

## Group Theory and the Near-UV Absorption Spectrum of Gas-phase Benzene

**Author:** Bryce E. Williamson

### Practical:

**Summary:** Students measure the (1B<sub>2u</sub> 1A<sub>1g</sub>) absorption spectrum of gas-phase benzene. With the guidance of the demonstrator and the provided student notes, they interpret the spectrum and assign individual vibronic bands. On the basis of these assignments, they measure some of the excited-state vibrational frequencies and relate them to physical differences between the electronic ground and excited states.

The aims of the experiment are to introduce the students to the practical application of quantum mechanics and group theory to the interpretation of reasonably complicated spectral data. It is particularly relevant to students who are considering graduate- (including honours-) level study in physical chemistry. It introduces students to concepts that are commonly applied in molecular (polyatomic) spectroscopy and will help them to determine if they have an interest in pursuing research in this field.

This experiment is an effective learning tool since it requires the student to apply theoretical concepts that they have met in lectures to real data obtained from real chemical systems obtained with real equipment. The spectrum is reasonably complicated and most students are initially daunted by its appearance. The exercises incorporated in the experiment show that the joint use of group-theoretical and quantum-mechanical principles allows the experimenter to understand essentially all of the features of the spectrum and to deduce a good deal of information about the molecule. Moreover, the results are seen to be in accord with notions (for examples bonding/antibonding orbitals) that students might reasonably be expected to have assimilated from other branches of chemistry.

**Author:** Bryce E. Williamson

**Publisher:** Australian Physical Chemistry Enhanced Laboratory Learning Project

**Date:** Published by LTSN Dec 2003

**Reference:** [http://www.apcell.org/apcell\\_main.htm](http://www.apcell.org/apcell_main.htm)

**Discipline:** Chemistry

**Abstract**

This experiment was developed to illustrate the utility of group theory to the analysis of polyatomic spectra. It is best used in conjunction with lectures that cover representation theory, reduction methods, direct products and applications of group theory to the symmetry classification of molecular vibrations and determination of spectroscopic selection rules. It also requires knowledge of spectroscopic principles such as general selection rules, the Born-Oppenheimer approximation and the Franck-Condon principle. Students would be advantaged by previous exposure to the concepts of vibronic intensity stealing and hot bands.

Students should have covered group theory to the level of (for example) Atkins, Physical Chemistry or higher. They should have an awareness of the Born-Oppenheimer approximation and Franck-Condon principle. Some knowledge of angular momentum coupling, the Clebsch-Gordan series and the exclusion principle would be helpful.

**Duration**

Prior to Lab     none

In Laboratory    8 hours

After Laboratory none

**Further comments**

This experiment has been reproduced with kind permission from the Australian Physical Chemistry Enhanced Laboratory Learning (APCELL) Project. Further details about this experiment, all supporting documentation and background information is freely available from the APCELL website ([www.apcell.org](http://www.apcell.org)). You are requested to register for access but all details are used for the sole purpose of the project to ensure a high quality of service.