Developing the “Effective Electrons” Model to Improve the Calculation Method of Valence-shell Electron-pair

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According to the traditional VSEPR theory, the calculation method of the number of central atom’s valence shell electron pair is limited. When studying the geometry of molecule (ion), people have to make some special rules for exceptions. Also, the traditional VSEPR theory can be only used for predicting the molecular (ionic) geometry of ABm or ABmEn type. For solving these problems, I decided to further study the valence bond theory, the hybrid orbital theory, VSEPR theory and the theory of coordinate bond and initiated the research on "improving the calculation method of the valence shell electron pairs ". During my project, I found that when the covalent bond is formed between the central atom A and the ligating atom B, the molecular geometry’s formation of the electron pairs provided by the atom B is sometimes valid, while sometimes invalid. Based on this opinion, I set up a new theoretical model, that is, the “Effective Electrons” Model. So I define the electrons that ligating atom donates as "effective electrons", and based on VESPR theory and the model of “coordination atom providing the central atom with effective electrons”, the calculation formula of the valence shell electron pair can be figured out as follows: The number of the valence shell electron pair of the central atom = (the number of valence shell electrons of the central atom + the number of the effective electrons provided by the surrounding coordination atoms ±charge number of central atom) /2 With this method, people can not only analyze the molecular (ionic) geometry of ABm or ABmEn type, but also the molecules that have multiple central atoms, and the molecular geometry with coordinate bonds, which enlarges the applied scope of VSEPR theory.

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