



Identification of Commercial Sweetener (süssina) Components and Investigation of Aspartame and Saccharin Using Raman Spectroscopy

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Abstract: Artificial sweeteners are being used extensively especially by diabetes and obesity and have entered most of the food industries, some of them contain natural compounds, but they are low in sweetness. Others are classified as high in sweetness, which are dangerous and harmful to health because they contain chemical additives, which are still under study, also in markets there are pure sweeteners or sweeteners mixed with these industrial chemical additives. A selection of one common and commercially available table-top artificial Sweetener in Sudanese Markets (süssina) was considered. The study was conducted by using Raman spectroscopy Model Horiba LabRAM HR 3D to examine the components of these industrial chemicals additives in the normal situation and after heating at boiling point of water. The study showed the presence of sorbitol ($C_6H_{14}O_6$), a natural component of corn, Aspartame ($C_{14}H_{18}N_2O_3$) and saccharin ($C_7H_4NNaO_3S$) which are artificial chemical additives.

Keywords: Artificial Sweeteners, Natural Sweeteners, Laser Raman Spectroscopy

1. Motivation

Artificial sweeteners are functional food additives that impart sweetness in food. Also they are known as sugar substitutes, which contain zero-calorie or low-calorie. Uses of sweeteners, have largely increased in the past 20 years. Nowadays sweeteners occupy a large portion of commercial space on supermarkets worldwide. The use of these (zero calorie) sweeteners has increased dramatically these days particularly for diabetics, weight maintenance in food and drinks. The sweetening capacity of these artificial sweeteners ranging from hundreds to thousands of times more than that of the natural sugar [1-2].

Some of them contain natural compounds that include the monosaccharide polyols such as (sorbitol, sucrose, fructose...), but they are low in sweetness. Others are classified as high in sweetness that are actually artificial chemical additives include aspartame, acesulfame-K,

neotame, saccharin, sucralose, cyclamate, and alitame, which are dangerous and harmful to health, which are still under study [3].

Most artificial sweeteners are not metabolized by the body and are therefore considered safe. However, scientists disagree about safety because the metabolites of the "nonmetabolized" compounds have been shown to produce deleterious effects in mice, rats, and dogs [4].

The objective of this study is to investigate whether these sweeteners content industrial chemical additives or just natural ingredients or mixture of these components, which is important for food quality.

Because the most common use of these materials is in the daily tea, so the sample (süssina) was added to mineral water in the boiling point and after cooling to the room temperature HCl acid (pH 3.1) was added to detect the change that occurs in the composition of this substance when it enters intervention inside the stomach. (pH of HCl inside the

stomach range from 2 to 3.5) [5].

Several previous studies have been conducted to study the artificial sweeteners using another techniques such as FT-IR spectroscopy, surface enhanced Raman spectroscopy (SERS) to investigate saccharin, Aspartame, sorbitol accesulfame-k, xylitol, sodium cyclamate, Dextrose, Sucrose and Maltodextrin. [1, 2, 7-9, 12].

The obtained results from these previous studies have been also obtained in this study by using Raman spectroscopy.

Raman technique has proven that it is a precision technique with high efficiency and accuracy in Artificial sweeteners analysis and easy to use. Raman technique does not require any previous preparation; the analysis can be done on a small amount of sample (parts of the milligrams) whether the sample is liquid or dry, the analysis lasts short time within seconds Whereas the other techniques needs pre preparation to be processed also samples are needed in large quantities And longer time for analysis.

2. Raman Spectroscopy

Raman Effect or Raman phenomenon is defined as an inelastic scattering of Light by matter (Molecule). When a monochromatic wave (Laser light) is scattered by a matter, two types of interaction happens and result into two distinctive types of scattered light. One type of interaction does not involve energy transfer or exchange between the incident light and the matter (molecules), or atoms; of matter In This case the type of scattered light is elastic and referred to as Rayleigh scattering. This type of scattering is elastic in nature and referred to as Rayleigh scattering. The second type of interaction involves energy exchange between the incidents Light and the material (molecules) The scattered light will have a New frequency which is simply equal to the sum or the difference between the frequencies of the incident light and the natural frequency vibration of the material (molecules), in this case the scattering light is known as an inelastic, and is called Raman Effect [1].

