PGOPHER IN THE CLASSROOM AND THE LABORATORY

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PGOPHER[ab] is a general purpose program for simulating and fitting rotational, vibrational and electronic spectra. As it uses a graphical user interface the basic operation is sufficiently straightforward to make it suitable for use in undergraduate practicals and computer based classes. This talk will present two experiments that have been in regular use by Bristol undergraduates for some years based on the analysis of infra-red spectra of cigarette smoke and, for more advanced students, visible and near ultra-violet spectra of a nitrogen discharge and a hydrocarbon flame. For all of these the rotational structure is analysed and used to explore ideas of bonding. The talk will discuss the requirements for the apparatus and the support required. Other ideas for other possible experiments and computer based exercises will also be presented, including a group exercise.

The PGOPHER program is open source, and is available for Microsoft Windows, Apple Mac and Linux. It can be freely downloaded from the supporting website http://pgopher.chm.bris.ac.uk. The program does not require any installation process, so can be run on student's own machines or easily setup on classroom or laboratory computers.

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[a] PGOPHER, a Program for Simulating Rotational, Vibrational and Electronic Structure, C. M. Western, University of Bristol, http://pgopher.chm.bris.ac.uk

[b] PGOPHER version 8.0, C M Western, 2014, University of Bristol Research Data Repository, doi:10.5523/bris.huflggvpcuc1zvliqed497r2