



## Study of Solid-State Radiolysis of Behenic, Fumaric, and Sebacic Acids for their Possible Use as Gamma Dosimeters Measured Via ATR-FT-IR Spectroscopy

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### ABSTRACT

The intensive use of ionizing radiation has promoted the constant investigation of adequate dosimetric systems in the measurement of doses applied in irradiated products. The objective of this work is to propose gamma dosimetric systems, using carboxylic acids in a solid state and measuring the change via infrared spectroscopy (carboxylic acid/ATR-FT-IR<sup>1</sup>). We worked with three systems: (1) behenic acid/ATR-FT-IR, (2) sebacic acid/ATR-FT-IR, and (3) fumaric acid/ATR-FT-IR. The change in absorbance corresponding to the stretching vibration frequency of the carbonyl group to the absorbed dose (in the range of kGy) was measured. The results showed that the acid/ATR-FT-IR systems have a linear response with respect to the absorbed dose, for behenic acid/ATR-FT-IR from 0 to 122 kGy, for ATR-FT-IR sebacic acid from 0 to 61 kGy, and for fumaric acid/ATR-FT-IR from 0 to 34 kGy. The results indicated that the linear response of the absorbance dose in the three systems allows us to continue studying other variables to be able to propose them as chemical dosimeters.

## 1. Introduction

Different chemical dosimetry systems have been proposed. The most popular is the Fricke dosimeter, measured via UV-VIS spectrophotometry at 304 nm [1]. Other dosimeters are based on the use of amino acid films on PET<sup>2</sup> measured by EPR<sup>3</sup>, such as the alanine dosimeter [2] or the aspartic acid dosimeter [3]. However, no universal dosimeter exists due to the different physical and chemical variables of each dosimetric system—for example, temperature, sensitivity, linear response interval, analysis time, type of radiation, etc. For this reason, it is crucial to investigate diverse possible dosimetry systems to be able to measure doses in various circumstances. Several authors studied the stability of carboxylic acids against gamma radiation. Their primary decomposition in the solid state via gamma radiolysis is a decarboxylation reaction, forming a corresponding hydrocarbon with one fewer carbon atom and carbon dioxide (CO<sub>2</sub>) [4-5], with radiochemical yield G (CO<sub>2</sub>) values of about 3 [6]. The objective of this work is to propose dosimetric systems for gamma radiation using carboxylic acids, specifically behenic acid (C<sub>22</sub>H<sub>44</sub>O<sub>2</sub>), sebacic acid (C<sub>10</sub>H<sub>18</sub>O<sub>4</sub>), and fumaric acid (C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>), measuring in the signal corresponding to the carbonyl bond stretch (C = O)

monitored by ATR-FT-IR spectroscopy. For this purpose, the change in absorbance corresponding to the stretching of the carbonyl bond (C = O) was measured via ATR-FT-IR spectroscopy at 1700 cm<sup>-1</sup> for behenic acid, 1685 cm<sup>-1</sup> for sebacic acid, and 1660 cm<sup>-1</sup> for fumaric acid. The results indicated that carboxylic acid-ATR-FT-IR systems show a linear response to the dose of gamma radiation from Gy to the order of kGy at room temperature (20°C).

## 2. Experimental

### 2.1 Chemicals and Materials

The reagents used were purchased from Sigma-Aldrich® (USA) and were of a higher commercially available purity. To avoid contamination in the glass vials, they were treated with a hot mixture of HNO<sub>3</sub> and H<sub>2</sub>SO<sub>4</sub> for 30 minutes, followed by a wash with distilled water. Then, they were heated at 300 °C for 24 hours.

### 2.2 Irradiation of Samples

The gamma irradiation of the samples was carried out at room temperature with a dose rate of 170 Gy/min in a

“Gammabeam PT 651” irradiator equipped with a high-intensity  $^{60}\text{Co}$  source, at Instituto de Ciencias Nucleares, UNAM.

