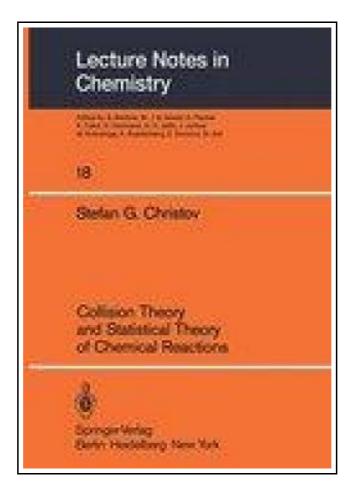
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COLLISION THEORY AND STATISTICAL THEORY OF CHEMICAL REACTIONS



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Springer Jul 1980, 1980. Taschenbuch. Book Condition: Neu. 24.4x17x cm. This item is printed on demand - Print on Demand Neuware - Since the discovery of quantum mechanics, more than fifty years ago, the theory of chemical reactivity has taken the first steps of its development. The knowledge of the electronic structure and the properties of atoms and molecules is the basis for an un derstanding of their interactions in the elementary act of any chemical process. The increasing information in this field during the last decades has stimulated the elaboration of the methods for evaluating the potential energy of the reacting systems as well as the creation of new methods for calculation of reaction probabili ties (or cross sections) and rate constants. An exact solution to these fundamental problems of theoretical chemistry based on quan tum mechanics and statistical physics, however, is still impossible even for the simplest chemical reactions. Therefore, different ap proximations have to be used in order to simplify one or the other side of the problem. At present, the basic approach in the theory of chemical reactivity consists in separating the motions of electrons and nu clei by making use of the Born-Oppenheimer adiabatic approximation to obtain electronic energy as an effective potential for nuclear motion. If the potential energy surface is known, one can calculate, in principle, the reaction probability for any given initial state of the system. The reaction rate is then obtained as an average of the reaction probabilities over all possible initial states of the reacting ~articles. In the different stages of this calculational scheme additional approximations are usually introduced. 322 pp. Englisch.



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