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The bestselling computational chemistry text, newly updated and expanded  
Because of advances in technology, PC users can now model chemical phenomena which only a few years earlier required a supercomputer. With processing capabilities moving forward so rapidly, a current introduction to computational chemistry should utilize today's generally available machines.

Computational Chemistry Using the PC, Third Edition takes the reader from a basic mathematical foundation to beginning research-level calculations, avoiding expensive or elaborate software in favor of PC applications. Geared toward an advanced undergraduate or introductory graduate course, this Third Edition contains revised and expanded coverage of molecular mechanics, molecular orbital theory, molecular quantum chemistry, and semi-empirical and ab initio molecular orbital calculations. Features of the text include:

A mathematical introduction emphasizing matrix algebra

Practice problems, lab exercises, and small research projects suitable for a one-semester course

Instruction on conducting research-level calculations using readily available software

Learning tools available on an accompanying Web site

Extensive bibliography with references ranging from the historically significant to contemporary research

With significant changes made to adjust for improved technology and increased computer literacy of today's student, Computational Chemistry Using the PC, Third Edition gives its readers the tools they need to translate theoretical principles into real computational problems, then proceed to a computed solution. Students of computational chemistry, as well as professionals interested in updating their skills in this fast-moving field, will find this book to be an invaluable resource.

DONALD W. ROGERS, PhD, is Professor Emeritus at Long Island University. For forty years, Professor Rogers has taught academic courses in physical chemistry, thermodynamics, general chemistry, computational chemistry, and microcomputer interfacing. He publishes regularly in the Journal of Physical Chemistry and elsewhere, and his work has been supported for the last

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