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## Preface to the Second Edition

## Preface to the First Edition

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It is five years since the first edition was published, and many things have moved on sufficiently to warrant a second edition.

Some things have changed. I have left the elementary chapters alone and I still believe that Appendix A on the variational method is the correct place for you to start your studies.

Some topics have not changed in the last five years. Density functional theory (and especially the B3LYP method of Becke and Perdew) has become the workhorse of modern computational chemistry. I have now started to do problems and expanded the text as appropriate.

I have also started to return to a few of the older topics. For example, everyone can now do chemical drawing, so I do not need to teach it. Thankfully that part of our lives the Z-matrix has all but disappeared, I still have fond memories of struggling to get cyclic structures to work, and now gets a page of discussion.

I have completely rewritten the chapters dealing with Moete Carlo and molecular dynamics, the On model, transition states and solvent models. I have also added a completely new chapter called 'Getting Out the Energy', and I hope you will enjoy reading it.

It is fashionable to have an associated website with any new teaching text, and I have therefore added a website at

<http://www.vcl.ac.uk/~chem/college/hinchliffe>

where you will find a number of problem sets and their solutions. Feel free to use them any way you like. I used them in my own teaching. Perhaps you have a corresponding set that you would like to share with the rest of us? Let me know.

I did all the drawings of molecules using either Gaussian 03 or HyperChem; these were done either on a machine in my Vcl laptop or on the University of Manchester's High Performance Computing Centre's supercomputer, a Bull Itanium2 system.

As always, I welcome comments and can be reached at: [Alan.Hinchliffe@manchester.ac.uk](mailto:Alan.Hinchliffe@manchester.ac.uk)

Alan Hinchliffe  
Manchester, UK