PGOPHER: A GENERAL PURPOSE PROGRAM FOR SIMULATING ROTATIONAL STRUCTURE

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The PGOPHER program is a general purpose program for simulating and fitting rotational structure of any type. It represents a distillation of several programs written and used over the past decade or so within the Bristol laser group and elsewhere, and the current version is a re-write from scratch to produce a general purpose and flexible program. It is designed to be easy to use; it uses a standard graphical user interface and the program is currently in use for undergraduate practicals and workshops as well as research work. Features include:

- Simulates linear molecules and symmetric and asymmetric tops
- Open and closed shell systems and hyperfine structure
- Raman, multiphoton and forbidden transitions as well as multiple components of standard electric dipole transitions
- Models perturbations between multiple states
- Fits to line positions, line intensities or overall band contours
- Flexible input format for line lists, allowing data from several files to be combined
- Can overlay numerical spectra and images from pdf files or other sources (even absorption plates) on to simulated spectra
- Calibration mode for experimental spectra, including built in Ne, Fe and I_2 spectra as calibration sources.
- Matrix elements can be displayed in symbolic form

A second full release is being made available this summer. The program is freely downloadable from a supporting web site at Bristol (http://pgopher.chm.bris.ac.uk), for Windows, with beta versions available for Linux and Apple Mac. The program is released as open source, and can be compiled with open source tools. Comments, both good and bad, are very welcome at help-pgopher@bristol.ac.uk; these have been invaluable in developing PGOPHER.