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Physical, Thermal and Spectral Properties of Biofield Treated 1,2,3-Trimethoxybenzene

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Abstract

Study background: 1,2,3-Trimethoxybenzene is an important compound used for the synthesis of chemicals and pharmaceutical agents. The objective of this study was to investigate the influence of biofield energy treatment on the physical, thermal and spectral properties of 1,2,3-trimethoxybenzene.

Methods: The study was performed by dividing the sample into two groups (control and treated). The control group remained as untreated, while the treated group received Mr Trivedi's biofield energy treatment. The control and treated 1,2,3-trimethoxybenzene samples were then characterized by X-ray diffraction (XRD), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), Fourier transform infrared (FT-IR) spectroscopy, and ultra violet-visible spectroscopy (UV-Vis) analysis.

Results: XRD studies revealed the significant increase in crystallite size of treated sample by 45.96% as compared to the control sample. DSC analysis showed a decrease in melting temperature of the treated sample (45.93°C) with respect to control (46.58°C). Additionally, the substantial change was evidenced in latent heat of fusion of treated sample by 64.18% as compared to the control. TGA analysis indicated a decrease in maximum thermal decomposition temperature (T_{max}) of treated sample (151.92°C) as compared to the control sample (154.43°C). This indicated the decrease in thermal stability of the treated sample as compared to the control. FT-IR spectroscopic analysis showed an increase in the frequency of C-O bond in treated sample (1105→1174 cm^{-1}) as compared to the control sample. However, UV analysis showed no changes in absorption peaks in treated sample as compared to the untreated sample.

Conclusion: Overall, the result indicated that biofield energy treatment has altered the physical, thermal and spectral properties of the treated sample as compared to control. Hence, the treated sample could be used as an intermediate in the synthesis of organic compounds.

Keywords: X-ray diffraction; Thermal analysis; Fourier transform infrared (FT-IR) spectroscopy; Ultra violet-visible spectroscopy (UV-Vis) analysis

Abbreviations: XRD: X-ray diffraction; DSC: Differential scanning calorimetry; TGA: Thermogravimetric analysis; FT-IR: Fourier transform infrared; UV-Vis: Ultra Violet-Visible spectroscopy analysis; CAM: Complementary and alternative medicine

Introduction

Benzene-based compounds are used as an intermediate for the synthesis of pesticides and other chemicals. Methoxybenzene derivatives such as anisole (methoxybenzene) and veratrole (1,2-dimethoxybenzene) are widely used in perfumes, insect pheromones, pharmaceuticals [1] and synthesis of organic compounds [2]. 1,2,3-Trimethoxybenzene is an organic compound with excellent physical properties due to its interesting chemical structure [3]. It has been used to study the effect of solvent on photo-induced electron transfer reactions [4]. 1,2,3-Trimethoxybenzene was used as an intermediate for the synthesis of 2,4-diamino-5-benzylpyrimidines and analogues for antimicrobial applications [5]. However, 1,2,3-trimethoxybenzene based compounds are potentially toxic in nature and causes enormous health problems. These compounds are found in many hazardous waste sites that have been proposed for inclusion in the environmental protection agency (EPA) national priority list [6]. The distribution and degradation of the chemicals entirely depend on physicochemical properties of the chemicals. These properties are namely molecular weight, solubility, volatilization, and polarity [7,8]. It was reported that by improving volatilization of the chemicals it might accelerate the degradation by reacting with photochemically-produced free radicals [9]. Chakraborty *et al.* used

anaerobic degradation of benzene derivatives by *Dechloromonas* strain [10]. However, these methods are not cost effective. Thus, some alternate strategies should be designed which can increase the degradation of 1,2,3-Trimethoxybenzene, ultimately it might reduce the health problems associated with this compound. Recently, biofield energy treatment was used as potential strategy to alter the physical, chemical and thermal properties of metals [11,12], ceramic [13], organic compounds [14,15], and organic products [16,17]. Therefore, authors planned to investigate the influence of biofield energy treatment on physical, thermal and spectral properties of 1,2,3-trimethoxybenzene.

The National Centre for Complementary and Alternative Medicine (NCCAM), which is a part of the National Institute of Health (NIH), endorses the use of Complementary and Alternative Medicine (CAM) therapies as an alternative in the healthcare sector, and about 36% of Americans regularly uses some form of CAM [18]. CAM includes numerous energy-healing therapies; biofield therapy is one of the energy medicine used worldwide to improve overall health.

