Mutagenic Effects in DNA from Carbon-14 Decay: Quantum Chemistry Calculations

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The potential for radioactive Carbon-14 to have biological effects has long been recognized. Every second, the human body is subjected to 20–30 radiocarbon decays within the base pairs and sugar groups of DNA. We used density functional theory to examine the kinetic and electronic effects of transmuting a carbon atom into nitrogen within DNA fragments. The dynamical studies use ab intio molecuar dynamics to measure the recoil radiation stability and show that the recoil energy of the Nitrogen-14 daughter nucleus is sometimes sufficient to break chemical bonds. For the most part, however, radiocarbon decay simply creates a nitrogen atom on a carbon site.

Static calculations were subsequently performed to examine how radiocarbon transmutation modifies the hydrogen bonds between DNA base pairs. We find that the presence of the transmuted nitrogen can break bonds, alter the strength of the bond substantially, and shuttle protons between bases. The latter has the potential to be particularly significant, as proton transfer is a well-known chemical process that can disrupt base-pairing and replication in DNA.