# Colloquium

## SFB 956

Conditions and Impact of Star Formation

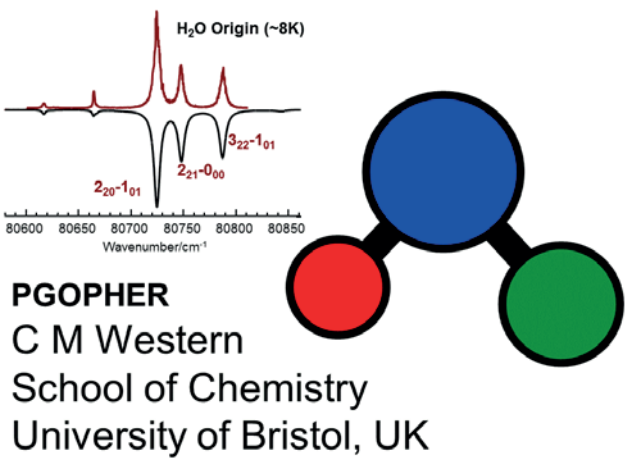
**23 April 2018**

Monday 3:00 pm

**Physikalische Institute Köln**

Lecture Hall III

Zülpicher Straße 77 | 50937 Köln




**Colin M. Western**

School of Chemistry, University of Bristol, UK

## PGOPHER – A Program for Rotational, Vibrational and Electronic Spectra

GOPHER is a general-purpose program for simulating and fitting rotational, vibrational and electronic molecular spectra. It can be used with many different spectroscopic techniques, including microwave, infra-red, Raman, visible, ultra-violet and multiphoton spectra. It can handle many different types of molecule and interactions, including linear, symmetric and asymmetric tops, fine and hyperfine structure and perturbations. It can handle many states and species simultaneously. It is designed to be used both for analyzing unknown spectra and extracting information such as temperature and state populations from observations on known species. It is an open source program, and can be freely downloaded from a supporting website.(http://pgopher.chm.bris.ac.uk)

The talk will start with a tutorial style introduction to what the program can do, and how calculations can be set up, including an example of its use in undergraduate teaching labs. This will be followed by presentation of recent developments in the program for automatic and semi-automatic assignment of unknown spectra. Assignment of spectra remains a significant problem; it is not unusual for high resolution spectra to have 20,000 lines needing assignment, with little or no obvious pattern to the lines. PGOPHER has recently gained several tools to help with this, including several different types of plot, and methods of trying many different trial assignments, and these will be discussed.

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