Basic Consideration

Raman Effect is explained using the classical theory of scattering as follows; let us assume a monochromatic light wave Propagating with an oscillating electric field in the x direction, with amplitude E_x of an electric field at a time (t) can be expressed as follows;

$$E_x = E_x^0 \cos(2\pi\nu_0 t) \quad (1)$$

E_x^0 is the amplitude of the electric field component, ν_0 is the electromagnetic wave frequency (laser light). as an explanation we can consider a diatomic molecule (in this case it is a material) with a Vibration frequency ν_V it is called natural frequency with a normal vibration vector q_V can be expressed as a function of time as;

$$q_V = q_V^0 \cos 2\pi\nu_V t \quad (2)$$

When the electromagnetic wave (Laser light) interacts with the Molecule, electrons of the molecule will be

polarized by the laser light to induce a dipole moment (μ) where α is known as the polarizability in bellow equation;

$$\mu = \alpha E \quad (3)$$

The induced dipole will oscillate at three different frequencies as a result it will emit light (scattered light). These different frequencies can be identified by

Expanding the polarizability tensor (α) by the mathematical Taylor's series form for the component of (q_V) as;

$$\alpha = \alpha^0 + \left(\frac{d\alpha}{dq_V}\right) q_V + \dots \quad (4)$$

By substituting the above equations the dipole moment can be expressed as;

$$\mu = E_x^0 \alpha^0 \cos(2\pi\nu_0 t) + E_x^0 \left(\frac{d\alpha}{dq_V}\right)_0 q_V^0 \{ \cos[2\pi(\nu_0 - \nu_V)t] + [2\pi(\nu_0 + \nu_V)t] \} \quad (5)$$

The frequencies that, the scattered light will have are (ν_0), ($\nu_0 - \nu_V$), ($\nu_0 + \nu_V$) the scattered light at the same frequency (ν_0), there is no energy loss or gain due to interaction with the molecule and it is known as elastic scattering or Rayleigh scattering. The other two components would have experienced a gain or loss of energy equal to the energy of the molecular vibration; this is known as inelastic scattering or Raman scattering represented ($\nu_0 - \nu_V$), ($\nu_0 + \nu_V$) which are known as Stokes and anti-Stokes lines respectively and they are fundamentally important as a finger print for molecular vibrations frequencies figure 1 illustrates stokes and anti-stokes Raman scattering [1].

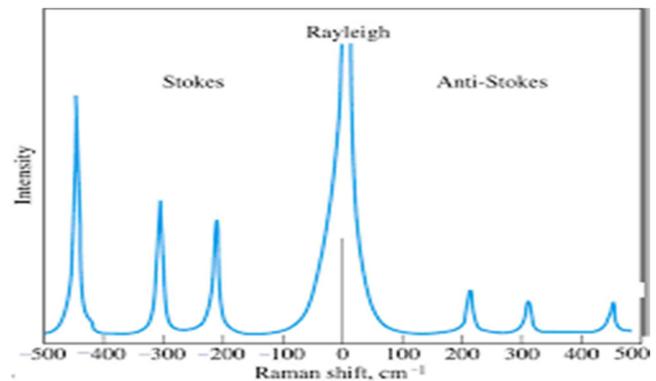


Figure 1. Stokes and anti-Stokes Raman scattering.

3. Materials & Methods

Two samples of commercial sweetener, (Süssina) were investigated in this work by laser Raman spectrometer in the Range from 50 cm^{-1} to 4000 cm^{-1} for both powder and solution.

3.1. Equipment

In this work laser Raman Microscope spectrometer Model Horiba Lab RAMHR 3D shown in the Figure 2 was used. The laser wavelength is 532 nm and output power of 6 mW.

The Raman shift in wave number, and the change in intensities of the scattered light were compared with data in the references and previous studies.

