

Theory of Chemical Bonds in Metalloenzymes XIV.
Six States Model for Hydroxylation Reactions of Alkanes by P450.

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Abstract

Previous four states model (one quartet and three doublet states) [1] for hydroxylation reactions of alkanes by P450 has been extended to six states model (one sextet, two quartet and three doublet states) for theoretical elucidation of state correlation diagrams of the ground and lower excited states along the reaction pathways. The six states model [1] was found to be useful enough for systematic and unified understanding of electronic structures of transition structures and intermediates of the reactions revealed by our group and several other groups. The state correlation diagrams based on the model have indeed provided reasonable reaction mechanisms of the hydroxylations. Implications of the six states model were also discussed in relation to our electrophilic (SE2), singlet and triplet diradical models [2]-[4] for reaction mechanisms of P450.

References

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