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Researchers have shown that when atoms undergo any translation, vibration, rotation and quantifiable motion a measurable electromagnetic radiation is generated which is evident by acoustic or vibrational spectroscopy [19]. Likewise, the cells present in the human body are consisting of the electron, proton, neutron and fundamental particles that always remain in a state of vibratory motion [19]. Additionally, neurons that are present in the human central nervous system have the ability to transmit the information in the form of electrical signals [20-23]. Thus, human biofield is referred as an energetic field or matrix that surrounds the human body. This energetic field is identical to superhighway that allows DNA in our cells to communicate faster than light and maintain coherent, holistic intelligence in the organism [24]. Therefore, it is envisaged that human beings have the ability to harness the energy from the environment/ Universe and can transmit into any object (living or non-living) around the Globe. The object(s) will always receive the energy and responding in a useful manner that is called biofield energy. Mr Trivedi is known transform the characteristics of various living and non-living things using his unique biofield energy. This biofield energy treatment is also known as 'The Trivedi Effect'. It is known to alter phenotype characteristics of microbes [25,26] and improved the growth and anatomical characteristics of medicinal plants [27,28].

After considering the potential of biofield energy treatment and chemical properties of 1,2,3- trimethoxybenzene, this study was conducted to investigate the influence of this treatment on physical, thermal and spectral properties of the compound.

Materials and Methods

1,2,3-Trimethoxybenzene was procured from S D Fine Chemicals Ltd., India. The sample was divided into two parts; one was kept as a control sample while the other was subjected to Mr Trivedi's unique biofield energy treatment and coded as treated sample. The treated group was in sealed pack and handed over to Mr Trivedi for biofield energy treatment under standard laboratory conditions. Mr Trivedi has given the energy treatment through his energy transmission process to the treated samples without touching the sample. The control and treated samples were characterized by X-ray diffraction, Differential scanning calorimetry, Thermogravimetric analysis, Fourier transform infrared spectroscopy, and Ultra violet-visible analysis.

Characterization

X-ray diffraction (XRD) study: The XRD analysis of control and treated 1,2,3-trimethoxybenzene were carried out using Phillips, Holland PW 1710 X-ray diffractometer system, which contains a copper anode with nickel filter. The radiation of wavelength used by the XRD system was 1.54056 Å. The XRD results obtained were presented in the form of a chart of 2θ vs. intensity. The average crystallite size (G) was calculated by using formula:

$$G = k\lambda / (b \cos\theta)$$

Here, λ is the wavelength of radiation used; b is full-width half-maximum (FWHM) of peaks and k is the equipment constant (=0.94). Percentage change in average crystallite size was calculated using following formula:

$$\text{Percent change in average crystallite size} = [(G_t - G_c) / G_c] \times 100$$

Where, G_c and G_t are the average crystallite size of control and treated powder samples respectively.

Differential scanning calorimetry (DSC): The control and treated 1,2,3-trimethoxybenzene samples were analysed using a Pyris-6 Perkin

Elmer DSC at a heating rate of 10°C/min under air atmosphere, and the air was flushed at a flow rate of 5 mL/min. Predetermined amount of sample was kept in an aluminium pan and closed with a lid. A blank aluminium pan was used as a reference. The percentage change in latent heat of fusion was calculated using following equations:

$$\% \text{ change in Latent heat of fusion} = \frac{[\Delta H_{\text{Treated}} - \Delta H_{\text{Control}}]}{\Delta H_{\text{Control}}} \times 100$$

Where, $\Delta H_{\text{Control}}$ and $\Delta H_{\text{Treated}}$ are the latent heat of fusion of control and treated samples, respectively.

Thermogravimetric analysis-Differential thermal analysis (TGA-DTA): The thermal stability of control and treated 1,2,3-trimethoxybenzene were analysed by using Mettler Toledo simultaneous TGA and Differential thermal analyser (DTA). The samples were heated from room temperature to 400°C using a heating rate of 5°C/min under air atmosphere.

FT-IR spectroscopy: The FT-IR spectra were recorded on Shimadzu's Fourier transform infrared spectrometer (Japan) with the frequency range of 4000-500 cm^{-1} . The analysis was accomplished to evaluate the effect of biofield treatment at an atomic level like dipole moment, force constant and bond strength in chemical structure [29]. The treated sample was divided into two parts T1 and T2 for FT-IR analysis.