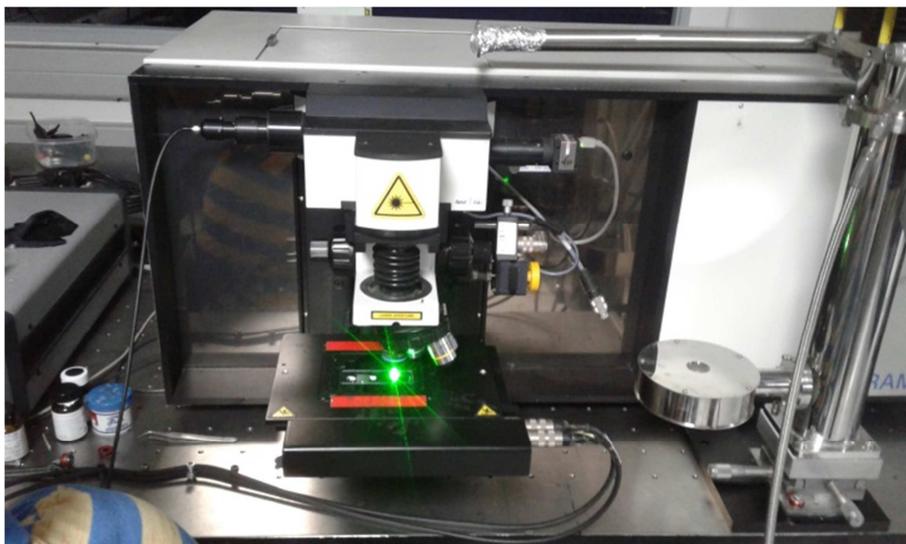


Figure 2. Schematic diagram of laser Raman microscope spectrometer.

3.2. Samples Preparation

Samples were prepared as follows:

Sample:

(a) (süssina) powder.

(b) 5g of (süssina) powder dissolved in a boiling mineral water (25 mL) 100C⁰ with HCl acid 5mL (PH 3.1)

4. Results & Discussion

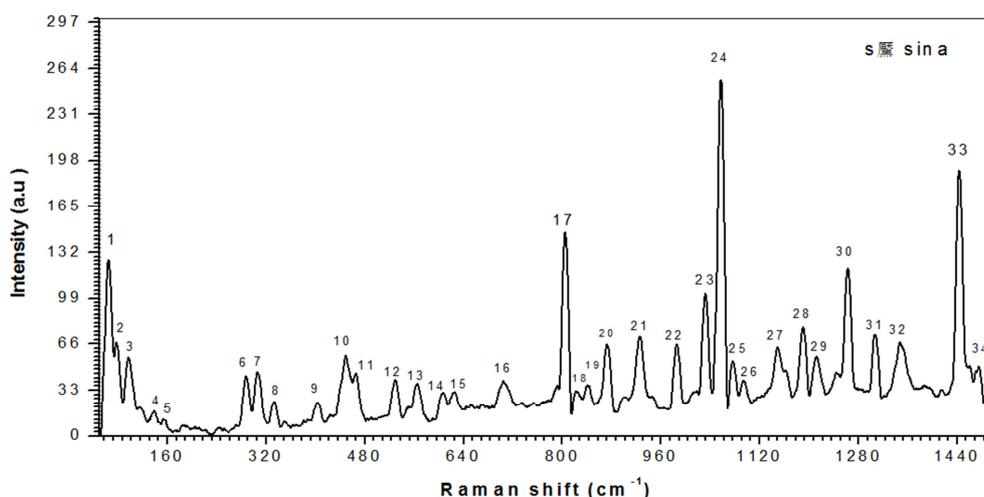


Figure 3. Raman spectrum of (süssina) powder in the range from 50 to 1500cm⁻¹.

Figure 3 illustrates Raman spectrum of the sample (süssina) in the range from 50 to 1500cm⁻¹.

Table 1 lists the main frequencies of the Raman spectra and the vibrational assignment.

Table 1. The analyzed data of Raman spectrum of (süssina) from 50 to 1500cm⁻¹.

| Peak NO | Raman shift (cm ⁻¹) | Assignment | Reference |
|---------|---------------------------------|-----------------------------|-----------|
| 1 | 67 | Skeldef | [6] |
| 2 | 78.2 | - | - |
| 3 | 97.3 | - | - |
| 4 | 140 | Stretching (O-Ag-O) | [6] |
| 5 | 153.7 | - | - |
| 6 | 288 | C-CH ₃ sci | [10] |
| 7 | 306 | Torsion (N ₂ OH) | [11, 9] |
| 8 | 334 | - | - |

