

Characterization of Biofield Energy Treated 3-Chloronitrobenzene: Physical, Thermal, and Spectroscopic Studies

Mahendra Kumar Trivedi¹, Alice Branton¹, Dahry Trivedi¹, Gopal Nayak¹, Ragini Singh² and Snehasis Jana^{2*}

¹Trivedi Global Inc., 10624 S Eastern Avenue Suite A-969, Henderson, NV 89052, USA

²Trivedi Science Research Laboratory Pvt. Ltd., Hall-A, Chinar Mega Mall, Chinar Fortune City, Hoshangabad Rd., Bhopal- 462026, Madhya Pradesh, India

Abstract

The chloronitrobenzenes are widely used as the intermediates in the production of pharmaceuticals, pesticides and rubber processing chemicals. However, due to their wide applications, they are frequently released into the environment thereby creating hazards. The objective of the study was to use an alternative strategy i.e. biofield energy treatment and analysed its impact on the physical, thermal and spectral properties of 3-chloronitrobenzene (3-CNB). For the study, the 3-CNB sample was taken and divided into two groups, named as control and treated. The analytical techniques used were X-ray diffraction (XRD), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), UV-Visible (UV-Vis), and Fourier transform infrared (FT-IR) spectroscopy. The treated group was subjected to the biofield energy treatment and analysed using these techniques against the control sample. The XRD data showed an alteration in relative intensity of the peak along with 30% decrease in the crystallite size of the treated sample as compared to the control. The TGA studies revealed the decrease in onset temperature of degradation from 140°C (control) to 120°C, while maximum thermal degradation temperature was changed from 157.61°C (control) to 150.37°C in the treated sample as compared to the control. Moreover, the DSC studies revealed the decrease in the melting temperature from 51°C (control) →47°C in the treated sample. Besides, the UV-Vis and FT-IR spectra of the treated sample did not show any significant alteration in terms of wavelength and frequencies of the peaks, respectively from the control sample. The overall study results showed the impact of biofield energy treatment on the physical and thermal properties of 3-CNB that can further affect its use as a chemical intermediate and its fate in the environment.

Keywords: Biofield energy treatment; 3-Chloronitrobenzene; X-ray diffraction study; Thermogravimetric analysis; Differential scanning calorimetry; UV-Visible spectroscopy; Fourier transform infrared spectroscopy

Abbreviations: 3-CNB: 3-Chloronitrobenzene; NCCAM: National Centre for Complementary and Alternative Medicine; NIH: National Institute of Health; XRD: X-ray diffraction; TGA: Thermogravimetric analysis; DTG: Derivative thermogravimetry; FT-IR: Fourier transform infrared

Introduction

Chlorobenzene is an aromatic, colourless, and flammable organic compound present in the form of liquid, that is widely used as intermediate for the manufacturing of other chemicals. The chlorination of benzene results in the production of monochlorobenzene that has been used for the synthesis of diphenyl oxide, chloronitrobenzenes (CNBs), and sulfone polymers. Apart from that, it is also used in the manufacturing of phenol, pigment intermediate, and dioctyl phenol [1,2]. CNBs that are an important end product of monochlorobenzenes possess three isomeric forms i.e. 2- CNB, 3- CNB, and 4- CNB. These isomers structurally differ from each other in terms of the position of the nitro group in the benzene ring with respect to the chloro group; however they possess similar chemical, pharmacological, and toxicological properties [3,4]. They are used as intermediates in the manufacturing of substitute phenyl carbamates, pharmaceuticals (e.g. acetaminophen), pesticides (e.g. parathion and carbofuran), and rubber-processing chemicals [5-7]. Moreover, 3-chloronitrobenzene (3-CNB), a yellow crystalline solid, plays a very important role as precursor due to the presence of two reactive sites. It can be chlorinated for producing pentachloronitrobenzene that is used as a fungicide and in the manufacturing of various agrochemicals. 3-chloroaniline (Orange GC Base), a dye intermediate, is produced from 3-CNB via hydrogenation process [8]. Due to their wide application in the chemical industry, the

