

Qualitative Valence-Bond Descriptions of Electron-Rich Molecules: Pauling "3-Electron Bonds" and "Increased-Valence" Theory: Pauling "3-Electron ... Theory (Lecture Notes in Chemistry)

R. D. Harcourt

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This book provides qualitative molecular orbital and valence-bond descriptions of the electronic structures for electron-rich molecules, with strong emphasis given to the valence-bond approach. Electron-rich molecules form an extremely large class of molecules, and the results of quantum mechanical studies from different laboratories indicate that qualitative valence-bond descriptions for many of these molecules are incomplete in so far as they usually omit "long-bond" Lewis structures from elementary descriptions of bonding. For example, the usual representation for the electronic structure of the ground-state for 03 involves resonance between the (+1 o and Until standard Lewis structures ~ (-I . b:" ~d· , recently, any contribution to resonance of the "long-bond" (or spin-paired o •• / •• , . . has been largely ignored. diradica~ Lewis structure However, it :0 . 0 . . e- _ ____ " has now been calculated to be a very important structure. For the ground-states of numerous other systems, calculations also indicate that "long-bond" structures are more important than is usually supposed, and therefore they should frequently be included in qualitative valence-bond descriptions of electronic structure. The book describes how this may be done, and some of the resulting consequences for the interpretation of the electronic structure, bond properties and reactivities of various electron-rich molecules. When appropriate, molecular orbital and valence bond descriptions of bonding are compared, and relationships that exist between them are derived.



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