/HRLIF.htm.

[a] These libraries are OpenSource and available at http://www.kde.org.
[b] This program is based on the program blzyrot, Blaise B. Champaigne and David W. Pratt, private communication, 1994.