



Computational Methods in Chemistry (Paperback)

By Joachim Bargon

Springer-Verlag New York Inc., United States, 2013. Paperback. Condition: New. Language: English . Brand New Book ***** Print on Demand *****.The papers collected in this volume were presented at an international symposium on Computational Methods in Chemistry. This symposium was sponsored by IBM Germany and was held September 17-19, 1979, in Bad Neuenahr, West Germany. According to Graham Richards [Nature 278, 507 (1979)] the Third Age of Quantum Chemistry has started;-where the results of quantum chemical calculations have become so accurate and reliable that they can guide the experimentalists in their search for the unknown. The particular example highlighted by Richards was the successful prediction and subsequent identification of the relative energies, transition probabilities and geometries of the lowest triplet states of acetylene. The theoretical predictions were based chiefly upon the work of three groups: Kammer [Chern. Phys. Lett. ~, 529 (1970)] had made qualitatively correct predictions; Demoulin [Chern. Phys. 11, 329 (1975)] had calculated the potential energy curves for the two lowest triplet states (3 and 3) of B A acetylene; and Wetmore and Schaefer III [J. Chern. Phys. ~ 1648 (1978)] had determined the geometries of the cis (3B and ~A) and the trans (3B...



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