UV-Vis spectroscopic analysis: UV spectra of the control and treated 1,2,3-trimethoxybenzene samples were acquired on Shimadzu UV-2400 PC series spectrophotometer with 1 cm quartz cell and a slit width of 2.0 nm. Methanol was used as a solvent and the analysis was carried out using wavelength in the range of 200-400 nm. The UV spectra were analysed to determine the effect of biofield treatment on the energy gap of highest occupied molecular orbital and lowest unoccupied molecular orbital (HOMO-LUMO gap) [29]. The treated sample was divided in two parts T1 and T2 for the analysis.

Results and Discussions

X-ray diffraction

The XRD was used to investigate the crystalline nature of control and treated 1,2,3-trimethoxybenzene sample. The XRD diffractogram of control and treated 1,2,3-trimethoxybenzene are presented in Figure 1. XRD diffractogram of control 1,2,3-trimethoxybenzene showed intense crystalline peaks at 2θ equal to 13.05°, 13.29°, 13.54°, 19.54°, 21.67°, 22.75°, 25.55°, 25.77°, 26.78° and 27.20°. Whereas, the treated 1,2,3-trimethoxybenzene also showed XRD peaks at 2θ equal to 13.50°, 13.68°, 19.24°, 22.99°, 26.03°, 27.09° and 27.31°. The comparative evaluation of the XRD diffractograms showed the decrease in intensity of XRD peaks of treated samples with respect to the control. It is assumed that biofield energy treatment might disturb the long-range pattern of the 1,2,3-trimethoxybenzene molecules that led to a reduction in crystallinity of the sample.

The crystallite size of control and treated 1,2,3-trimethoxybenzene was computed using Scherrer formula, and data are depicted in Figure 2. The crystallite size is known as a group of molecules or atoms having orientation in the same plane. It was reported that crystallite size directly influences the materials properties, and it is one of the crystallographic parameters linked with the formation of dislocations and point defects in a crystal structure [30]. The crystallite size of control 1,2,3- trimethoxybenzene was 67.23 nm, and it was substantially increased up to 98.13 nm in the treated sample. The result indicated 45.96% increase in the crystallite size of treated compound as compared to the control sample. Pang and Bao reported that due

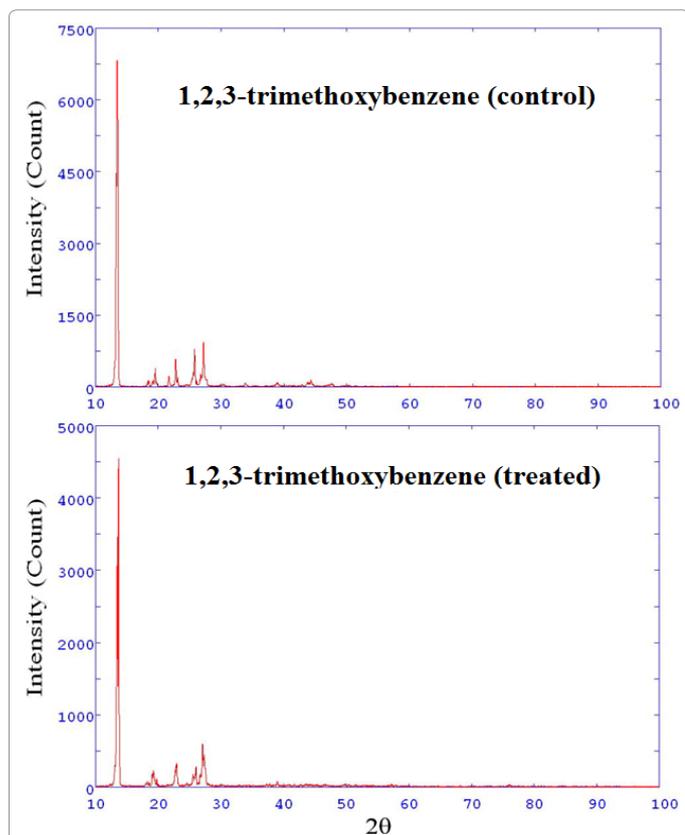


Figure 1: XRD diffractograms of control and treated 1,2,3-trimethoxybenzene.

