

Abstract Submitted
for the 4CF09 Meeting of
The American Physical Society

A Method to Calculate Protein Dipole Moments BRETT MELLOR, BRIAN MAZZEO, Brigham Young University — The electric dipole moments of globular proteins, determined experimentally by dielectric relaxation spectroscopy, contribute to both protein function and structure. Numerical computations of dipole moments can be obtained from structures in the Protein Data Bank. However, previous computations in literature have agreed with experimental results for only a limited number of proteins. This paper presents a method to compute the pH-dependent dipole moment. The protein molecule is considered as an array of electrical point charges in aqueous solution. The dipole moment is calculated as the vector sum of two components: (1)the core dipole moment which emerges from the unequal sharing of electrons in covalent bonds; (2)the surface charge dipole moment resulting from pH-dependent side chain partial charges. pKa shifts for each side chain amino acid are determined by the H++ server employing the Poisson-Boltzmann equation. The net charge and dipole moment over a range of pH are calculated. The Oncley equation is used to predict the dielectric increment at arbitrary pH, temperature, and protein concentration.

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Date submitted: 24 Sep 2009

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