https://doi.org/10.33805/2639-6734.106
Volume 1 • Issue 1 | Page 1 of 8

EDELWEISS PUBLICATIONS
OPEN ACCESS

Journal of Heterocyclics

Research Article ISSN: 2639-6734

Characterization of Physical, Thermal and Spectroscopic Properties of Biofield Treated Ortho-Toluic Acid

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Abstract

Toluic acid isomers are widely used as a chemical intermediate in manufacturing of dyes, pharmaceuticals, polymer stabilizers, insect repellent and other organic synthesis. The aim of present study was to evaluate the impact of biofield treatment on physical, thermal and spectroscopic properties of ortho isomer of toluic acid (OTA). The OTA sample was divided into two groups, served as control and treated. The treated group received Mr. Trivedi's biofield treatment. Subsequently, the control and treated samples were evaluated using X-ray diffraction (XRD), differential scanning calorimetry (DSC), thermogravimetric analysis/ derivative thermogravimetry (TGA/DTG), Fourier transform infrared (FT-IR) and ultraviolet-visible (UV-Vis) spectroscopy. XRD result showed 26.66% decrease in crystallite size in treated OTA sample as compared to control. Furthermore, DSC analysis result showed that latent heat of fusion was considerably reduced by 6.68% in treated OTA sample as compared to control. However, an increase in melting point was observed in treated sample. The melting point of treated OTA sample was found to be 107.96°C as compared to control (105.47°C) sample. Moreover, TGA/DTG studies showed that T_{max} (temperature, at which sample lost its maximum weight) was decreased by 1.21% in treated OTA sample as compared to control. It indicates that vaporisation of treated OTA sample might increase as compared to control. The FT-IR and UV-Vis spectra did not show any significant changes in spectral properties of treated OTA sample as compared to control. These findings suggest that biofield treatment has significantly altered the physical and thermal properties of OTA, which could make it more useful as chemical intermediate.

Keywords: Biofield Energy Treatment; *o*-Toluic Acid; X-Ray Diffraction Study; Differential Scanning Calorimetry; Thermogravimetric Analysis; Fourier Transform Infrared Spectroscopy; Ultraviolet-Visible Spectroscopy

Introduction

Toluic acids are closest homologues to benzoic acid. It is basically available in three isomeric forms *i.e.* ortho, meta, and para isomers. All three isomers are colourless and crystalline substances, which are virtually insoluble in water but soluble in organic solvents such as ethyl alcohol, diethyl ether etc. Toluic acids can be obtained from toluidines and oxidation of xylenes [1]. It is used as a raw material in the production of various pharmaceutical drugs as well as an additive to the nutrient medium which is used in cultivation of mold for production of benzylpenicillin [2].

The ortho isomer of toluic acid *i.e.* *o*-toluic acid (OTA) is used as an intermediate for polymer stabilizers and pesticides. It is also used in production of animal feed supplements and other organic chemicals like pharmaceuticals, pigments and dyestuffs. It is used as raw material in production of *o*-toluoyl chloride, *o*-tolunitrile etc. It is also used as intermediate in production of 5-iodo-2-methylbenzoic acid [3].

OTA is used as intermediate in various chemical reactions, where its rate of reaction plays a crucial role. Carballo *et al.* reported that rate of reaction in organic compounds can be controlled by modulating the crystallite size [4]. Since, OTA is generally used as chemical intermediate in various reactions, some alteration in its crystallite size and thermal stability may affect the reaction kinetics and ultimately the percentage yield of end product [5]. After considering the properties and applications of OTA, authors wanted to investigate an economically safe approach that could be beneficial in order to modify its physical and thermal properties.

