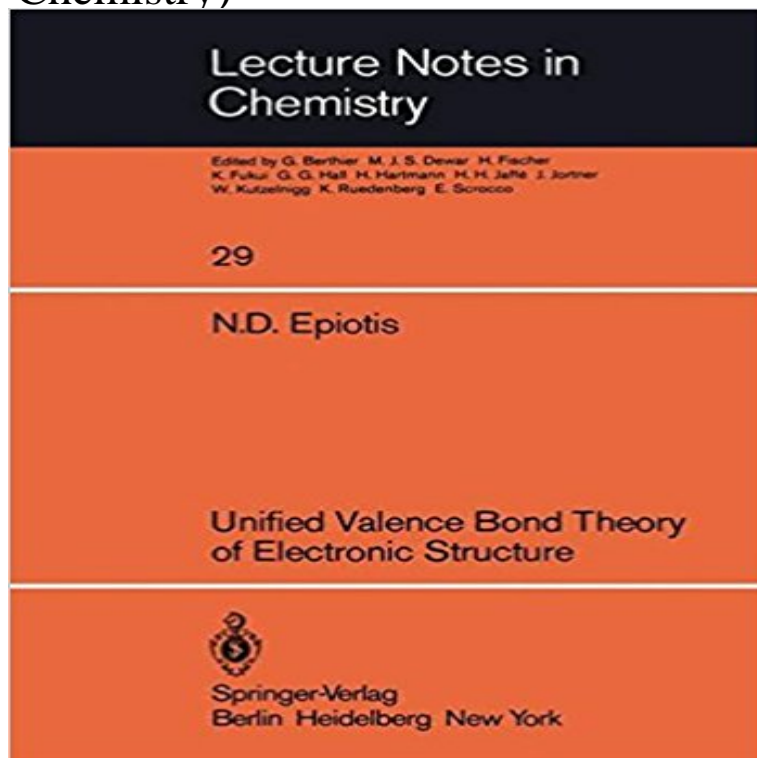


Unified Valence Bond Theory of Electronic Structure (Lecture Notes in Chemistry)



In the last fifty years, computational chemistry has made impressive strides. Huckel MO computations were rapidly succeeded by semiempirical monodeterminantal Self Consistent Field (SCF) MO calculations which now give way to high quality ab initio calculations of the poly-determinantal SCF-MO and Generalized VB variety. By contrast, no analogous progress has been made in the area of the qualitative theory of chemical bonding. In fact, more than a half-century after the exposition of Huckel MO theory the conceptual superstructure of chemistry is still founded on it. This is made glaringly evident by the fact that highly sophisticated computations are still interpreted with primitive Huckel MO theory, despite the fact that most chemists are well aware of its formal deficiencies. The current popularity of qualitative MO theory among experimentalists is not the result of recent advances, rather the consequence of stimulating application of old MO theoretical concepts. . . . This work attempts to improve this situation by outlining a qualitative theory of chemical bonding which operates at a high level of theoretical sophistication. It was first presented at the NATO Advanced Study Institute on Topics in Theoretical Organic Chemistry in Gargnano, Italy, in June 1979, and in other international meetings and conferences, colloquia, and informal gatherings in the period of time following the Gargnano meeting. It was also presented in a seminar given at the University of Washington in October 1980.

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