CNBs are directly released into the environment. Their presence has been mainly found in water and fishes [9]. 3-CNB has the ability to enter in the environment through the chlorination of drinking water. Moreover, Rivera et al. found 3- CNB as a main pollutant during their research in Spain [10]. All these circumstances create a need for some alternative strategy which could be helpful for these chemicals to improve the yield efficiency and reducing the environmental hazards. Biofield energy treatment recently came in focus due to its ability to make alterations in various living organisms and non-living objects. It is a type of energy healing therapies that are also recommended by National Institute of Health (NIH)/National Centre for Complementary and Alternative Medicine (NCCAM) [11]. The term 'biofield' is related to the biological energy field central to the life and thought to be produced from the physical processes, emotions and thoughts of the human being [12]. It may interact with the environmental processes and the emissions of other individuals. The frequency of these radiations depends on the physiological, mental, emotional, and spiritual state of the person [13]. The non-living objects also possess the energy aura in the form of electromagnetic radiations due to their atomic and molecular

***Corresponding author:** Snehasis Jana, Trivedi Science Research Laboratory Pvt. Ltd., Hall-A, Chinar Mega Mall, Chinar Fortune City, Hoshangabad Rd., Bhopal-462026, Madhya Pradesh, India, Tel: 91-755-6660006; E-mail: publication@trivedieffect.com

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vibrations. The non-living objects cannot change this energy parameter by more than 2%, whereas, the human being can change it drastically by the natural exchange process from the environment [14,15]. Thus, the human has the ability to harness the energy from the environment or universe and can transmit it to any living or non-living object(s) around the Globe. The objects always receive the energy and responding to the useful way. This process is known as biofield energy treatment. Mr. Trivedi is well known to possess a unique biofield energy treatment (The Trivedi Effect) that has been reported for causing alterations in various research field viz. microbiology [16], agriculture [17], and biotechnology [18]. Besides that, the impact of biofield treatment was also reported on physical, thermal and spectral properties of various metals and organic compounds [19-21]. Hence, the current study was conceptualized to evaluate the impact of Mr. Trivedi's biofield energy treatment on the physical, thermal and spectral properties of 3-CNB using various analytical methods.

Materials and Methods

3-chloronitrobenzene (3-CNB) was procured from Loba Chemie Pvt. Ltd., India. The sample was divided into two parts; the first one was kept as a control while another was subjected to Mr. Trivedi's biofield energy treatment and coded as treated sample. The treated group was handed over to Mr. Trivedi in sealed pack for biofield treatment under standard laboratory condition. Mr. Trivedi provided the treatment to the treated group without touching the sample through his energy transmission process. The biofield treated sample was further characterized using the standard protocols of X-ray diffraction, thermogravimetric analysis, differential scanning calorimetry, UV-Vis, and FT-IR spectroscopic characterization.

Characterization

X-ray diffraction (XRD) study: X-ray powder diffractogram were obtained on Phillips, Holland PW 1710 X-ray diffractometer system. The X-ray generator was equipped with a copper anode with nickel filter operating at 35kV and 20 mA. The wavelength of radiation used by the XRD system was 1.54056 Å. The data were collected in the 2θ range of 10° - 99.99° . The step size was 0.02° and the counting time was kept at 0.5 seconds per step. The data obtained from the XRD analysis was in the form of a chart of 2θ vs. intensity. It data showed a detailed table that contains peak intensity counts, d value (Å), peak width (θ), and relative intensity (%).

The crystallite size (G) was calculated from the Scherrer equation with the method based on the width of the diffraction patterns obtained in the X-ray diffracted in the crystalline region.