### 3. Analysis of Samples

#### 3.1 ATR-FT-IR

The analysis of the samples via infrared spectrometry was performed in a PerkinElmer® Spectrum 100 FT-IR spectrometer with ATR sampling operated by the Spectrum™ software v.10.0, in absorbance mode from 650 to 4000  $\text{cm}^{-1}$ , using 50-gauge pressure and 16 scan, at Instituto de Ciencias Nucleares, UNAM.

### 4. Results

The main pathway of decomposition in the solid-state gamma radiolysis of carboxylic acids was the decarboxylation reaction of the acid, forming as the main product hydrocarbon with one less carbon atom and  $\text{CO}_2$  [3].

#### 4.1 Behenic Acid

##### 4.1.1 Infrared spectroscopy analysis

Behenic acid ( $\text{C}_{21}\text{H}_{43}\text{COOH}$ ) is a monocarboxylic acid with a molecular weight of 340.59 g/mol characterized by infrared spectroscopy, mainly by bands at 2915 and 2850  $\text{cm}^{-1}$  that correspond to the frequency of stretching of the methylene group, and a band at 1700  $\text{cm}^{-1}$  that corresponds to the stretching frequencies of the carbonyl group (Figure 1). After the irradiation, the results showed a

linear dependence between the band intensity at 1700  $\text{cm}^{-1}$  with respect to the absorbed dose in a range of 0 to 120 kGy (Figure 2 and Figure 3).

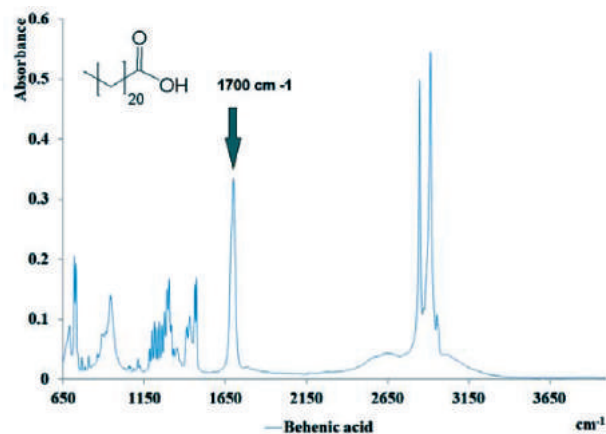


Figure 1. Infrared spectrum of behenic acid.

#### 4.2 Sebacic Acid

##### 4.2.1 Infrared spectroscopy analysis

Sebacic acid ( $\text{C}_{10}\text{H}_{18}\text{O}_4$ ) is a dicarboxylic acid with a molecular weight of 202.25 g/mol characterized by infrared spectroscopy, mainly by bands at 2915 and 2850  $\text{cm}^{-1}$  that correspond to the frequency of the stretching of the methylene group, and a band at 1685  $\text{cm}^{-1}$  that corresponds to the stretching frequencies of the carbonyl group (Figure 4). The results showed a linear dependence between band intensity at 1685  $\text{cm}^{-1}$  with respect to the absorbed dose in a range of 0 to 61 kG (Figure 5 and Figure 6).

