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Quantum chemical studies for estimation of pKa and redox potential

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Abstract

We have proposed a new scheme for estimating the acid dissociation constant (pK_a) based on quantum-chemical calculations combined with a polarizable continuum model, where a parameter is determined for small reference molecules. pK_a values of variously sized molecules were evaluated ranging from several organic molecules, amino acids, and a protein consisting of 300 atoms. Our scheme can predict a semiquantitative pK_a value for specific chemical groups and discuss the influence of the surroundings on the pK_a values. Applications to pK_a value of the side chain of amino acids almost reproduced the experimental value. We also showed the influence of hydrogen bonds on the pK_a values in the case of tripeptides, which decreases the pK_a value by 3.0 units for serine in comparison with those of the corresponding monopeptide. Finally, with some assumptions, we derived the pK_a values of tyrosines and serines in chignolin and a tryptophan cage. We obtained quite different pK_a values of adjacent serines in the tryptophan cage; the pK_a value of the OH group of Ser13 exposed to bulk water is 14.69, whereas that of Ser14 exposed not to bulk water is 20.80 because of the internal hydrogen bonds. We also apply the same methodology to estimate standard hydrogen electrode and redox potentials for several ractions. This scheme also reproduces well the redox potentials of several typical reactions within almost 0.1 V. Density functional theory-based methods also give excellent redox potentials of the same reactions with almost the same accuracy with our new computational scheme.

Biography

Yasuteru Shigeta has received Ph.D. (2000) degrees in chemistry from Osaka University, Osaka, Japan. He was selected as Japan Society for the Promotion of Science (JSPS) Research Fellowship for Young Scientists from up to 2003. He became an Assistant Professor at the University of Tokyo in 2003, a Lecture of Physics at University of Tsukuba in 2007, and an Associate Professor of Chemical Engineering, Osaka University in 2010. He has received several awards for his outstanding efforts in theoretical chemistry. He has published more than 120 papers in reputed journals.