

## RECENT CHANGES IN PGOPHER: A GENERAL PURPOSE PROGRAM FOR SIMULATING ROTATIONAL STRUCTURE

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Key features of the PGOPHER program include the simulation and fitting of the rotational structure of linear molecules and symmetric and asymmetric tops, including effects due to unpaired electrons and nuclear spin. The program is written to be as general as possible, and can handle many effects such as multiple interacting states, predissociation and multiphoton transitions. It is designed to be easy to use, with a flexible graphical user interface. PGOPHER has been released as an open source program, and can be freely downloaded from the website at <http://pgopher.chm.bris.ac.uk>.

Recent additions include a mode which allows the calculation of vibrational energy levels starting from a harmonic model and the multidimensional Franck-Condon factors required to calculate intensities of vibronic transitions. PGOPHER takes account of both the displacement along normal co-ordinates and mixing between modes (the Duschinsky effect).  $I$  matrices produced from ab initio programs can be directly read by PGOPHER or the mode displacements and mixing can be fit to observed spectra.

In addition the effects of external electric and/or magnetic fields can now be calculated, including plots of energy level against electric field suitable for predicting Stark deceleration, focussing and trapping of molecules. The figure shows a typical plot, showing the electric field tuning of the  $M = 0$  levels of  $2_{02}$ ,  $1_{11}$  and  $1_{10}$  levels of  $(\text{NO})_2$ .

Other new features include fits to combination differences, simulation of the Doppler split peak typical of Fourier transform microwave spectroscopy, specifying a nuclear spin temperature independent of rotational temperature and interactive adjustment of parameter values with the mouse in addition to typing values.