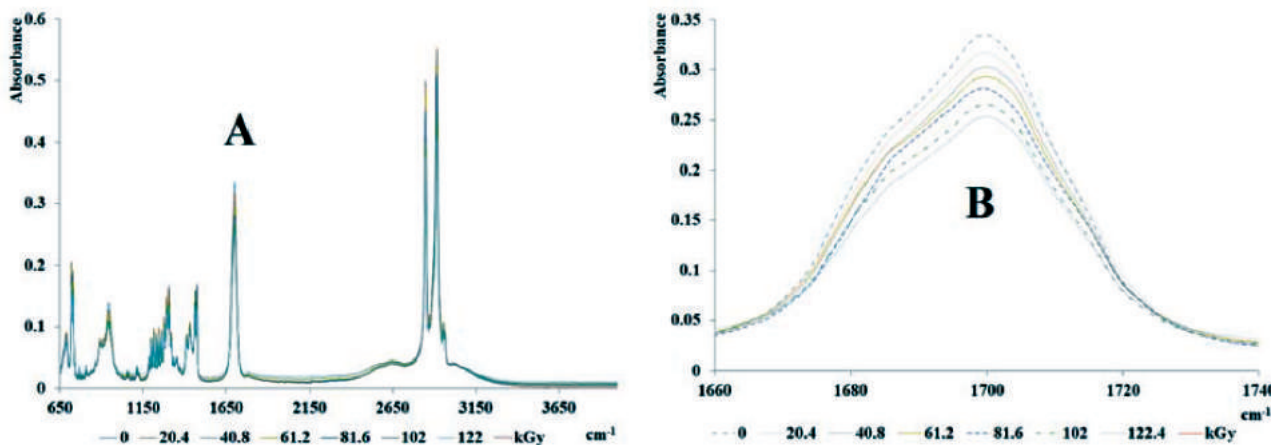


Figure 2. “A” corresponds to the infrared spectrums of behenic acid at various doses. “B” corresponds to the stretching band of the carbonyl group at 1700 $\text{cm}^{-1}$ .

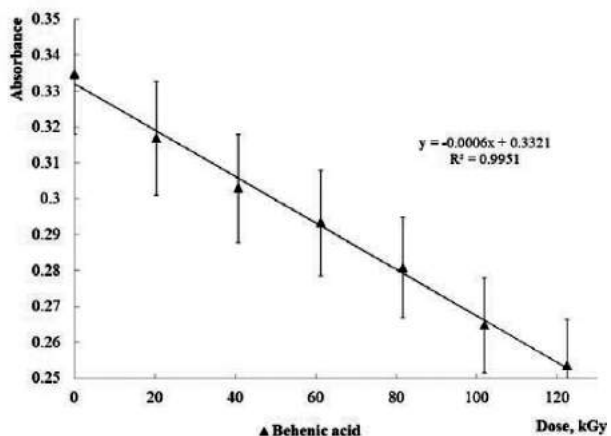


Figure 3. Relationship between the absorbance of the carbonyl group band and the absorbed dose.

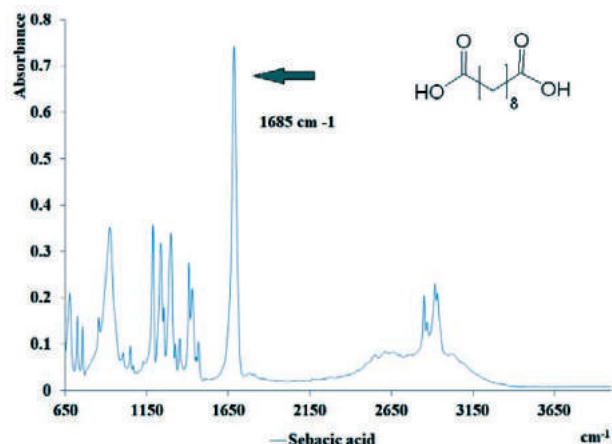


Figure 4. Infrared spectrum of sebacic acid.

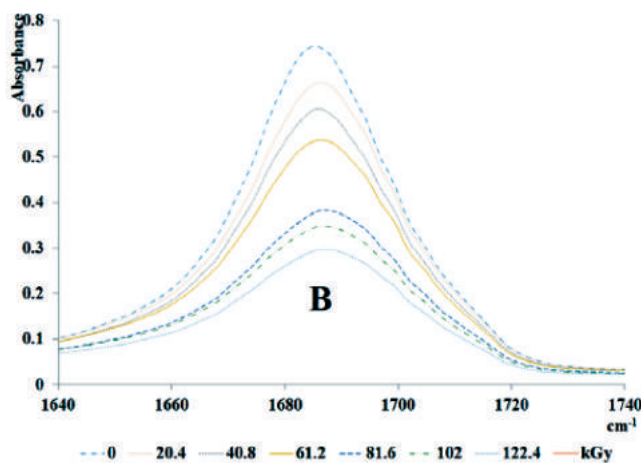
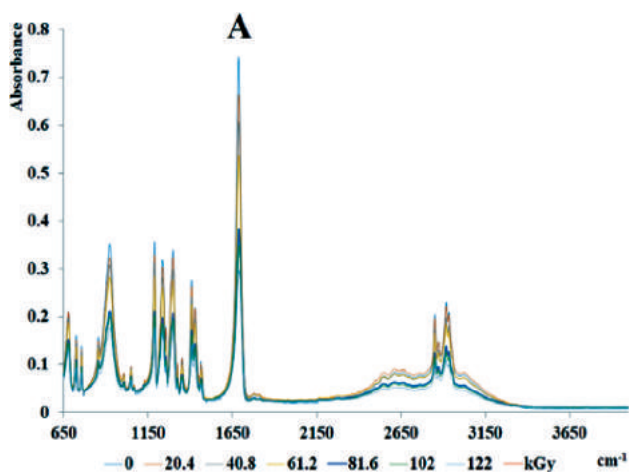