Biofield is the name given to the electromagnetic field that permeates and surrounds

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Citation: Trivedi MK, Branton A, Trivedi D, Nayak G, Singh R, et al. (2016) Characterization of Physical, Thermal and Spectroscopic Properties of Bio field Treated Ortho-Toluic Acid. J O Heterocyclics 106: 21-28

Received: Oct 25, 2015
Accepted: Feb 20, 2016
Published: Feb 27, 2016

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living organisms [6]. It is scientifically termed as the biologically produced electromagnetic and subtle energy field that provides regulatory and communication functions within the human organism. Biomagnetic fields present around human body can be measured through various techniques such as electromyography, electrocardiography and electroencephalogram [7]. Thus, a human has the ability to harness the energy from environment or Universe and can transmit into any living or non-living object(s). The objects always receive the energy and responding into useful way that is called biofield energy and the process is known as biofield treatment. The concept of human bioenergy has its origin thousands of year back, till date many recent biofield therapies are in practice for their possible therapeutic potentials such as enhanced personal well-being, improved functional ability of arthritis patient, decreased pain and anxiety [8-10]. Biofield therapies are very popular in holistic medicine heath care systems and are included in the National Center for Complementary and Alternative Medicine (NCCAM), which is part of the National Institute of Health (NIH). NCCAM places biofield therapy (putative energy fields) as a subcategory of energy medicine among complementary and alternative medicines [11,12]. These healing treatments suggest their mechanism upon modulating patient-environmental energy fields. Mr. Trivedi's biofield treatment (The Trivedi Effect®) is well known and significantly studied in different fields such as microbiology, agriculture, and biotechnology [13-19]. Recently, impact of biofield treatment on atomic, crystalline and powder characteristics as well as spectroscopic properties of different materials was studied and alteration in physical, thermal and chemical properties was reported [20-22]. Hence, based on the outstanding results obtained after biofield treatment on different materials and considering the applications of OTA, the present study was undertaken to evaluate the impact of biofield treatment on physical, thermal and spectroscopic properties of OTA.

Materials and Methods

o-Toluic acid (OTA) was procured from S D Fine Chemicals Pvt. Ltd., India. The sample was divided into two parts; one was kept as a control, while other was subjected to Mr. Trivedi's biofield treatment and coded as treated sample. The treatment group in sealed pack was handed over to Mr. Trivedi for biofield treatment under standard laboratory conditions. Mr. Trivedi provided the treatment through his energy transmission process to the treated group without touching the sample. The biofield treated samples were returned in the similar sealed condition for further characterization using XRD, DSC, TGA, FT-IR and UV-Vis spectroscopic techniques.

X-ray diffraction (XRD) study

XRD analysis was carried out on Phillips, Holland PW 1710 X-ray diffractometer system, which had a copper anode with nickel filter. The radiation of wavelength used by the XRD system was 1.54056 Å. The data obtained were in the form of a chart of 2θ vs. intensity and a detailed table containing peak intensity counts, d value (Å), peak width (θ°), relative intensity (%) etc.

The crystallite size (G) was calculated by using formula:

$$G = k\lambda/(b\text{Cos}\theta)$$

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). However, percent change in crystallite size was calculated using the following equation:

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

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

Differential scanning calorimetry (DSC) study

For studies related to melting temperature and latent heat of fusion of OTA, Differential Scanning Calorimeter (DSC) of Perkin Elmer/Pyris-1, USA with a heating rate of 10°C/min under air atmosphere and flow rate of 5 ml/min was used. Melting point and latent heat of fusion were obtained from the DSC curve.

Percent change in melting point was calculated using following equations:

$$\%\ \text{change in melting point} = \frac{[T_{\text{Treated}} \quad T_{\text{Control}}]}{T_{\text{Control}}} \times 100$$

Where, T_{Control} and T_{Treated} are the melting point of control and treated samples, respectively.

Percent 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/ Derivative Thermogravimetry (TGA/DTG)

Thermal stability of control and treated samples of OTA was analysed by using Mettler Toledo simultaneous Thermo-gravimetric analyser (TGA/DTG). The samples were heated from room temperature to 400°C with a heating rate of 5°C/min under air atmosphere. From TGA curve, onset temperature T_{onset} (temperature at which sample start losing weight) and from DTG curve, T_{max} (temperature at which sample lost its maximum weight) was recorded.

Percent change in temperature at which maximum weight loss occur in sample was calculated using following equation:

$$\%\ change\ in\ T_{max} = \left[\left(T_{max,\ treated} - T_{max,control}\right) / T_{max,control}\right] \times 100$$

Where, $T_{max,\ control}$ and $T_{max,\ treated}$ are temperature at which maximum weight loss occurs in control and treated sample, respectively.

