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A Resource for Introducing Molecular Modelling into the Undergraduate Chemistry Curriculum

Abstract

Computational methods including molecular modelling are becoming an essential aspect of chemistry. As such there is a pressing need to introduce this methodology at the undergraduate level. In this communication we give our experience of developing an appropriate course using formal lectures and practical workshop sessions. The emphasis is on practical applications. While the essential background theoretical aspect is introduced it is recognised that overemphasis and reliance on theoretical understanding can discourage many students. Our approach is to treat molecular modelling similarly to spectroscopic interpretation where an intelligent interpretation of an NMR spectrum does not always require a deep appreciation of background NMR theory.

Introduction

Over the past few years, molecular modelling has evolved from a specialised research tool of limited availability to an important and essential means of chemistry exploration. Software to perform molecular modelling is now widely available on desktop PCs using ubiquitous operating systems such as *Microsoft Windows*. This widespread availability can now be exploited to introduce molecular modelling into the undergraduate curriculum.

While the mathematical background to certain molecular modelling tools, such as electronic structure calculations, can be daunting this also applies to spectroscopy which has been taught for many years at undergraduate level. The key is to teach molecular modelling as a practical tool. In this respect learning to use modern graphics based molecular modelling software is certainly no more difficult than learning to operate an IR or NMR spectrometer. In essence the student needs to be able to appreciate intelligently the type of information that can be obtained from molecular modelling and to recognise its limitations. The student can achieve this by a practical hands-on approach.

Molecular modelling can be used therefore to learn and understand chemistry. It can do this in isolation or in combination with experimental approaches. Molecular modelling can be used to explore relationships between molecular structure and molecular properties. This theme of structure property relationships pervades almost every stage of a chemist's education.

Description

While numerous textbooks exist on theoretical chemistry there are very few textbooks which teach molecular modelling directed specifically at undergraduate level. This is partly due to the arrival only very recently of suitable software for such purposes available campus-wide. It is therefore of benefit to have a resource introducing the background to the principles involved accompanied by a series of practical exercises. This material can be used unaltered or adapted to suit a particular emphasis.

Lecture material in the form of *Powerpoint* slides is therefore accompanied by workshop exercises to be completed using *Gaussian 03* and *Gaussview*. The *Gaussian* program is the leading electronic structure software both in academia and industry; *Gaussview* is a graphical interface to the program allowing molecular preparation and graphical display of calculated molecular properties. Both programs are made available on a campus site - license at reasonable cost.

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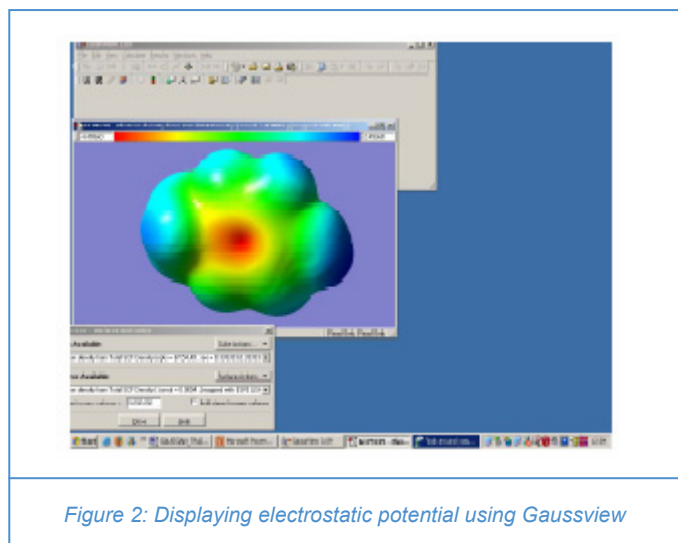
Content

The lectures cover introductory molecular modelling and computational chemistry. Major topics covered include:

- General introduction to the methods of computational chemistry
- Extension from qualitative molecular orbital methods to qualitative methods
- Types of electronic structure methods available
- Practical aspects of performing electronic structure calculations as opposed to detailed theoretical foundations
- Choice of level of electronic structure theory
- Basis set definitions and explanations
- Factors influencing choice of basis set
- Factors to consider in choosing an appropriate method
- Interpreting output from electronic structure calculations
- Graphical representation of orbital electron density, spin density and electrostatic potential
- Geometry optimisation
- Calculation of vibrational frequencies
- Methods for evaluating charge distribution and their performance
- Calculation of spin densities and hyperfine couplings
- Transition state calculations and their characterisation
- Fundamentals of molecular mechanics
- Forcefield expressions for a typical forcefield
- Minimisation
- Conformational Analysis
- Molecular dynamics

The workshop exercises are aimed at enhancing the lecture content, stimulating the students and providing practical hands-on training.

Examples from the workshops are shown in Figures 1 and 2.



Feedback/Evaluation

The resource was used in the teaching of molecular modelling at the School of Chemistry in the academic year 2005/2006. Based on completed student questionnaires the vast majority of students found the resource of significant use and it greatly increased their appreciation of molecular modelling. The availability of parallel practical workshops to the lecture material helped the students appreciate the applications of the technique to real problems. Many students also took the opportunity to use the *Gaussian* software loaded on the University network to explore some of the more advanced workshop aspects in their own time. In addition I have had contacts from students outside Manchester commenting on the usefulness of the workshop exercises in learning how to use the *Gaussian* program.

For more information

<http://www.manchester.ac.uk/chemistry>

or more specifically

<http://www.chemistry.manchester.ac.uk/staff/staffprofile.php?un=omalley>