Figure 5. “A” corresponds to the infrared spectrums of sebacic acid at various doses. “B” corresponds to the stretching band of the carbonyl group at 1685cm<sup>-1</sup>.

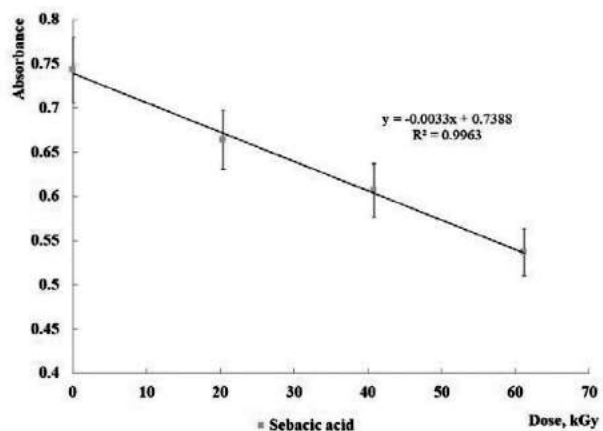


Figure 6. Relationship between the absorbance of the carbonyl group band and the absorbed dose.

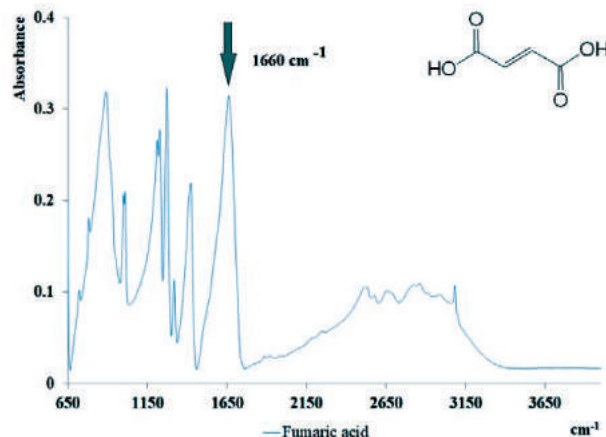


Figure 7. Infrared spectrum of fumaric acid.