Spectroscopic studies

For determination of spectroscopic characters, the treated sample was divided into two groups *i.e.* T1 and T2. Both treated groups were analysed for their spectral characteristics using FT-IR and UV-Vis spectroscopy as compared to control OTA sample.

FT-IR spectroscopic characterization

FT-IR spectra were recorded on Shimadzu's Fourier transform infrared spectrometer (Japan) with frequency range of 4000-500 cm^{-1}. The FT-IR spectroscopic analysis of OTA (control, T1 and T2) were carried out to evaluate the impact of biofield treatment at atomic and molecular level like bond strength, stability, rigidity of structure etc.

UV-Vis spectroscopic analysis

The UV-Vis spectral analysis was measured using Shimadzu UV-2400 PC series spectrophotometer over a wavelength range of 200-400 nm with 1 cm quartz cell and a slit width of 2.0 nm. This analysis was performed to evaluate the effect of biofield treatment on structural property of OTA sample. The UV-Vis spectroscopy give the preliminary information related to skeleton of chemical structure and possible arrangement of functional groups [23].

Results and Discussion

X-ray diffraction

X-ray diffraction study was conducted to study the crystalline nature of the control and treated samples of OTA. Figure A1 showed the XRD diffractogram of control and treated samples of OTA. The control sample showed intense crystalline peaks at 2θ equals to 16.20°, 22.45°, 24.14°, 25.57°, 25.70° and 27.68°. Intense peaks indicated the crystalline nature of OTA. Whereas, the XRD diffractogram of treated OTA showed peaks with altered intensity as compared to control sample. The XRD diffractogram of treated OTA showed crystalline peaks at 2θ equals to 16.17°, 22.40°, 24.07°, 25.31°, 25.60° and 27.61° (Figure 1). In addition, the crystallite size was found to be 93.03 and 68.23 nm in control and treated OTA, respectively (Figure 2). It indicates that crystallite size was decreased by 26.66% in treated OTA as compared to control.

It is presumed that biofield energy may be absorbed by the treated OTA molecules which may lead to formation of more symmetrical crystalline long range pattern; that caused increase in intensity of some peaks. Also treated samples of OTA showed decreased crystallite size as compared to control, which suggest that biofield energy might induce strain in lattice and that possibly results into fracturing of grains into sub grains and hence results decreased crystallite size. As OTA is used as intermediate in synthesis of many pharmaceutical compounds, the decrease in crystallite size may lead to fasten the rate kinetics which ultimately enhances the percentage yield of end products [5].

DSC analysis

Differential scanning calorimetry (DSC) was used to determine the latent heat of fusion and melting temperature in control and treated sample of OTA. The DSC thermograms of control and treated samples of OTA are shown in Figure 3. In a solid, substantial amount of interaction force exists in atomic bonds to hold the atoms at their positions, thus a sufficient amount of energy is required to change the phase from solid to liquid, known as latent heat of fusion (ΔH). Further, the energy supplied during phase change *i.e.* ΔH is stored as potential energy of atoms. However, melting point is related to kinetic energy of the atoms [24]. Data showed that ΔH was reduced from 126.63 J/g (control) to 118.17 J/g in treated OTA. It indicates that ΔH was decreased by 6.68 % in treated sample as compared to control. However, the melting point of treated OTA was increased from 105.47°C (control) to 107.96°C. Thus, data suggest that melting point was increased by 2.36% as compared to control (Figure 4). Previously, our group reported that biofield treatment has altered the latent heat of fusion and melting point in lead and tin powder [25]. The reduction in ΔH revealed that treated OTA probably have extra internal energy in form of potential energy as compared to control, which might be transferred through biofield treatment. This potential energy might be stored in treated OTA molecules, which results in lowering of ΔH in treated sample as compared to control. Besides, the increase of melting point in treated OTA suggests that kinetic energy and thermal vibrations of molecules probably altered after biofield treatment. In addition, the sharpness of the

