Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Molecular dynamics study of the Mg - AMP interaction in water DON BRUGESS, Asbury College, IOAN KOSZTIN, University of Missouri - Columbia — The conformational states of Mg^{++} complexed with adenosine monophosphate (AMP) in water solution is analyzed using classical molecular dynamics (MD) simulations. Relevant portions of the 3D *potential of mean force* (PMF) of Mg^{++} is reconstructed by employing two distinct methods: (1) equilibrium MD simulations using the umbrella sampling and weighted histogram analysis method, and (2) non-equilibrium steered MD simulations using a recently developed method based on the Jarzynski equality. Withing computational errors, both methods yield the same results. Two topologically distinct sets of equilibrium conformations of Mg^{++} in the vicinity of the phosphate moiety are found. The free energy difference between the states within a given set is about 1 kT, and are separated by potential barriers of $\sim$ 10 kT in height. However, the free energy difference between states from the two distinct sets are found to be unrealistically high ($\sim$ 10 kcal/mol). Also, the calculated dissociation energy of Mg++ from AMP exceeds several times the corresponding experimental value. Possible sources of this discrepancy are discussed, and alternative methods to improve the accuracy of the calculations are proposed.

Ioan Kosztin
University of Missouri - Columbia

Date submitted: 01 Dec 2004

Electronic form version 1.4