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

Where, k is the equipment constant (0.94), λ is the X-ray wavelength (0.154 nm), b in radians is the full-width at half of the peak and θ the corresponding Bragg angle. However, percent change in crystallite size was calculated using the following equation:

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

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

Thermogravimetric analysis/ Derivative Thermogravimetry (TGA/DTG): It showed the effect of temperature on the stability of the control and treated samples of 3-CNB. The samples were analysed using Mettler Toledo simultaneous thermogravimetric analyser (TGA/DTG) and heated from room temperature to 350°C with a heating rate

of $5^\circ\text{C}/\text{min}$ under air atmosphere. From TGA/DTG curve, the onset temperature T_{onset} (temperature at which sample start losing weight) and T_{max} (maximum thermal degradation temperature) were recorded.

Differential scanning calorimetry (DSC) study: DSC analysis of control and treated sample was done to analyse the melting behaviour of sample, and it was carried out using Perkin Elmer/Pyris-1. Each sample was accurately weighed and hermetically sealed in aluminium pans and heated at a rate of $10^\circ\text{C}/\text{min}$ under air atmosphere (5 mL/min). The thermogram was collected over the temperature range of 45°C to 250°C . An empty pan sealed with cover pan was used as a reference sample.

UV-Vis spectroscopic analysis: For UV-Vis spectroscopic analysis, the treated sample was divided into two groups, served as T1 and T2. The analysis was measured using Shimadzu UV-2400 PC series spectrophotometer. The spectrum was recorded with 1 cm quartz cell having a slit width of 2.0 nm over a wavelength range of 200-400 nm. In this method, the wavelength of light absorbed by the sample depends on the structure of the sample. With UV-Vis spectroscopy, it is possible to investigate electron transfer between orbitals or bands of atoms, ions and molecules from the ground state to the first excited state [22].

Fourier transform-infrared (FT-IR) spectroscopic characterization: For FT-IR characterization, the treated sample was divided into two groups named T1 and T2. The samples were crushed into fine powder for analysis and followed by mixing in the spectroscopic grade KBr in an agate mortar. Then the sample was pressing into pellets with a hydraulic press. FT-IR spectra were recorded on Shimadzu's Fourier transform infrared spectrometer (Japan). FT-IR spectra are generated by the absorption of electromagnetic radiation in the frequency range 4000 - 400 cm^{-1} . With the help of FT-IR analysis, the impact of biofield treatment on bond strength, rigidity and stability of 3-CNB compound can be analysed [23].

Results and Discussion

XRD study

The XRD diffractograms of control and treated 3-CNB are presented in Figure 1. The XRD diffractogram of control 3-CNB showed the occurrence of intense crystalline peaks at 2θ equal to 15.62° , 15.81° , 17.35° , 17.47° and 25.29° . However, the treated sample showed XRD peak at 2θ equal to 25.20° . The sharp peaks on the diffractograms of the control and treated samples confirm the crystalline nature of 3-CNB [24]. Moreover, a single sharp peak observed in the treated sample as compared to multiple peaks in the control. It is possible that the crystalline planes may reoriented in the same direction after biofield treatment and that might be the probable cause for the emergence of single diffraction peak in the treated sample. In addition, the relative intensity of the diffracted peak in the treated sample was higher as comparison to the control. It is reported that the alteration in relative intensities of the peaks may occur due to change in the crystal morphology [25]. Thus, it is assumed that the energy was transferred through the biofield treatment, and it probably altered the morphology of the 3-CNB molecules. Besides, the average crystallite size was found as 121.67 nm in the control and 84.8 nm in the treated sample of 3-CNB. The percentage reduction in crystallite size was 30.30%. It is assumed that there is presence of severe internal strain due to biofield energy treatment that might be a reason for fracturing the grains into sub grains that lead to decrease in crystallite size of the treated sample [19]. It was reported that decrease in crystallite size might fasten the rate kinetics in the chemical reactions [26]. 3-CNB is used as a

precursor and intermediate in various chemical reactions. Hence, the decrease in crystallite size might enhance the percentage yield of end products by fastening the rate of chemical reaction. Besides, the smaller crystallite size exposed a higher crystallite edge surface that might help in increased rate of degradation [27]. Hence, the decreased crystallite size in biofield energy treated 3-CNB sample may fasten the rate of degradation of 3-CNB molecules from environment either through the process of volatilization or vaporization [28,29].

