Theory of ^{14}N and ^{17}O Nuclear Quadrupole Interactions in Polyglycine and Glycine in the Protein Chain of Cytochrome c

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As part of our ongoing investigations on hyperfine properties of nuclei and attached probes (like muon and muonium) in the protein chain of Cytochrome c (Cyt c), we have been studying the ^{14}N and ^{17}O nuclear quadrupole interactions in the amino acids in the protein chain at different sites where they occur. As a specific example of one of the amino acids in this context, we shall present our results on Glycine in the homo-molecular polymer Polyglycine and expectations for the hetero-molecular environment occurring at a particular region of the protein chain of Cyt c which is far enough away from the heme unit to make the results more characteristic of the chain.

In the Polyglycine polymer, our results for the ^{14}N and ^{17}O coupling constants e^2qQ and asymmetry parameters η for a central Glycine in a chain of odd numbered molecules are used to study how the e^2qQ and η vary with the chain length and to compare with the results for the isolated Glycine molecule. The aim is to study the convergence of the results with respect to chain length to find out the appropriate length at which the results become characteristic of the polymer chain. This conclusion is expected to provide insights into the chain length to be used in the protein to simulate the results for the protein chain in Cyt c. The Hartree-Fock Cluster procedure is being used for the investigations for all the results to be reported.

Key words: Hartree-Fock calculations; Polyglycine; Muon and Muonium Trapping; Nuclear Quadrupole Interactions.