## The Valence Bond Way in Chemistry

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*"Give us insight, not numbers"* was Coulson's admonition to theoretical chemists. My talk will show that Valence Bond (VB) theory provides insight and good numbers, and creates a great deal of order in Chemistry [1]. In this talk I will show its application to bioinorgnic and organic chemisry. Potentially, if time permits, I may cover the following two stories:

(a) The first story concerns the reactivity of the iron-oxo species of Cytochrome P450 in Habstraction, sulfoxidation, and aromatic hydroxylation, and how VB theory creates order and makes predictions in this complex field [2-4]. I will further teach how the VB model enables one to estimate H-abstraction barriers for reactions that range from  $H+H_2$  to the Ètard reaction, permanganate oxidation, and all the way to Cytochrome P450 oxidation. A bridge will be created between normal hydrogen atom abstraction (HAT) and the proton coupled electron transfer (PCET) mechanism [4].

(b) The story of the oxy complexes of Myoglobin and Hemoglobin (Mb.O<sub>2</sub>; Hb.O<sub>2</sub>), which were "discovered" about 333 years ago, and their bonding features, which were outlined first in 1936, remain disputed for 75 years. We shall see how VB theory resolves the dispute by transforming the CASSCF/MM wave function to a VB/MM wave function, which shows clearly the bonding mechanism of O<sub>2</sub> to the ferrous heme complex [5].

It will be argued that VB theory and VB reading of the wave function is a productive future paradigm in chemistry.

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