TGA studies

The TGA thermogram of the control and treated 3-CNB are shown in Figure 2, and data is reported in Table 1. The control 3-CNB showed the occurrence of one step thermal degradation pattern. The thermal degradation commenced at 140°C and completed at 182°C. During this process, the sample showed major weight loss (52.13%) that might be due to vaporization of the 3-CNB molecules. The temperature at which maximum vaporization occurred in the control sample (T_{max}) was observed at 157.61°C; as shown by the DTG thermogram. The TGA thermogram of the treated 3-CNB showed single step thermal degradation between 120°C-179°C. During this thermal event, the treated sample showed rapid vaporization and weight loss (78.23%). The DTG thermogram of treated 3-CNB showed a decrease in T_{max} and it was observed at 150.37°C. Moreover, the thermal stability was reported to be directly related to the crystallite size [30]. Hence, it was assumed that the decrease in crystallite size due to biofield energy treatment might be responsible for the decrease in thermal stability of the treated sample as compared to the control. Moreover, it was previously reported

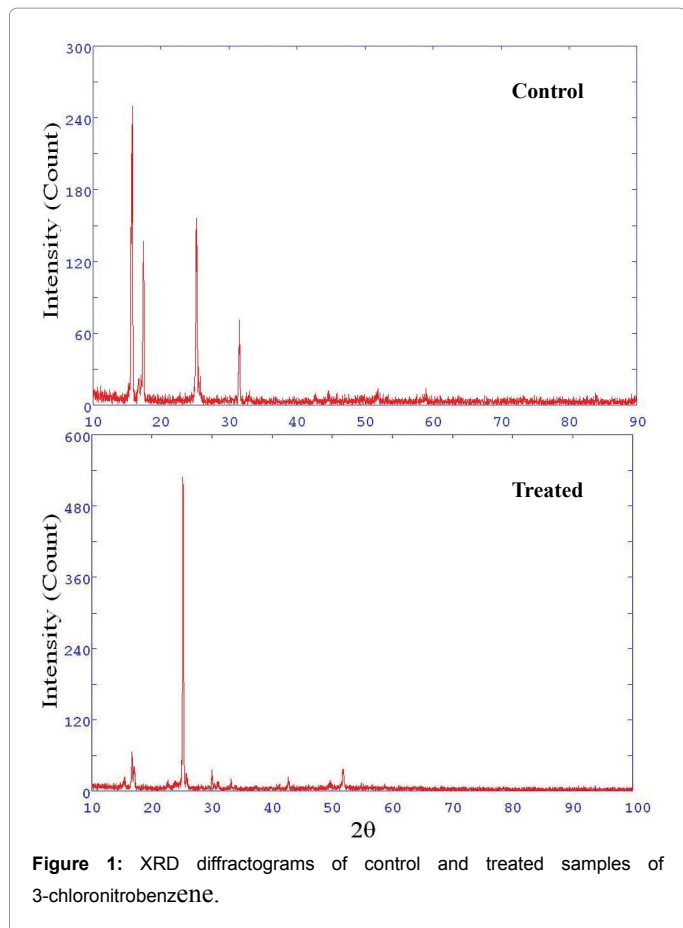


Figure 1: XRD diffractograms of control and treated samples of 3-chloronitrobenzene.