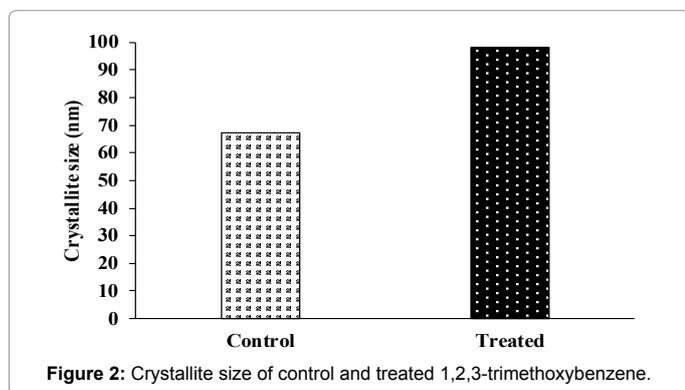


Figure 2: Crystallite size of control and treated 1,2,3-trimethoxybenzene.

to synthesis temperature and ripening on hydroxyapatite causes an increase in crystallite size [31]. Rey *et al.* [32] and Drouet *et al.* [33] reported an increase in crystal size with increase in temperature and pH. Hence, it is presumed here that biofield treatment might provide thermal energy to the treated 1,2,3-trimethoxybenzene atoms or molecules that lead to a reduction in dislocation density and increase in crystallite size as compared to the control. Carballo *et al.* reported that the rate of reaction can be significantly improved by an increase in crystallite size [34]. Thus, it is assumed that the increased crystallite size of treated 1,2,3-trimethoxybenzene might accelerate its reaction rate and percentage reaction yield during the synthesis of compounds. Additionally, the increased crystallite size can be correlated with increase in particle size and hence decrease solubility [35]. Hence, it is assumed that this might increase the volatilization leading to faster degradation of the treated sample as compared to control.

Thermal analysis

DSC study: DSC was used to investigate the latent heat of fusion and melting nature of the control and treated samples. DSC thermogram of control and treated 1,2,3-trimethoxybenzene are presented in Figure 3. The DSC thermogram of control 1,2,3-trimethoxybenzene showed a sharp endothermic inflexion at 46.58°C that was due to melting temperature of the sample. However, the treated 1,2,3-trimethoxybenzene showed an endothermic peak at 45.93°C. This indicated the decrease in melting temperature of the treated sample with respect to the control. It was reported that if the molecules contributing to a lattice are rigid, compact and symmetrical they tend to maximize the intermolecular interactions. Thus, a compound with less compact molecular arrangement has a low melting temperature than compactly arranged compound *i.e.*, more energy is needed to separate the molecules [36]. Hence, it is assumed that biofield treated sample might have a less compact arrangement that lead to the decrease in melting temperature.

The latent heat of fusion was computed from the DSC thermogram and data are presented in Table 1. The control compound showed a latent heat of fusion of 104.28 J/g and it was increased significantly to 171.21 J/g in the treated sample. The results indicated a significant increase in latent heat of fusion by 64.18% as compared to the control sample. The latent heat of fusion is considered as the energy required to overcome

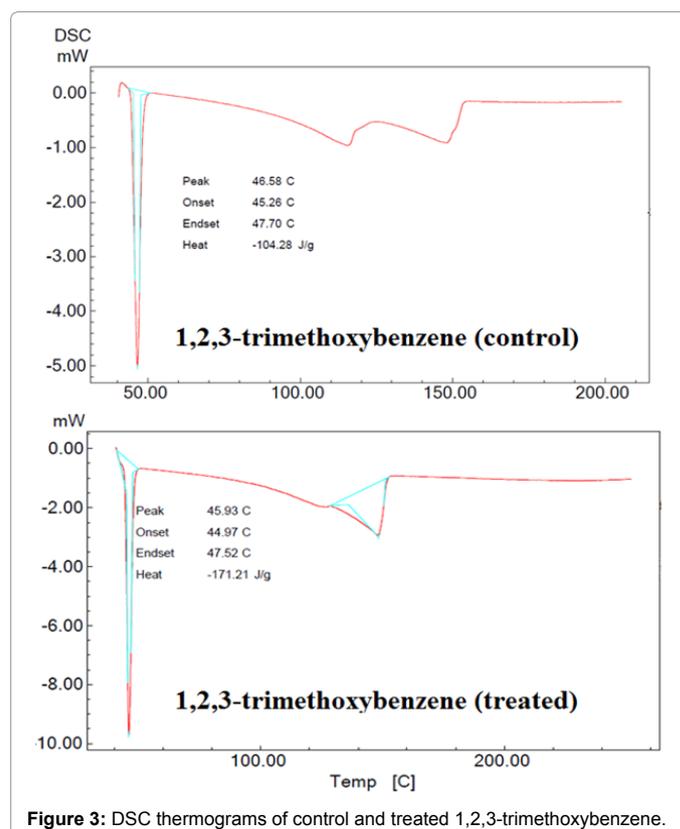


Figure 3: DSC thermograms of control and treated 1,2,3-trimethoxybenzene.