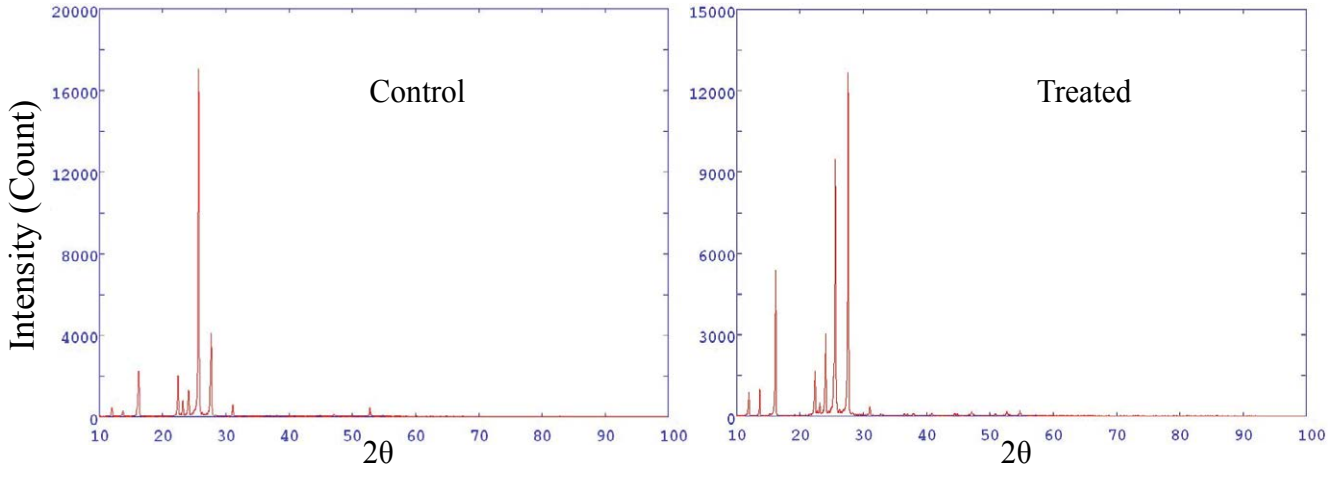

Figure 1: XRD diffractogram of control and treated sample of *o*-toluic acid.

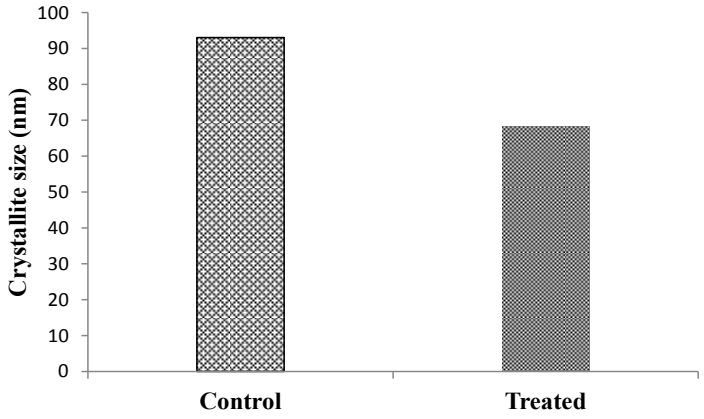

Figure 2: Crystallite size of control and treated sample of *o*-toluic acid.