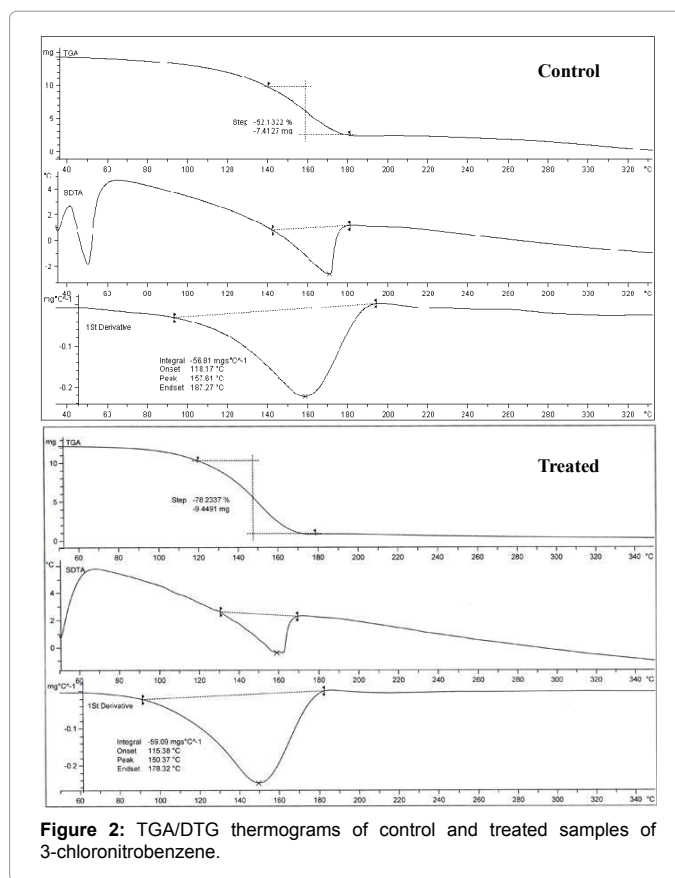


Figure 2: TGA/DTG thermograms of control and treated samples of 3-chloronitrobenzene.

| Parameter | Control | Treated | Percent change |
|-------------------------|---------|---------|----------------|
| Onset temperature (°C) | 140 | 120 | -14.29 |
| Endset temperature (°C) | 182 | 179 | -1.65 |
| T _{max} (°C) | 157.61 | 150.37 | -4.59 |
| Percent weight loss (%) | 52.13 | 78.23 | 46.23 |
| Melting point (°C) | 51 | 47 | -7.84 |

Table 1: Thermal analysis of control and treated samples of 3-chloronitrobenzene. T_{max}: temperature at which maximum vaporization occur

that the rate of reaction was affected by the state of reactant, and gases reacts faster than solids and liquids. On the other hand, the decreased vaporization temperature indicates that the molecules of 3-CNB may change their phase at low temperature [31]. Also, the percent weight loss was more in the treated sample (78.23%) than the control sample (52.13%), which also supports the fast vaporization of the treated sample. Hence, it was assumed that the decrease in vaporization temperature and increased vaporization process in biofield treated sample might fasten the reaction kinetics. Besides, the environmental fate of 3-CNB from the aquatic surface and the moist soil surface is expected through the volatilization and vaporization process [28,29]. Through this process, the 3-CNB molecules reached in the atmosphere in vapour phase and degrade there by reacting with photochemically

produced hydroxyl radicals [32]. Hence, due to the decrease in vaporization temperature, the biofield treated 3-CNB molecule may get easily vaporised from the water and soil surface. This process may help the fast degradation of 3-CNB from the environment by decreasing the volatilization and vaporization half-life.

DSC analysis

The result of DSC analysis was reported in Table 1. The control sample exhibited a sharp endothermic peak at 51°C, whereas the treated sample showed a sharp peak at 47°C. The peaks were due to the melting of control and treated samples, respectively of 3-CNB. The result showed about 8% decrease in melting temperature of the treated sample as compared to the control. It was reported that the melting points of the samples increased due to an increase in crystallite size and *vice versa* [33]. It might be a possible reason for the decrease in melting temperature of the treated sample as it was evident from XRD studies that crystallite size was reduced in treated sample as compared to the control. The decrease in melting temperature might be advantageous for 3-CNB to be used as a chemical intermediate as it helps in accelerating the reaction rate.