Parameter	Control	Treated
Latent heat of fusion ΔH (J/g)	104.28	171.21
Melting temperature (°C)	46.58	45.93
T_{max} (°C)	154.43	151.92
Weight loss (%)	53.93	57.04

Table 1: Thermal analysis data of control and treated 1,2,3-trimethoxybenzene. T_{max} : Maximum thermal decomposition temperature.

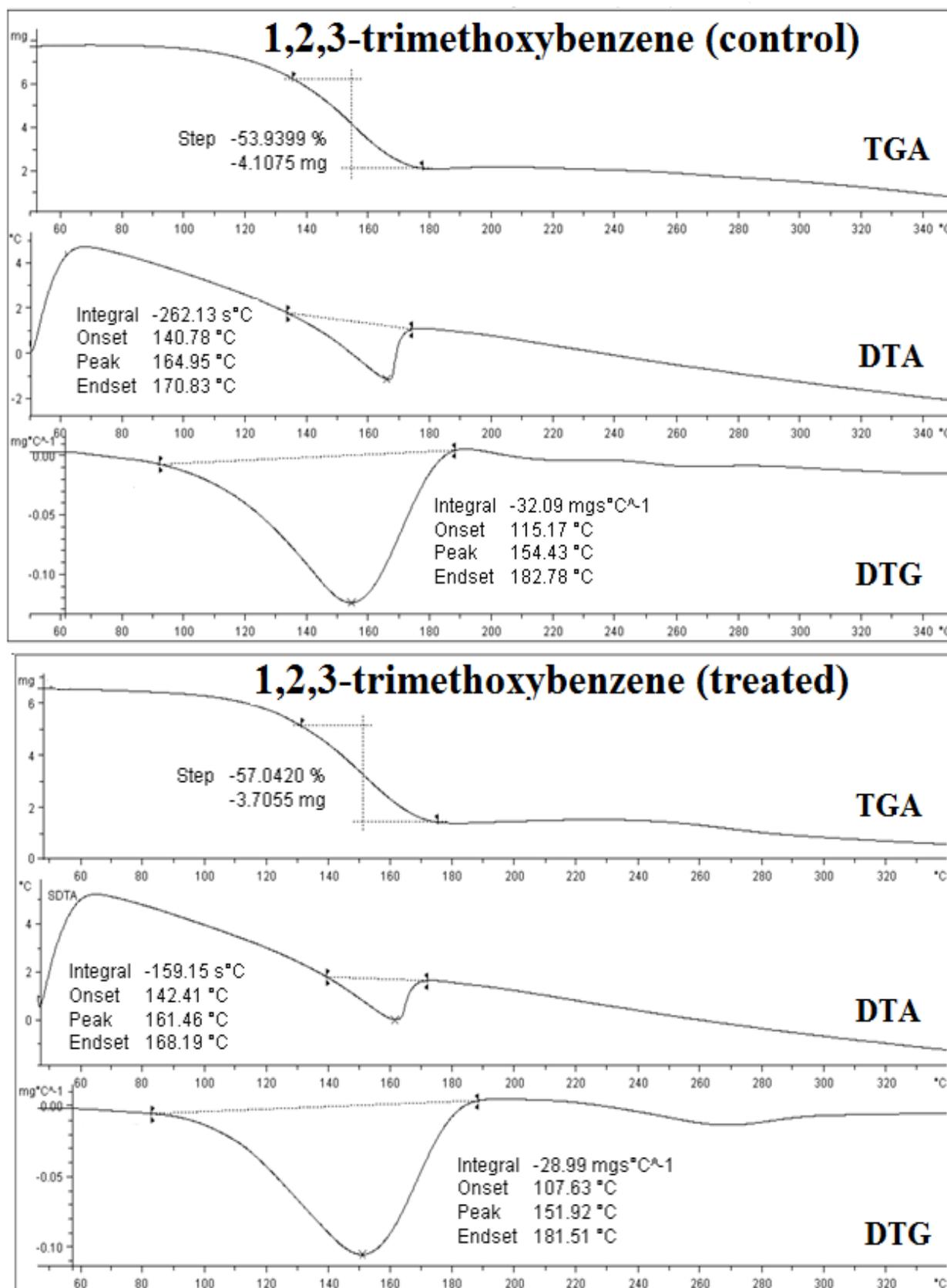


Figure 4: TGA thermograms of control and treated 1,2,3-trimethoxybenzene.

