Kernel Energy Method: Application to DNA

Lulu Huang*, Lou Massa [†], and Jerome Karle*

*Laboratory for the Structure of Matter, Naval Research Laboratory Washington, D.C. 20375-5341

[†]Hunter College and the Graduate School, City University of New York, New York, New York 10021

Abstract

The Kernel Energy Method (KEM) has been used in recent papers to calculate the quantum mechanical *ab-inito* molecular energy of peptides and the protein insulin. It was found to have good accuracy. The computational difficulty of representing a molecule increases only modestly with the number of atoms. The calculations are simplified by adopting the approximation that a full biological molecule can be represented by smaller "kernels" of atoms. In this paper the accuracy of the KEM is tested in application to DNA, whose basic kernels, chemical bonding, and overall molecular structure are quite different from peptides and proteins. The basic kernel in the case of peptides and proteins is an amino acid. The basic kernel in the case of DNA is a nucleotide consisting of a phosphate-sugar-base. The molecular energy is calculated for all 3 basic types of DNA, i.e., B, A, and Z configurations of DNA. The results give an accuracy that is comparable to that achieved with peptides and proteins. Thus the KEM is found to be applicable to major types of biological molecules.