DESCRIPTION

• 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.

ABOUT THE AUTHOR

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NEW TO EDITION

• Completely revised and updated

• Website featuring dryer supporting material, background information, full colour illustrations, questions and answers tied into the text and Visual Basic packages and many realistic examples with solutions

• Sections on Monte Carlo and Molecular Dynamics completely rewritten and expanded

• Dryer material moved onto website

• New material added to chapters on ‘sharing out the energy’, ‘Empirical models’ and ‘Dealing with the solvent’

FEATURES

• Provides a comprehensive introduction to this evolving and developing field

• Focuses on the essentials, including MM, MC, and MD, along with a chapter devoted to QSAR and Discovery Chemistry.

• Includes many real chemical applications combined with worked problems and solutions provided in each chapter.

• Ensures that up-to-date treatment of a variety of chemical modeling techniques are introduced.

• Hands-on approach using state of the art software packages G03/W and/or Hyperchem, both in the text and in more detail on the website much more detail on the site. For example, Gaussian .gjf files and sample outputs.

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