the intermolecular force exist between atoms or molecules during a phase change from solid to liquid. Thus, it is assumed that biofield energy treatment has possibly altered the intermolecular force between the 1,2,3-trimethoxybenzene molecules that led to substantial increase in latent heat of fusion. It was reported that benzene compounds have a high density as compared to alkanes and fatty acids. Moreover, these compounds form the solid solutions with the narrow gap between the solidus (temperature below which a substance is completely solid) and liquidus (temperature above which material is completely liquid) [37]. Thus, it allows obtaining required phase change material with desired melting temperature. Hence, stable melting temperature and high latent heat of fusion may confer better phase change nature to biofield energy treated 1,2,3-trimethoxybenzene.

TGA study: TGA analysis was used to investigate the thermal stability of control and treated 1,2,3-trimethoxybenzene samples. TGA thermogram of control and treated sample are depicted in Figure 4. The

TGA thermogram of control 1,2,3-trimethoxybenzene sample showed onset thermal degradation at around 137°C and it terminated at 178°C. During this thermal step, the control sample lost 53.93% of the initial weight. Nevertheless, the treated sample started the onset of degradation at 134°C, and the thermal degradation stopped at 176°C. The treated sample lost around 57.04% of its weight during this process. Hence, rapid thermal degradation was found in treated sample indicating the low thermal stability of the sample as compared to the control.

DTA thermogram of control and treated 1,2,3-trimethoxybenzene are presented in Figure 4. The DTA thermogram of control 1,2,3-trimethoxybenzene showed an endothermic peak at 164.95°C due to thermal decomposition of the sample. However, the treated sample showed a reduction in thermal decomposition temperature (161.46°C) as compared to the control.

This was further affirmed by DTG analysis of the samples. The rate of maximum thermal degradation (T_{max}) was recorded and data are

