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Theoretical study of ^{14}N pure quadrupole resonance in amino acids

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Abstract. The theoretical hybridization model of Vega is adapted to the tetrahedral environment around the nitrogen nucleus in eleven amino acids to estimate the orbital occupation numbers using the experimental values of the quadrupole coupling constant and asymmetry parameter of ^{14}N quadrupole resonance and the results are discussed.

Keywords. Electric field gradient; quadrupole coupling constant; occupation number; hybrid orbitals; amino acids.

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1. Introduction

The study of the nuclear quadrupole coupling constants (QCC) helps in calculating the electric field gradients (EFG) and also provides useful information about the concepts of chemical bonds like ionic character, occupation numbers, double bond character etc. The theoretical interpretation of QCC in terms of the chemical bonds was first given by Townes and Dailey (1949) and has been applied to N-heteroaromatics (Scrocco 1965), hydrazines and hydrazides (Sauer and Bray 1972), azines (Sauer *et al* 1972) and amino acids (Edmonds and Summers 1973). Later Vega (1974) proposed a theoretical model relating the EFG components, the electronic occupation numbers and degrees of hybridization in sp^3 tetrahedral configuration around the nitrogen nucleus, without recourse to the assumptions involved in Townes and Dailey theory. In the present work, the treatment proposed by Vega (1974) has been adapted to nitrogen resonance in various amino acids to calculate the occupation numbers of hybrid orbitals and the results are discussed.

2. Theory

To correlate the EFG components with the charge distribution in the molecule, Vega (1974) considered tetrahedral configuration around the resonating nucleus and assumed reflection symmetry for the two equivalent hybrids ϕ_1 and ϕ_2 with the occupation number a_1 which make an angle $2\theta(>\pi/2)$ with each other while the other two hybrids ϕ_3 and ϕ_4 with occupation numbers a_3 and a_4 lie in the symmetry plane as shown in figure 1. An orthogonal coordinate system $\xi\eta\zeta$ is chosen such that ζ-axis is perpendicular to the symmetry plane, η-axis bisecting the ϕ_1 and ϕ_2 orbits and ξ-axis