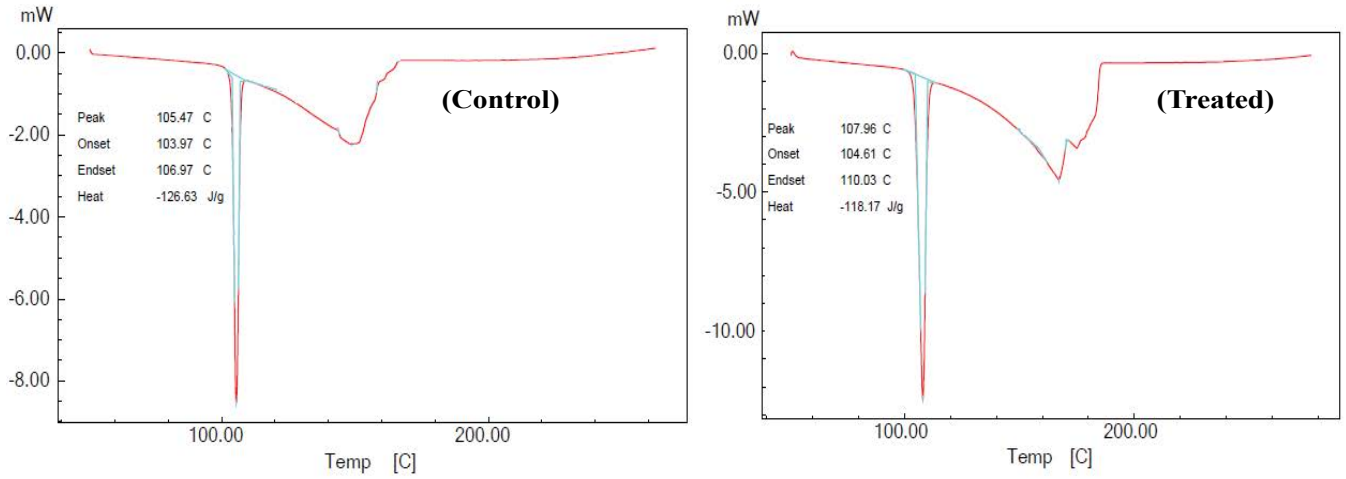

Figure 3: DSC thermogram of control and treated sample of *o*-toluic acid.

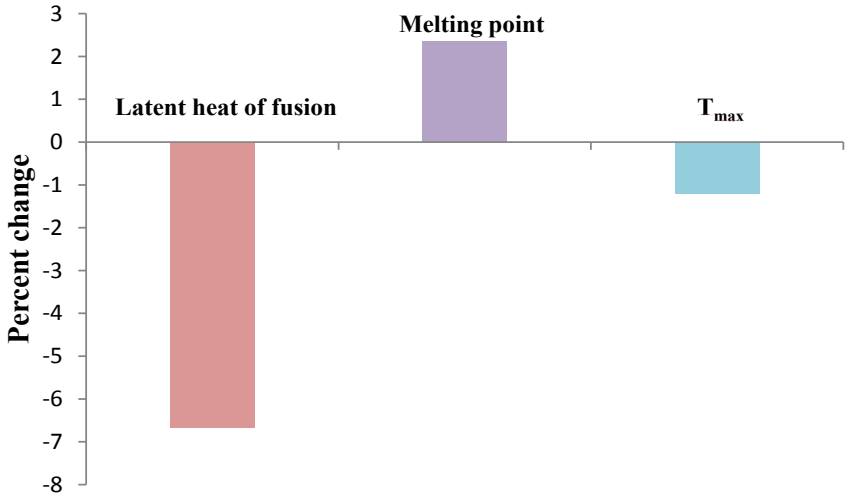

Figure 4: Percent change in latent heat of fusion, melting point, and T*max* of treated sample of *o*-toluic acid as compared to control.

