

THE PROSPE DATABASE OF PROGRAMS FOR ROTATIONAL SPECTROSCOPY

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The database "PROSPE - Programs for ROTational SPEctroscopy" is a freely available collection of programs for various aspects of the rotational spectroscopy problem.^a The aim has been to collect well tested and well documented programs, ranging from 'state of the art' solutions to specific problems, to simple 'calculators'. The programs are subdivided into ten different thematic sections and are all provided as source code for own compilation and modification, and as ready to run executables for 'black-box' use.

Several recent additions/enhancements to programs in the database will be discussed. These include ASCP - a general viewing program for spectroscopic predictions, STRFIT - a general structure fitting program, QSTARK - a Stark effect program for molecules with up to one quadrupolar nucleus. Many programs provide a route for generating publication quality PostScript diagrams. The database also aims to cater for those relatively new to the field and, as an example, contains a special subsection of post-processing programs as well as a *Crib-sheet* to the popular SPFIT/SPCAT package of H.M.Pickett. Contribution of tested programs to the database is encouraged and the required minimum is the listing, the executable, specimen data, and output for the specimen data. Provision of concise but clear documentation, and of a reference to a published work for an example of use/citation, is also recommended.

^aavailable at <http://www.ifpan.edu.pl/kisiel/prospe.htm>