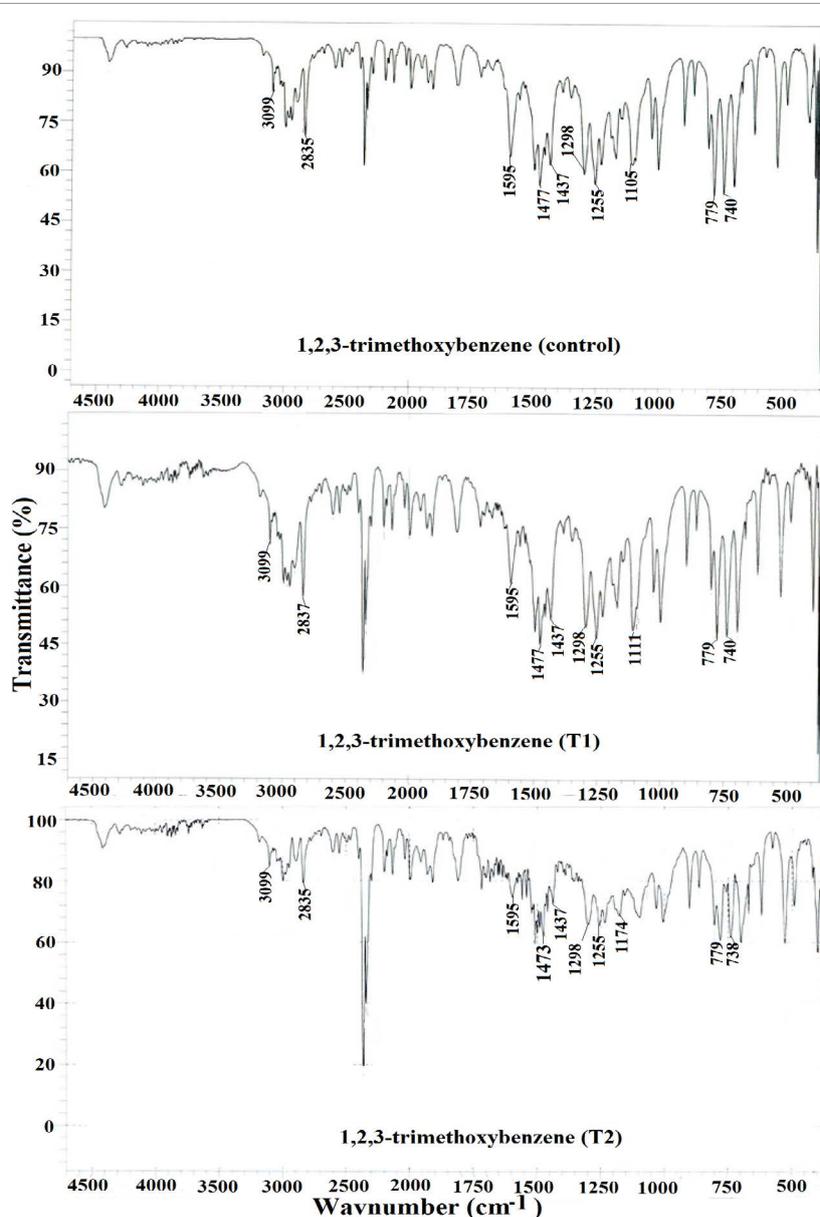


Figure 5: FT-IR spectra of control and treated 1,2,3-trimethoxybenzene (T1 and T2).

reported in Table 1. The control sample showed a T_{max} at 154.43°C, and it was decreased up to 151.92°C in the treated sample. Overall, the result showed that thermal stability of treated 1,2,3-trimethoxybenzene sample was decreased as compared to control. It is presumed that decrease in thermal stability might increase the volatilization of the treated sample. This may increase the vaporization and degradation of the treated sample in the environment as compared to control sample.

FT-IR spectroscopy

FT-IR spectra of control and treated 1,2,3-trimethoxybenzene samples are presented in Figure 5. The FT-IR spectrum of control and treated samples (T1 and T2) showed C-H aromatic stretching at 3099 cm^{-1} . Vibration peaks for methyl group stretching were observed at 2835 cm^{-1} in control and T2 sample; whereas in T1 sample it was evidenced at 2837 cm^{-1} . The $-C=C$ aromatic stretch was observed at 1595 cm^{-1} in the control and treated samples. The absorption peak in the region of 1105-1255 cm^{-1} were due to C-O stretch in the control 1,2,3-trimethoxybenzene sample. The T1 and T2 samples showed C-O stretching peak from 1111-1255 cm^{-1} and 1174-1255 cm^{-1} , respectively. The C-H asymmetric bending peaks were observed at 1437-1477 cm^{-1}

in control and T1 samples. Whereas, the T2 sample showed these bending peak in the region of 1437-1473 cm^{-1} . The C-H out of plane deformation peaks were observed in the region of 740-779 cm^{-1} in the control and T1 sample. However, in case of T2 sample the C-H out of plane bending vibrations were noticed at 738-779 cm^{-1} . Overall, the result showed an increase in frequency of the C-O bond 1105→1174 cm^{-1} in T2 sample as compared to the control sample. It was previously suggested that increase in the frequency of any bond causes a possible enhancement in force constant of the respective bond [29]. Hence, it is assumed that biofield energy treatment might altered the dipole moment or force constant of the C-O bond in treated 1,2,3-trimethoxybenzene sample as compared to the control sample.

UV-visible spectroscopy

UV spectra of control and treated 1,2,3-trimethoxybenzene are presented in Figure 6. The UV spectrum of control 1,2,3-trimethoxybenzene showed absorption peaks at 267 and 207 nm. The treated 1,2,3-trimethoxybenzene (T1) showed absorption peaks at 266 and 206 nm. Whereas the treated (T2) 1,2,3-trimethoxybenzene showed absorption peaks at 267 and 205 nm. The UV spectra of the treated 1,2,3-trimethoxybenzene showed no change in absorption