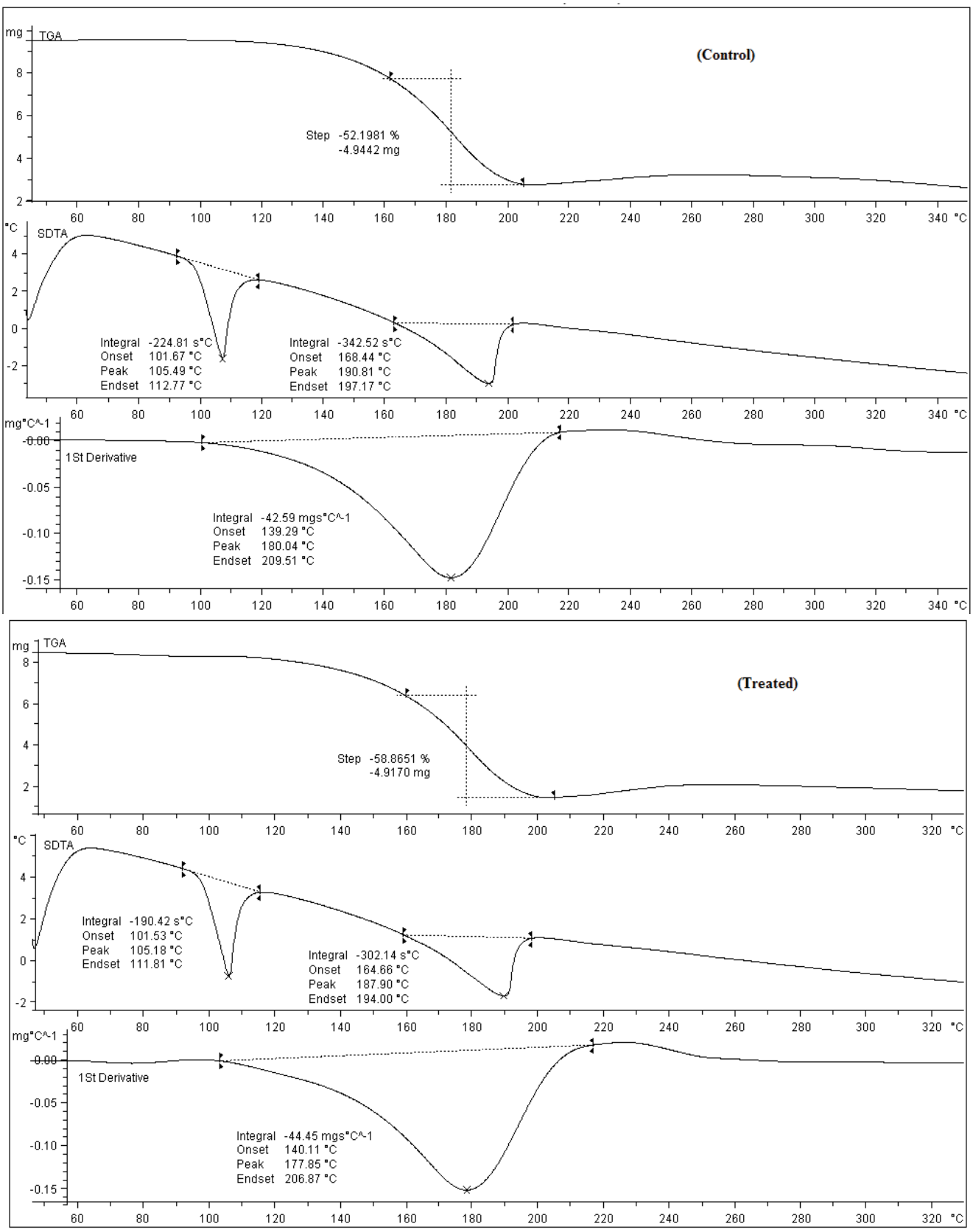

Figure 5: TGA thermogram of control and treated samples of *o*-toluic acid.

endothermic peaks showed good degree of crystallinity in control and treated samples of OTA.

TGA/DTG analysis

TGA/DTG thermogram of control and biofield treated samples are summarized in Table 1. TGA thermogram of control OTA sample (Figure 5) showed that it started losing weight around 160°C (onset) and stopped at 207°C (end set). However, the treated OTA also started losing weight near to 160°C (onset) and terminated at 207°C (end set). It indicates that no significant change was found in onset and endset temperature of treated OTA as compared to control. Furthermore, in this process, control sample lost 52.19% and treated OTA sample lost 58.86% of its weight, which could be due to vaporisation of OTA. Besides, DTG thermogram data showed that T_{max} was found at 180.04°C in control whereas, it was decreased to 177.85°C in treated OTA (Table 1). It indicates that T_{max} was decreased by 1.21% in treated OTA as compared to control. Furthermore, the reduction in T_{max} in treated sample of OTA with respect to control sample may be correlated with increase in vaporisation of treated sample of OTA after biofield treatment. It was previously reported that vapour phase reaction can be more advantageous as compared to liquid phase reaction in terms of reaction time, generation of objectionable amounts of odour and undesired by-products [26,27]. Hence, biofield treated OTA can be used in those reactions as decrease in vaporisation temperature may enhance the reaction kinetics and yield of end product.

