Theory of ^{14}N and ^{17}O Nuclear Quadrupole Interactions in the Single Amino Acids Occurring in the Protein Chain of Cytochrome c

R. H. Scheicher[a], D. Cammarere[a,b], N. Sahoo[a,c], K. Nagamine[d,e], and T. P. Das[a]

[a] Department of Physics, State University of New York at Albany, Albany, NY, 12222, USA
[b] Tamarac High School, Brittenkill, NY, USA
[c] Department of Radiation Oncology, Albany Medical College, Albany, NY, 12208, USA
[d] Muon Science Laboratory, RIKEN (The Institute of Physical and Chemical Research), Wako, Saitama 351-0198, Japan
[e] Meson Science Laboratory, Institute of Materials Structure Science, KEK, Tsukuba, Ibaraki 305-0801, Japan

Reprint requests to Prof. T. P. Das; Fax: 1-518-442-5260, E-mail: tpd56@albany.edu

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The understanding of electron transport in proteins based on a novel technique involving muon spin rotation (μSR) measurements is a topic of great current interest. The technique, which involves study of spin relaxation of a positive muon (μ^+) trapped in amino acids in protein chains due to the fluctuating magnetic field that the moving electron produces, is based on the premise that the electron is generated by ionization of a muonium (Mu) which was trapped at the same site as the μ^+ left behind. In attempting to test this premise from first-principles for the Cytochrome c (Cyt c) system in which recent μSR measurements have been made, we have carried out Hartree-Fock investigations of the electronic structures of the bare amino acids and amino acids with μ^+ and Mu trapped at the oxygen of the C=O group common to all amino acids. With the aim that the comparison of theoretically predicted experimental nuclear quadrupole interaction (NQI) parameters will provide a useful test of the electron distribution in the amino acids of Cyt c, we present results for the nuclear quadrupole coupling constants (e^2qQ) and asymmetry parameters (η) for the bare amino acids and the amino acids with trapped μ^+ and Mu. The trends in e^2qQ and η for ^{14}N and ^{17}O between the various amino acids, as well as the changes in these parameters in the presence of μ^+ and Mu are being analyzed. It would be helpful to have experimental data for e^2qQ and η to compare with our predictions for the amino acids as they occur in vitro in polycrystalline Cyt c in which the μSR measurements have been carried out. It is also hoped that the μSR technique will be able to provide experimental data on e^2qQ and η for the ^{14}N and ^{17}O nuclei to compare with our predictions.

Key words: Hartree-Fock Calculations; Amino Acid Molecules; Muon and Muonium Trapping; Nuclear Quadrupole Interactions.