UV-Vis spectroscopic analysis

The UV spectra of control and treated samples of 3-CNB are shown in Figure 3. The UV spectrum of control sample showed characteristic absorption peaks at 209 and 257 nm. The spectrum was well supported by the literature [34,35]. The treated sample also showed absorption of light at the similar wavelength. The peaks were appeared at 208 and 256 nm in T1 while in T2 sample, at 209 and 257 nm. It suggested that biofield treatment may not cause any change in structure or position of the functional group as well as the energy that is responsible for electronic transitions between highest occupied molecular orbital and

lowest unoccupied molecular orbital.

FT-IR analysis

The FT-IR spectra of the control and treated samples are shown in Figure 4. The spectra showed characteristic vibrational frequencies as follows:

Nitrogen- oxygen vibrations: In the present study, the NO₂ asymmetric stretching vibration was observed at 1523 cm⁻¹ in all three samples, *i.e.* control, T1, and T2. Similarly, the NO₂ symmetric stretching vibration was observed at 1348 cm⁻¹ in the control and 1346 cm⁻¹ in the treated (T1 and T2) samples. The peak responsible for NO₂ deformation was observed at 538 cm⁻¹ in control and T1 sample and 540 cm⁻¹ in T2 sample. Moreover, the NO₂ rocking vibration peak was appeared at 499 cm⁻¹ in all three samples, *i.e.* control and T1, and T2.

Carbon-hydrogen vibrations: The peak of aromatic C-H stretching was observed at 3101 cm⁻¹ in the control sample; similarly, in T1 sample the peak was observed at 3101 cm⁻¹ and in T2, 3101 cm⁻¹. Moreover, the peaks due to C-H out of plane bending were appeared at 748 and 732 cm⁻¹ in the control sample. These peaks were observed at 743 and 732 cm⁻¹ in T1 sample and 748 and 731 cm⁻¹ in T2 sample.

Ring vibration: Several bands from overtone and combination were appeared in the range of 1992-1732 cm⁻¹ due to *meta* di- substituted benzene in the control sample. The similar bands were observed in T1 and T2 samples in the range of 1992-1782 cm⁻¹ and 1990-1782 cm⁻¹, respectively. Moreover, the peak due to C=C aromatic stretching was

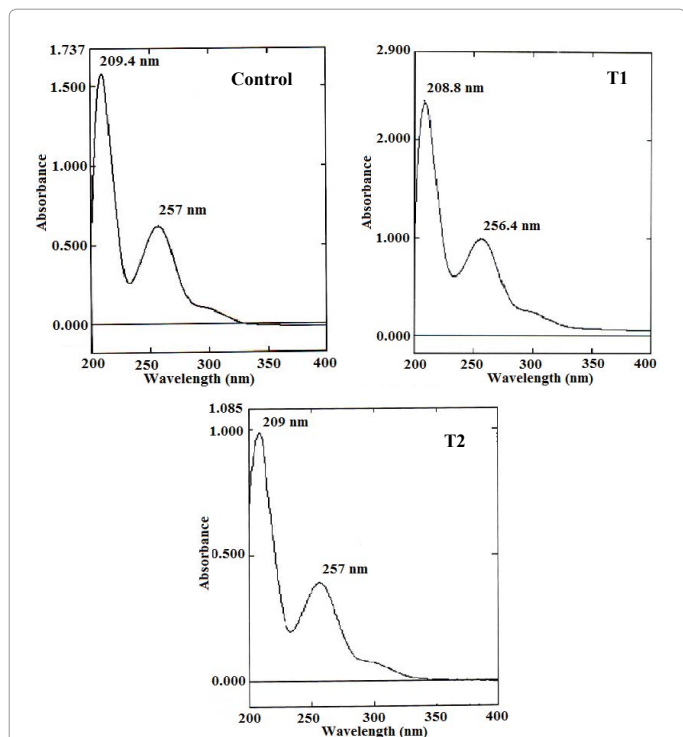


Figure 3: UV-Vis spectra of control and treated samples of 3-chloronitrobenzene.