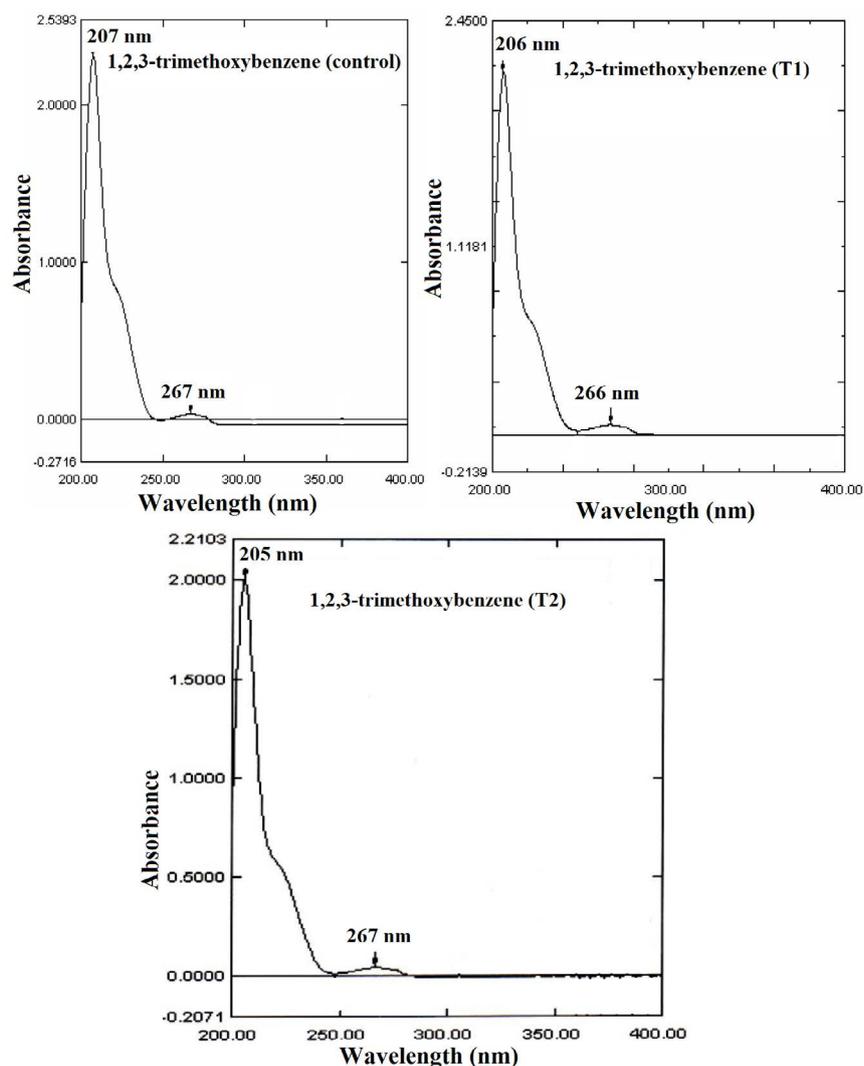


Figure 6: UV spectra of control and treated 1,2,3-trimethoxybenzene.

peaks as compared to the control. It is assumed that biofield energy treatment may not affect the energy gap of highest occupied molecular orbital and lowest unoccupied molecular orbital (HOMO-LUMO gap).

Though this was the first attempt to investigate the impact of biofield energy treatment on physicochemical properties of 1,2,3-trimethoxybenzene. However, future research will be conducted to elucidate the exact mechanism of biofield energy effect on physical, structural properties of the compound. Sophisticated analytical techniques such as NMR, GC-MS, and TGA-FTIR will be used to get further detailed insights about the structural/thermal changes in the biofield treated 1,2,3-trimethoxybenzene.

Conclusions

In summary, the XRD studies revealed the significant increase in crystallite size of treated 1,2,3-trimethoxybenzene as compared to the control. It is hypothesized that the biofield treatment might reduce the dislocation density that lead to the increase in crystallite size of the treated 1,2,3-trimethoxybenzene. DSC studies showed a substantial increase in latent heat of fusion of the treated sample by 64.18% as compared to the control sample. It was speculated that biofield energy might altered the intermolecular forces between the treated 1,2,3-trimethoxybenzene that leads to significant increase in latent heat of fusion. TGA analysis showed a decrease in T_{max} of treated sample as compared to the control sample. It showed the decrease in thermal stability of the treated sample as compared to the control. FT-IR spectroscopic analysis showed an alteration in C-O bond of the treated 1,2,3-trimethoxybenzene that might be due to changes in force constant or dipole moment. Overall, the result showed an alteration in physical, thermal and spectral properties of the treated 1,2,3-trimethoxybenzene. It is assumed that increased crystallite size and low thermal stability might improve the volatilization and fast degradation of the biofield treated sample as compared to the control sample.

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