Spectroscopic studies

FT-IR analysis

FT-IR spectra of control, T1 and T2 samples of OTA are shown in Figure 6. The aromatic C-H stretching peak was appeared at 3063, 3064 and 3063 cm^{-1} in control, T1 and T2 sample respectively. The C=O stretching (carboxylic acid) peak appeared at 1678 cm^{-1} in control and 1676 cm^{-1} in both T1 and T2 samples. The peak due to aromatic ring stretching was appeared at 1576, 1574 and 1575 cm^{-1} in control, T1 and T2 sample respectively. CH_3 bending peak appeared at 1456 cm^{-1} in control and T1, and at 1458 cm^{-1} in T2 sample. C-C stretching peak was found at 1408 cm^{-1} in all three samples *i.e.* control, T1 and T2. Similarly C-O stretching (carboxylic acid) peak appeared at 1315 cm^{-1} in all three samples *i.e.* control, T1 and T2. C-OH stretching peak appeared at 1273 cm^{-1} in control and T1 sample and at 1274 cm^{-1} in T2 sample. O-H bending peak was found at 916 cm^{-1} in control and 914 cm^{-1} in both T1 and T2 sample. The peak due to ortho substituted arene appeared at 740 cm^{-1} in all three samples (*i.e.* control, T1 and T2). The FT-IR spectra were well supported by reference data [28].

The FT-IR spectroscopic study showed that no alteration was found in terms of frequency of peaks of treated samples (T1 and T2) however, intensity of peaks in T2 sample was slightly increased as compared to control. It suggests that biofield treatment did not cause any alteration in structural and bonding properties like bond strength, stability, rigidity of structure etc.

Parameters	Control	Treated
Latent heat of fusion ΔH (J/g)	126.63	118.17
Melting point (°C)	105.47	107.96
T_{max} (°C)	180.04	177.85
Weight loss (%)	52.19	58.86

Table 1: Thermal analysis of control and treated sample of *o*-toluic acid.

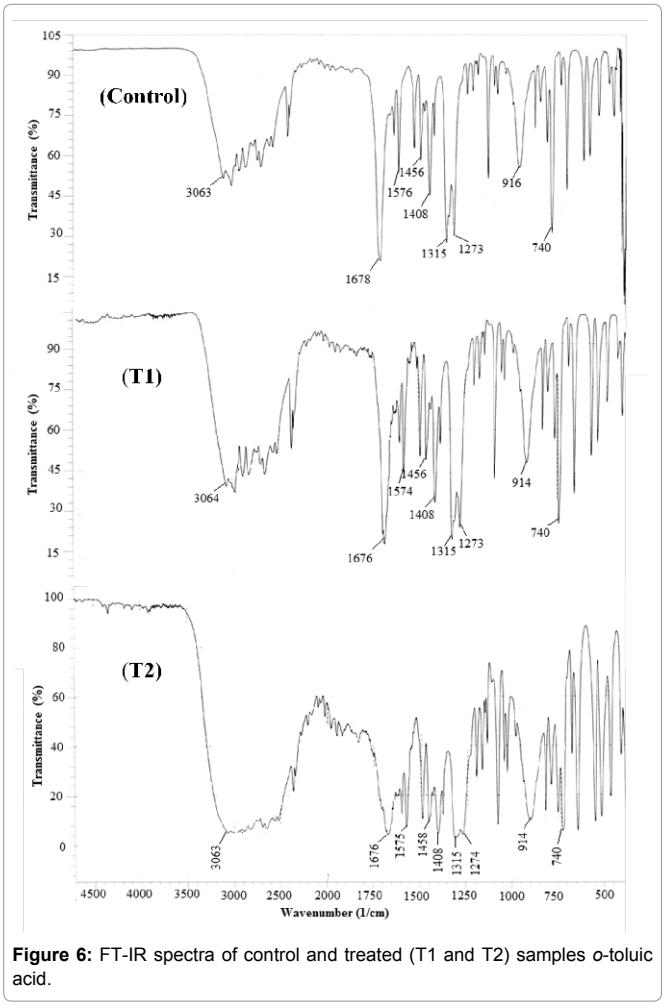

Figure 6: FT-IR spectra of control and treated (T1 and T2) samples *o*-toluic acid.

UV-Vis spectroscopic analysis

The UV spectra of control and treated samples (T1 and T2) of OTA are shown in Figure 7. The UV spectrum of control sample showed three absorption peaks *i.e.* at 202, 228 and 277 nm and the spectrum was well supported by literature data [29]. The UV spectrum of both treated samples of OTA (T1 and T2) also showed similar absorption peaks as compared to control. In T1 sample, absorption peaks appeared at 203, 228 and 278 nm whereas in T2 sample, peaks appeared at 203, 228 and 277 nm. It suggests that biofield treatment could not make any alteration in chemical structure or arrangement of functional groups of treated OTA samples.

