

EPR of Gamma Irradiated Single Crystals of N-Acetyl- and N-Carbamyl- α -Aminoisobutyric Acid

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The $(\text{CH}_3)_2\dot{\text{C}}\text{COOH}$ radical has been observed in the EPR spectra of γ -irradiated single crystals and powders of N-acetyl- α -aminoisobutyric acid and N-carbamyl- α -aminoisobutyric acid.

Key words: Electron Paramagnetic Resonance; Free Radical; α -Aminoisobutyric Acid Derivatives.

1. Introduction

EPR has been applied to study irradiation damage centers in carboxylic acid and its derivatives [1–5]. γ -irradiated single crystals of α -aminoisobutyric acid were investigated at room temperature [6] and X-irradiated single crystals at 77 K [7]. Furthermore, γ -irradiated single crystals of α -hydroxy isobutyric acid and α -aminoisobutyric acid hydrochloride were investigated between 113 and 300 K [8]. The radiation damage centers were attributed to $(\text{CH}_3)_2\dot{\text{C}}\text{COOH}$ radicals in four studies. In the present work we have applied EPR to γ -irradiated N-acetyl- α -aminoisobutyric acid, $(\text{CH}_3)_2\text{C}(\text{NHCOCH}_3)\text{COOH}$, NA, and N-carbamyl- α -aminoisobutyric acid, $(\text{CH}_3)_2\text{C}(\text{NHCONH}_2)\text{COOH}$, NC, in single crystal and powder form at room and low temperature to determine the irradiation damage centers and their properties.

2. Experimental

NA and NC single crystals were grown from acetone solution. In its single crystal form NA is monoclinic with space group $\text{P2}_1/\text{n}$, and unit cell dimensions $a = 10.165$, $b = 8.030$, $c = 9.712$ Å, $V = 736$ Å³, $\beta = 111.9^\circ$. The unit cell contains 4 molecules [9]. The single crystals and powders were irradiated with a Co^{60} γ -ray source of 0.3 Mrad h^{-1} at room temperature for 5 hours. The spectra were recorded with a Varian model E-109C EPR spectrometer, using 2 mW microwave power. The low temperature measurements were carried out using a Varian variable temperature control unit. The crystals were rotated on a lucite pillar about their crystallographic axes, and the angles of

Table 1. Principal values of the methyl groups for the $(\text{CH}_3)_2\dot{\text{C}}\text{COOH}$ radical in N-acetyl- α -aminoisobutyric acid (NA), and N-carbamyl- α -aminoisobutyric acid (NC). The values are given in mT.

Principal values (± 0.02 mT)	NA	NC
A_{xx}	2.34	2.26
A_{yy}	2.16	2.13
A_{zz}	2.1	2
a	2.2	2.13

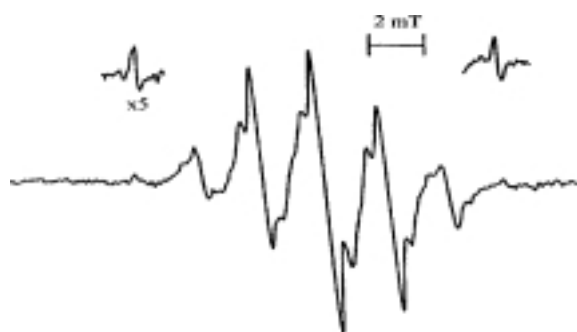


Fig. 1. EPR spectrum of γ -irradiated N-acetyl- α -aminoisobutyric acid powder at room temperature.

rotation were read on a scale in degrees. The g factors were found by comparison with a DPPH sample ($g = 2.0036$).

3. Results and Discussion

The EPR spectrum of γ -irradiated NA powder at room temperature is shown in Figure 1. The spectrum consists of 7 equally spaced (2.2 mT) lines with the relative intensity distribution 1 : 6 : 15 : 20 : 15 : 6 : 1. The single crystal spectrum of NA at room temperature is isotropic and equals the powder spectrum.