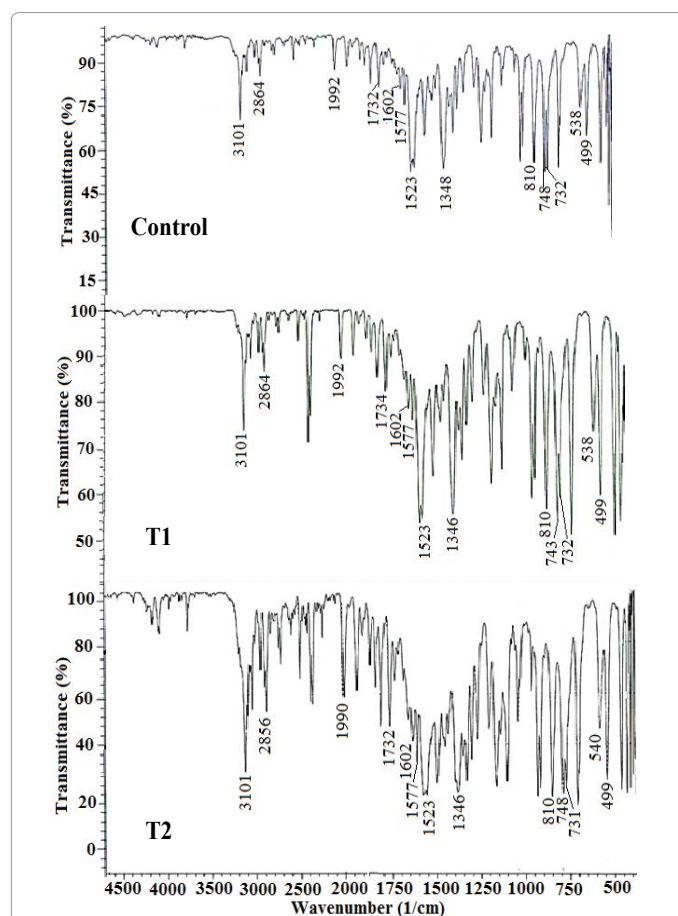


Figure 4: FT-IR spectra of control and treated samples of 3-chloronitrobenzene.

observed at 1602 cm^{-1} in all three samples, *i.e.* control and T1, and T2. Similarly, the peak due to ring stretching was observed at 1577 cm^{-1} in all three samples, *i.e.* control and T1, and T2.

C-Cl vibration: A prominent peak due to C-Cl stretching was observed at 810 cm^{-1} in all three samples, *i.e.* control, T1, and T2. The overall FT-IR analysis was supported by the literature data [36,37] and showed that there was no significant difference between observed frequencies of control and treated samples. Hence, it suggested that biofield energy treatment might not induce any significant change at bonding level.

Conclusion

From the overall study, it was observed that the crystallite size of the treated sample was reduced by 30% that suggests the probable increase in internal strain may be due to the impact of biofield energy treatment. The decreased crystallite size might help in fastening the reaction kinetics when used as intermediate as well as the enhanced rate of degradation of 3-CNB molecules. The XRD results were also supported by thermal analysis data. The TGA analysis revealed an increase in vaporization temperature and decrease in thermal stability of treated sample as compared to the control. It may occur due to the decrease in crystallite size of the treated sample, and it may help in the fast degradation of 3-CNB from the environment. The DSC analysis showed a decrease in melting temperature of the treated sample as compared to the control that might further relate with the decreased crystallite size of the treated sample. It also might advantageous for 3-CNB to be used as chemical intermediate as it helps in fastening the reaction rate. The study concluded the impact of Mr. Trivedi's biofield energy treatment on the physical and thermal properties of the 3-CNB sample that probably help in increasing the reaction kinetics of sample along with possible enhancement in its rate of degradation from the environment.

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