公開セミナー

日時：２０１２年８月３０日１３時ー１４時

場所：研究棟７３２号室

Quantum Chemical Modeling of Co-C Bond Activation in B_{12}-Dependent Enzymes

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The origin of the enormous catalytic activity of coenzyme B_{12}-dependent enzymes continues to be an outstanding problem in bioinorganic chemistry. During enzymatic catalysis the Co-C bond of coenzyme B_{12} (AdoCbl) is cleaved homolytically, leading to the formation of the 5'-deoxyadenosyl radical and cob(II)alamin. The rate of enzymatically accelerated homolytic cobalt-carbon bond cleavage of AdoCbl exceeds the rate observed in aqueous solution by about 12 orders of magnitude as a consequence of the coenzyme interaction with the substrate in the presence of apoenzyme. Despite the great effort that has been devoted to this problem, the mechanism of the catalytic activation is poorly understood. To the extent it has been addressed experimentally, evidence from model systems indicate that steric hindrance around coordinated alkyl ligands leads to a higher homolysis rate. Different models have been suggested, but none can be considered as fully satisfactory in light of a large body of experimental results.

In my presentation I will summarize recent progress in computational modeling of the catalytic activation of cobalt-carbon bond cleavage. The growing interest in modeling the structure and electronic properties of AdoCbl has demonstrated that computer simulations, in particular density functional theory (DFT) can be an important part of coenzyme B_{12} research.

上記セミナーを開催します。Pawel M. Kozlowski 教授はポルフィリンの理論化学的研究で著名な方です。この度、general chemistry audience 向けにビタミン B_{12} に関する研究についてお話し下さいます。奮ってご参加下さい。

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