

Simulation of Ginger EPR Spectra Obtained by X-Irradiation: Quantum Approach

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Abstract: The ginger sample has been exposed to X-rays at cumulative doses. The foodstuffs irradiation is used in particular to improve their hygienic qualities and increase their shelf lives. This process has been approved by various international organizations: FAO – AIEA – WHO. In the present work, we propose to reproduce by simulation, based on a quantum approach, of the ESR (Electron Spin Resonance) spectra. The semi-classical approach is valid for a simple system, but not for a complex system such as an atom with hyperfine structure. In this case a quantum approach, based on spin Hamiltonian, is essential to interpret the ESR spectra. The main result is that the simulated spectra are in good agreement with the experimental ones obtained before and after irradiation.

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1. Introduction

Electron paramagnetic resonance (EPR), also called electron spin resonance (ESR), was discovered in 1944 by Zavoisky [1] and has assumed an increasingly prominent position in various fields, especially in biochemistry-biology [2], chemistry [3], analysis of materials [4-6], geology and in medicine, or even in the two dimension imagery domain [7]. The phenomenon is based on the magnetic moment of an unpaired, spinning free electron.

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In a magnetic field, the unpaired electron, which has a spin quantum number $S = 1/2$ ($m_s = \pm 1/2$), precesses about the field axis (z-axis) with a component of its spin angular momentum either parallel ($m_s = +1/2$) or antiparallel ($m_s = -1/2$) to the z-axis. An oscillating magnetic field at right angles to the field axis induces transitions between the two spin states when the frequency of the field is at or near the Larmor frequency of the precessing electron. It is important to note that the EPR technic is an efficient and non-destructive method which is often applied to the quality control of irradiated foodstuffs [8-14]. Among species that are susceptible to give an EPR signal, we quote the transition-metal ions (oxidization state presenting the unpaired electrons), the organic radicals (CH_3, \dots), some inorganic radicals at the stable state ($\text{NO}_2, \text{NO}, \text{ClO}_2, \dots$) and the unstable atoms ($\text{H}, \text{OH}, \dots$). This method presents the advantage of important sensitivity which allows to detect 10^{11} unpaired electron spins by gram.

Recalling that, in a recent experimental work [15], a comparative analysis between ginger spectra observed before and after X-irradiation, permitted to follow the evolution, according to the dose absorbed by the sample, of the spectra shape and the amplitude. The signal of the unirradiated sample is characterized by a g-value of $2,0032 \pm 0,0005$, whereas after irradiation the observed signal present a weakly pick centered on the $g = 2,0028 \pm 0,0005$. These results show that free radicals are produced by irradiation in ginger.

To complete this study, we are concerned with simulation, based on a quantum approach, the ESR spectra obtained before and after irradiation of ginger. We found, in particular, that simulated spectra are in good agreement with the experimental ones notably after irradiation.

This paper is organized as follows : In section 2 we present a theoretical model, we show also the spectra simulation and their comparison with those obtained by the experience [15]. We draw some concluding remarks in section 3.

2. EPR spectra simulation

The spin Hamiltonian of ginger sample, expressed in energy units, (assuming no hyperfine interaction) is given by :

$$H_{spin} = g\beta\mathbf{H}_0\mathbf{S} \quad (1)$$

Where \mathbf{H}_0 is the external magnetic field vector, β denotes the Bohr magneton, g is the splitting factor and \mathbf{S} represents the electron spin operator.

Using spin functions based on the quantum number m_s , equation (1) can be used to compute energy levels. Equating energy differences for the allowed transitions ($\Delta m_s = \pm 1$) with the microwave photon energy,

$$E(m_s + 1) - E(m_s) = h\nu \quad (2)$$

with

$$E(m_s) = g\beta H_0 m_s \quad (3)$$

For a given frequency of radiation, ν absorption occurs at the resonant magnetic field, H_r , in units of Gauss, given by

$$H_r = \frac{h\nu}{\beta g} \quad (4)$$

Here h is the Planck's constant.

The radiofrequency microwave field \mathbf{H}_1 must be perpendicular to the external field \mathbf{H}_0 . For convenience, \mathbf{H}_1 is taken along z-direction.

The transition probability between two states $|i\rangle$ and $|f\rangle$ can be written as :

$$P_{if} = \frac{|\langle f|\beta H_1 g S|i\rangle|^2}{4\hbar^2} f(\nu - \nu_{if}) \quad (5)$$

with $f(\nu - \nu_{if})$ is the lineshape function, ν_{if} is the resonance frequency and H_1 is magnetic field amplitude of the radiation.

The lineshape function is expressed here in frequency. For experimental reasons, however, the microwave frequency is usually held constant in EPR experiment and the magnetic field is swept linearly. So, we must substitute the lineshape function $f(\nu - \nu_{if})$ by an another equivalent function F expressed in the terms of the magnetic field [20]

$$F(H - H_r) = \frac{2\Delta H}{\pi(\Delta H^2 + (H - H_r)^2)} \quad (6)$$

where ΔH is the full width at half intensity and H_r represents the resonance field.

