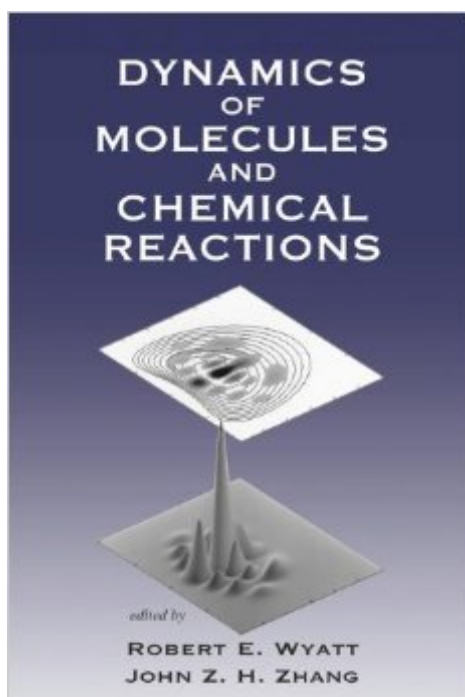


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Dynamics Of Molecules And Chemical Reactions



Synopsis

Covers both molecular and reaction dynamics. The work presents important theoretical and computational approaches to the study of energy transfer within and between molecules, discussing the application of these approaches to problems of experimental interest. It also describes time-dependent and time-independent methods, variational and perturbative techniques, iterative and direct approaches, and methods based upon the use of physical grids of finite sets of basic function.

Book Information

Hardcover: 704 pages

Publisher: CRC Press (June 27, 1996)

Language: English

ISBN-10: 0824795385

ISBN-13: 978-0824795382

Product Dimensions: 7.3 x 1.4 x 10.2 inches

Shipping Weight: 3.1 pounds (View shipping rates and policies)

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Chemical reactions generally happen between pairs of molecules. Those reactions always take place when the molecules collide, almost always either in a gas or in a liquid. Other, supposedly-simpler, things also happen when molecules collide:- kinetic energy gets transferred, and eventually a temperature (the average kinetic energy per molecule) settles out- drag and lift (the precursors of aviation, and of ballistics) are imposed on bodies passing through fluids- shock waves form when a body passes through fluid at greater than the "speed of sound" or an explosion occurs. After an adult lifetime of studying most of these effects, it's become apparent that the acoustical theory and indeed fluid mechanics in general, ignores crucial underpinnings that should have been available from first principles. The simplifying assumptions in such theory are at variance with the basic physics at molecular level, and thus are at grave risk of being wrong, outright. We know so little, and have apparently come so far on a substrate of baloney. So I bought this book in

an attempt to start from first principles (statistical mechanics and the like) to see whether the Quantum Mechanical view of the very-small can get us all back on the rails. I've only read the first chapter (I have nearly 100 other books on various subjects, all clamoring to be read...) but it looks very good so far.

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