| Peak NO | Raman shift (cm ⁻¹) | Assignment | Reference |
|---------|---------------------------------|--|------------|
| 9 | 405 | -- | - |
| 10 | 451.4 | β OCC + γ NCCC | [8] |
| 11 | 467.3 | - | - |
| 12 | 530 | C – CL | [12] |
| 13 | 566 | Amide VI | [13] |
| 14 | 608.5 | - | - |
| 15 | 622.4 | Aryl ring deformation and C–H bending | [2] |
| 16 | 711 | Skeleton deformation | [2] |
| 17 | 805 | O-P-O | [14] |
| 18 | 843 | C – O – C | [12] |
| 19 | 818 | Aryl C–H wagging | [2] |
| 20 | 876 | Skeletal vibration and C–H twisting | [2, 7] |
| 21 | 919.5 | C–H bending and C–C stretching | [1] |
| 22 | 982 | melamine | [9] |
| 23 | 1034 | mannitol | [2, 7] |
| 24 | 1054 | Ring Stretching sodium saccharin | [15] |
| 25 | 1093.3 | C–C stretching and O–H bending | [2, 7] |
| 26 | 1154 | Aryl ring deformation and C–H bending C–C stretching | [2, 9] |
| 27 | 1196 | ν OC + β HOC+ β HNC+ β HCC | |
| 28 | 1210 | amide III | [9] |
| 29 | 1267.4 | C–H symmetric rock | [9] |
| 30 | 1300 | C–N stretching and C–H bending | [9, 2] |
| 31 | 1360 | C3H, C ₂ H ₂ | [6, 9, 16] |
| 32 | 1445 | C–C stretching | [13] |
| 33 | 1475 | ν (CC) stretching vibrations ν (CN) in-plane vibrations | [7] |

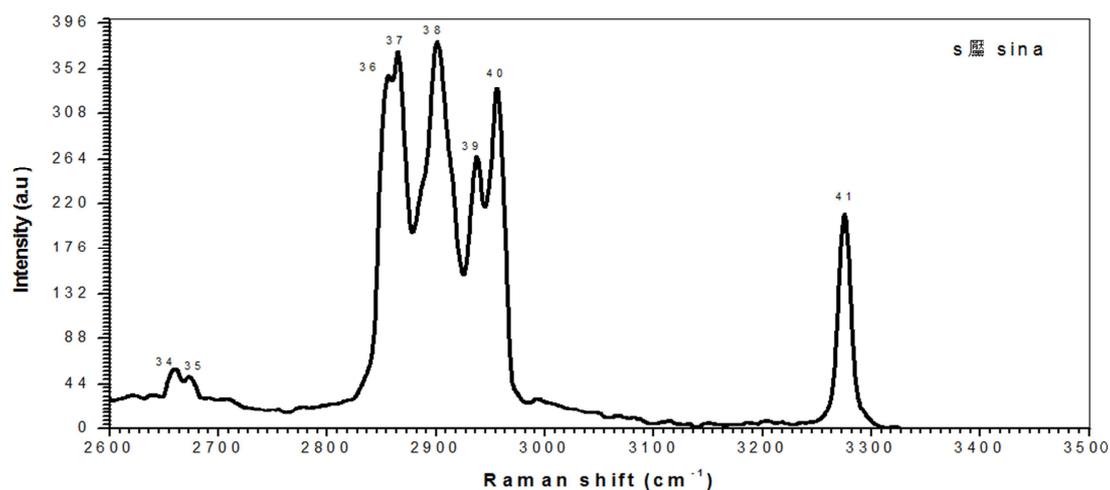


Figure 4. Raman spectrum of (süssina) powder in the range from 2600 to 3500 cm⁻¹.

Figure 4 illustrates Raman spectrum of the sample (süssina) frequencies of the Raman spectra and the in the range from 2600 to 3500cm⁻¹. Table 2 lists the main vibrational assignments.

Table 2. The analyzed data of Raman spectrum of (süssina) from 2600 to 3500cm⁻¹.

| Peak NO | Raman shift (cm ⁻¹) | Intensity (au) | Assignment | Reference |
|---------|---------------------------------|----------------|---------------|-----------|
| 34 | 2677 | 60.8 | H-bonds | [9] |
| 35 | 2673.1 | 52.3 | H-bonds | [6, 9] |
| 36 | 2852 | 347.4 | ν CH | [8] |
| 37 | 2864 | 370.4 | - | - |
| 38 | 2885 | 380 | (O–H stretch) | [11, 17] |
| 39 | 2936 | 267 | - | - |
| 40 | 2952 | 333.1 | ν CH | [8] |
| 41 | 3276.1 | 210.8 | Alkyne | [12] |