F is related to f by the relation [21]:

$$f(\nu - \nu_{if}) = \left| \frac{\partial H_r}{\partial \nu} \right| F(H - H_r) \quad (7)$$

Combining relations (5) and (7), the transition probability becomes :

$$P_{if} = \frac{|\langle f|\beta H_1 g S|i\rangle|^2}{4\hbar^2} \left| \frac{\partial H_r}{\partial \nu} \right| F(H - H_r) \quad (8)$$

3. Results and Discussion

Recall that, the ESR spectra of unirradiated and X-irradiated sample were recorded at room temperature with the exposition period of 12 h 30 min [15]] by EMS 104 (BRUKER), (X-band) spectrometer [16].

In figures 1 and 2, we show the simulation results of ESR spectra compared by experimental ones. The shape of the measured spectra after irradiation is comparable to those relative to the paprika [17] or red pepper [18] samples γ -irradiated.

The classical analysis [19] using the macroscopic equations gives an excellent approach to magnetic resonance, particularly because it gives a simple physical picture. It is rather less applicable to electronic paramagnetic than to nuclear paramagnetic substances because the case where the only major interaction is that with the external applied field tends to be the exception rather than the rule.

This approach is valid for a simple system, such as an atom with an electronic but no nuclear magnetic moment, or vice versa

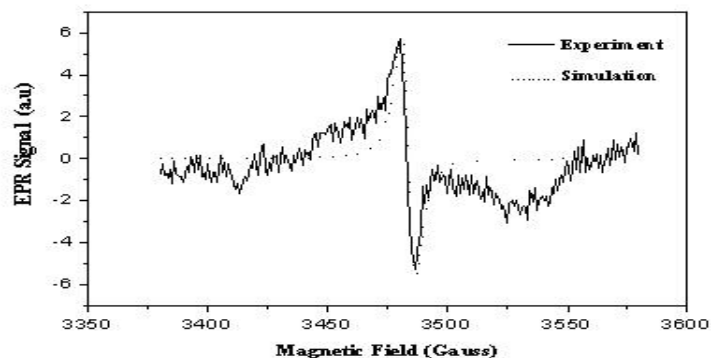


Fig. 1 ESR spectra before irradiation at room temperature

For a complex system such as an atom with hyperfine structure the semi-classical approach is not valid. In this circumstance a quantum mechanical approach is essential, and the resonance spectrum can only be interpreted in terms of spin Hamiltonian. The interaction considered in our simulation program for the ginger sample is the electronic Zeeman interaction which is the interaction of the magnetic moment of the electron with the externally applied magnetic \mathbf{H}_0 .

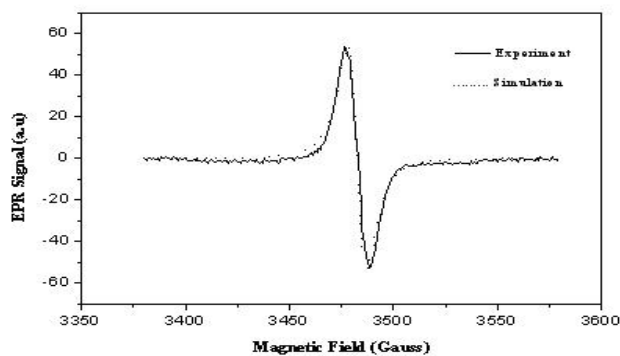


Fig. 2 ESR spectra 6 hours after irradiation at room temperature

We notice that the EPR spectra obtained by simulation are in good agreement with the experimental ones notably after irradiation. The parameters for the spectra simulation calculations shown in fig. 1 and 2 are given in Table 1.

<i>Spectral parameters</i>	<i>Before irradiation</i>	<i>After Irradiation</i>	<i>References</i>
<i>g – values</i>	2,0032	2,0028	[15]
<i>g – values</i>	2,0033	2,0029	<i>our parameters</i>
<i>Resonance field (G)</i>	3483,17	3482,69	<i>our parameters</i>

Table 1. Simulation parameters of ginger sample at room temperature.

3. Conclusion and Perspectives

In this work, we are concerned with simulation, based on quantum approach, of ESR spectra of ginger before and after X-irradiation. The ESR spectra are generated basically by finding the values of the magnetic field H_r at which, at a given value of the microwave frequency ν , there is a transition between energy levels. At that value, a line is produced by a lineshape function, typically Gaussian or Lorentzian. We determined the values of the spin Hamiltonian parameters for which the calculated spectrum best matches the observed spectrum. These parameters are not usually critical to the identification of the radicals that are present in irradiated foodstuffs.

The work concerned with simulation of the spin trap ESR (electron paramagnetic resonance) spectra is in progress. .

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