Conclusion

Overall study showed influence of biofield treatment on physical and thermal properties of OTA. XRD result showed that

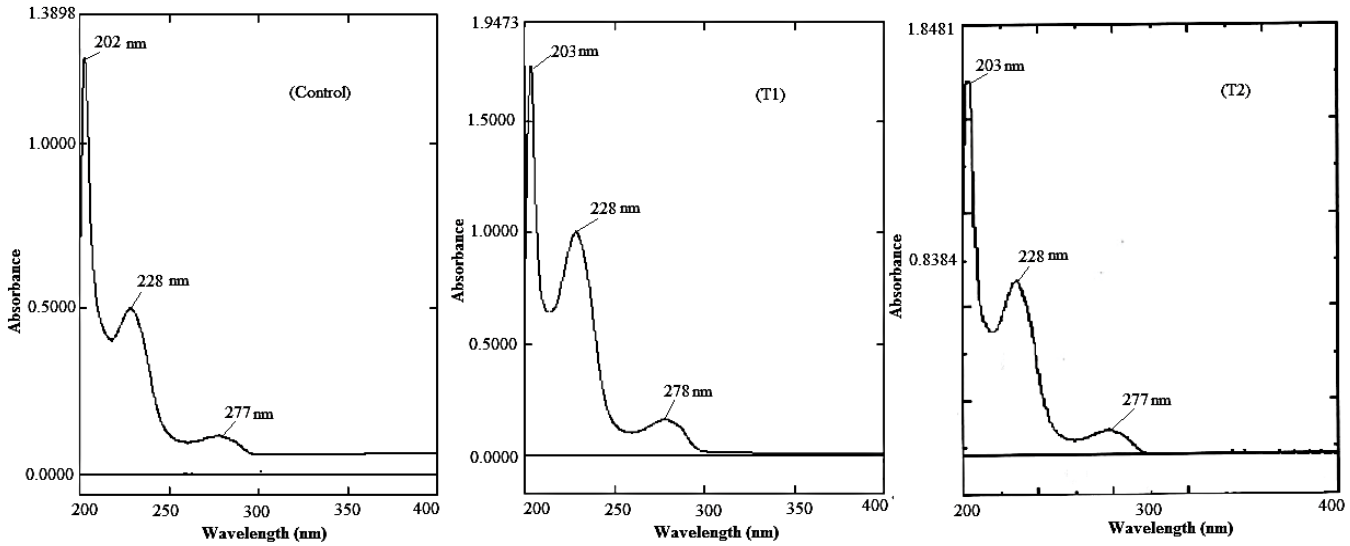

Figure 7: UV spectra of control and treated (T1 and T2) samples of *o*-toluic acid.

crystallite size was decreased by 26.66% in treated OTA sample as compared to control, which might be due to fracturing of grains into sub grains caused by lattice strain produced *via* biofield energy. The reduction in crystallite size may lead to increase in reaction kinetics of OTA which make it more useful as an intermediate compound. Thermal analysis data revealed that latent heat of fusion was reduced by 6.68% whereas, melting point was increased by 2.36% in treated OTA sample as compared to control. TGA/DTG studies showed that T_{max} was decreased by 1.21% in treated OTA samples. On the basis of reduction in T_{max}, it is hypothesized that vaporization temperature of treated OTA sample was decreased as compared to control which could make it more useful in those reactions where OTA was used in vapour state. Furthermore, the decrease in crystallite size and vaporisation temperature may lead to enhance the reaction kinetics. Therefore, it is assumed that biofield treated OTA could be more useful as an intermediate in production of various pharmaceutical products.

Acknowledgement

The authors would like to acknowledge the whole team of Sophisticated Analytical Instrument Facility (SAIF), Nagpur, Maharashtra and MGV Pharmacy College, Nashik for providing the instrumental facility. We are very grateful for the support of Trivedi Science, Trivedi Master Wellness and Trivedi Testimonials in this research work.

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