

Effect of Spin Degree of Freedom on the Reaction of O₂ with Hemoglobin

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Here, we report results of our study on the mechanism of spin-dependent O₂ reaction with hemoglobin [1]. O₂ reaction with hemoglobin, which we represent as FePIm (Fe = iron, P = porphyrin, Im = imidazole), involves the transition between two spin-dependent states, viz., the oxyhemoglobin state and the deoxyhemoglobin state. The deoxyhemoglobin state pertains to FePIm and a free O₂, while the oxyhemoglobin state pertains to an O₂ bound to FePIm. The deoxyhemoglobin and oxyhemoglobin systems have triplet and singlet total magnetizations, respectively. We found that a spin transition from triplet to quintet to singlet mediates the O₂ binding process, and this accelerates the reaction. We also found that the position of the Fe atom out of the porphyrin plane is an important indicator of O₂ affinity. These results indicate that spin transitions/crossings affect the activation energy barrier. Further details will be discussed at the meeting.

参考文献

- [1] *cf., e.g.*, D. Kurokawa, J.S. Gueriba, W.A. Diño, *Spin-Dependent O₂ Binding to Hemoglobin*, ACS Omega **3** (2018) 9241-9245.