



The New World of Quantum Chemistry: Proceedings of the Second International Congress of Quantum Chemistry Held at New Orleans, U.S.A., April 19-24. 1976

By -

Springer, Netherlands, 2011. Paperback. Book Condition: New. 244 x 170 mm. Language: English . Brand New Book \*\*\*\*\* Print on Demand \*\*\*\*\*.Bernard PULLMAN During a long period organic chemistry was one of the pre-ferred field of exploration for many quantum chemists. It still remains of major interest for a number of them, but altogether it seems as if the center of gravity of the quantum molecular theories became displaced towards different horizons. The displacement seems in fact to occur in two directions. On the one hand, we see a prominent development of very refined computations for relatively small and frequently inorganic molecular systems with the view of a better and better reproduction of their obser- vable properties and thus a better understanding of the fundamen- tal principles governing the electronic structure of molecules. On the other hand, there is a no less prominent development of frequently also no less refined computations towards the study of molecular systems which because of their dimensions or the com- plexity of the questions which they raise go beyond the usual treatment of organic molecules. These later studies involve in particular the penetration of quantum-mechanical concepts and me-thods into the realm of...



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