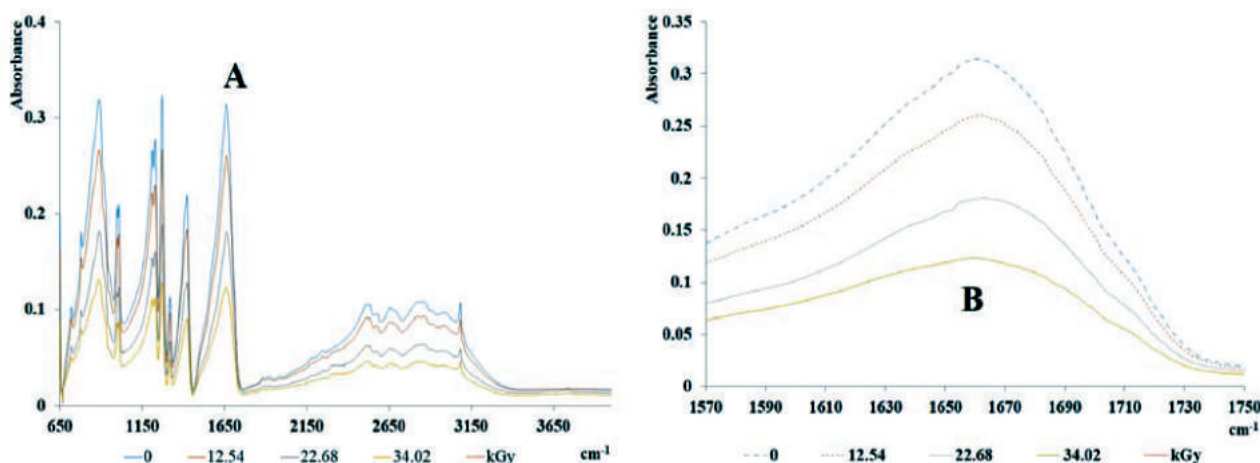


Figure 8. “A” corresponds to the infrared spectra of fumaric acid at various doses. “B” corresponds to the stretching band of the carbonyl group at 1660 cm<sup>-1</sup>.

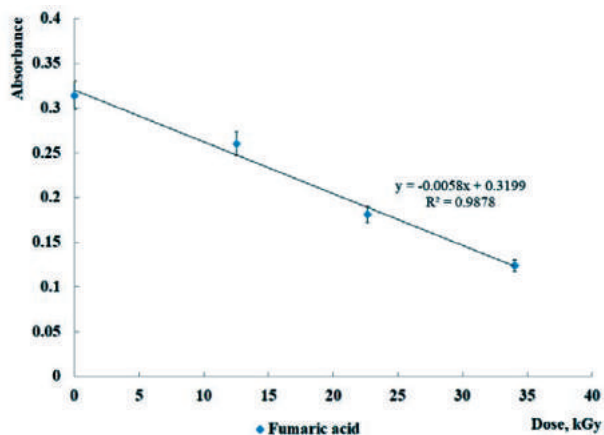


Figure 9. Relationship between the absorbance of the carbonyl group band and the absorbed dose.

### 4.3 Fumaric Acid

#### 4.3.1 Infrared spectroscopy analysis

Fumaric acid (C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>) is an unsaturated dicarboxylic acid with a molecular weight of 116.07 g/mol characterized by infrared spectroscopy, mainly by bands at 3150 cm<sup>-1</sup> that correspond to the frequency of stretch bond C-H sp<sup>2</sup>, and a band at 1665 cm<sup>-1</sup> that corresponds to the stretch frequencies of the carbonyl group. The results showed a linear dependence between band intensity at 1660 cm<sup>-1</sup> with respect to the absorbed dose in a range of 0 to 34 kG and Figure 6.

## 5. Remarks

The results indicated that the studied carboxylic acids show a linear response in different dose intervals up to the order

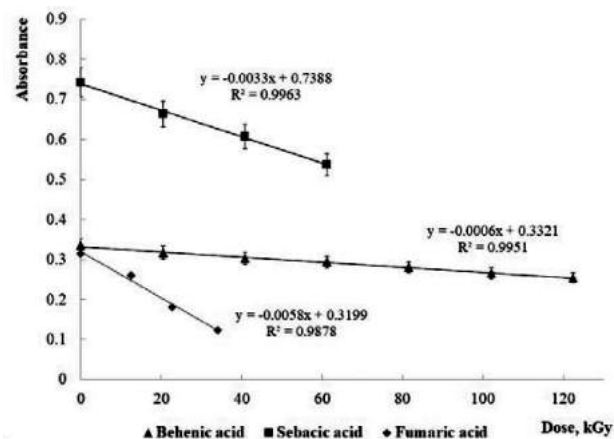


Figure 10. Range of linear response absorbance *vs* absorbed dose for various carboxylic acids.

of the kGy depending on the structure of the carboxylic acid (Figure 10), which suggests that these acids in conjunction with infrared spectroscopy can be proposed as a dosimetric systems for gamma radiation. However, more studies are still needed to determine if this system is independent of other physicochemical variables, such as dose intensity, temperature, etc.

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