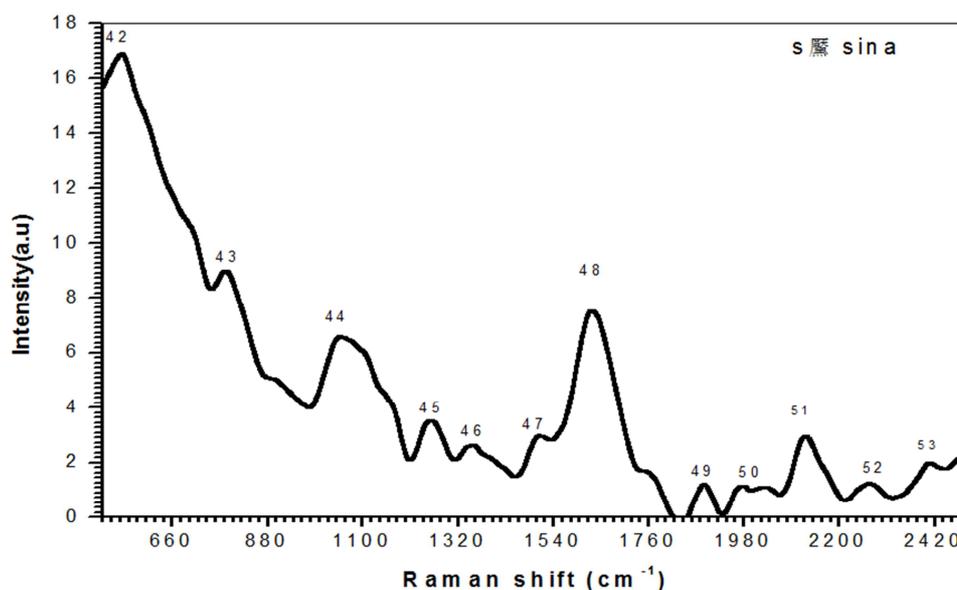


Figure 5. Raman spectrum of dissolved (süssina) in boiling mineral water and HCl acid (PH 3.1) in the range from 500 to 2500 cm^{-1} .

Figure 5 illustrates Raman spectrum of the dissolved (süssina) in the range from 500 to 2500 cm^{-1} . Table 3 lists the main frequencies of the Raman spectra and the vibrational assignments.

Table 3. The analyzed data of Raman spectrum of the dissolved (süssina) from 500 to 2500 cm^{-1} .

| Peak NO | Raman shift (cm^{-1}) | Intensity (au) | Assignment | Reference |
|---------|----------------------------------|----------------|--------------------------------------|-----------|
| 42 | 540 | 16 | disulphide bridges | [9] |
| 43 | 785 | 9 | twist CH_3 | [10] |
| 44 | 1056 | 6 | C–O stretching and O–H bending | [2] |
| 45 | 1271 | 3 | Torsion HCCN + torsion HCCO | [8, 6] |
| 46 | 1350 | 2.6 | - | - |
| 47 | 1513 | 3 | lycopene | [9] |
| 48 | 1632 | 7 | Asymmetric NH_2 deformation | [13] |
| 49 | 1899 | 1.1 | C = C | [12] |
| 50 | 2121 | 1.2 | sothiocyanate | [12] |
| 51 | 2275 | 2.9 | - | - |
| 52 | 2413 | 1.3 | - | - |
| 53 | 2408 | 2 | - | - |

5. Discussion

Through the analysis of the two samples it was found that some of the vibration modes of the sweetener s appeared as follows:

- 1 Vibrations modes of (süssina powder) at (876.0 very strong, 1056.0, 1093.0, 1134.0) cm^{-1} , which were attributed to the Sorbitol ($\text{C}_6\text{H}_{14}\text{O}_6$).
- 2 Vibrational modes of the powder (süssina) at (622.4, 818.0) cm^{-1} are attributed to the Aspartame ($\text{C}_{14}\text{H}_{18}\text{N}_2\text{O}_3$).
Vibrational modes at (711.0, 1032, 1154.0, 1300.0) cm^{-1} are attributed to Saccharin ($\text{C}_7\text{H}_4\text{NNaO}_3\text{S}$).
- 3 In the dissolved sample vibrational modes at (540, 1513, 2121) cm^{-1} are attributed to disulphide bridges, lycopene and sothiocyanate respectively.

6. Conclusion

The results presented in this work show that

Ramanspectroscopy technique is an efficient method to identify the compositions of the artificialsweeteners. It provides precise information about components found in the two samples of the commercial sweeteners.

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