

## **Molecular Modelling for Beginners**

Alan Hinchliffe



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#### Molecular Modelling for Beginners Alan Hinchliffe

- A concise, basic introduction to modelling and computational chemistry which focuses on the essentials, including MM, MC, and MD, along with a chapter devoted to QSAR and Discovery Chemistry.
- Includes supporting website featuring background information, full colour illustrations, questions and answers tied into the text, Visual Basic packages and many realistic examples with solutions
- Takes a hands-on approach, using state of the art software packages G03/W and/or Hyperchem, Gaussian .gjf files and sample outputs.
- Revised with changes in emphasis and presentation to appeal to the modern student.



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