
Experimental Investigation on Physical, Thermal and Spectroscopic Properties of 2-Chlorobenzonitrile: Impact of Biofield Treatment

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Abstract: 2-chlorobenzonitrile (2-CIBN) is widely used in the manufacturing of azo dyes, pharmaceuticals, and as intermediate in various chemical reactions. The aim of present study was to evaluate the impact of biofield treatment on physical, thermal and spectroscopic properties of 2-CIBN. 2-CIBN sample was divided into two groups that served as treated and control. The treated group received Mr. Trivedi's biofield treatment. Subsequently, the control and treated samples were evaluated using X-ray diffraction (XRD), surface area analyser, differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), Fourier transform infrared (FT-IR) and ultraviolet-visible (UV-Vis) spectroscopy. XRD result showed a decrease in crystallite size in treated samples *i.e.* 4.88% in 2-CIBN along with the increase in peak intensity as compared to control. However, surface area analysis showed a decrease in surface area of 64.53% in treated 2-CIBN sample as compared to the control. Furthermore, DSC analysis results showed a significant increase in the latent heat of fusion (28.74%) and a slight increase in melting temperature (2.05%) in treated sample as compared to the control. Moreover, TGA/DTG studies showed that the control and treated 2-CIBN samples lost 61.05% and 46.15% of their weight, respectively. The FT-IR spectra did not show any significant change in treated 2-CIBN sample as compared to control. However, UV-Vis spectra showed an increase in the intensity of peak as compared to control sample. These findings suggest that biofield treatment has significantly altered the physical, thermal and spectroscopic properties of 2-CIBN, which could make them more useful as a chemical intermediate.

Keywords: Biofield Treatment, 2-Chlorobenzonitrile, X-ray Diffraction, Surface Area Analysis, Differential Scanning Calorimetry, Thermogravimetric Analysis, Fourier Transform Infrared Spectroscopy, Ultraviolet-Visible Spectroscopy

1. Introduction

Benzonitrile is a colourless aromatic organic compound, had a sweet almond odour and derived from the reaction of benzoic acid with lead thiocyanate by heating [1]. They are widely used as an indispensable part in the production of dyes, rubber chemicals, pharmaceuticals, herbicides and natural products. They are present as important substructures in various biologically active agents like bicalutamide, fluvoxamine, fadrozole, *etc.* [2]. Benzonitriles and its derivatives are also used in manufacturing lacquers, polymers and anhydrous metallic salts [3]. Halogenated benzonitriles

are known to be used as intermediate in the synthesis of inhibitors of enzymes related to Chagas, Alzheimer and Parkinson disease [4-6] as well as inhibitors used in HIV and cancer treatment [7, 8]. 2-Chlorobenzonitrile (2-CIBN) is a halogenated benzonitrile derivative that is mainly used as an intermediate in the production of azo dyes by synthesizing dye intermediates like 2-cyano-4-nitroaniline. It is also used in palladium catalysed direct arylation of heteroaromatics, *e.g.*, 3-aminopicolinic acid and synthesis of antimalarial drug quetiapine nitrate [9]. 2-CIBN and its substituted derivatives *e.g.* 2,3-dichloro-6-nitrobenzonitrile also have potential anti-inflammatory properties [10]. Stability profile of any chemical compound is the most desired quality that

determines its shelf life and purity to be used as intermediate. The stability can be correlated to physical, thermal or structural and bonding properties of compound [11]. Currently, the stability of chemical compounds in pharmaceutical industries can be affected due to altering temperature and pH conditions [12]. Thus, it is important to search some alternate strategies, which could improve the stability of chemical compounds by altering their physical, thermal or structural and bonding properties.

It is already demonstrated that electrical current exists inside the human body in the form of vibratory energy particles like ions, protons, and electrons, and they generate a magnetic field in the human body [13, 14]. This electromagnetic field of the human body is known as biofield and energy associated with this field is known as biofield energy [15, 16]. It generates through internal physiological processes like blood flow, brain activity and heart function, and function for regulation and communication within the organism [17]. Currently, many biofield treatments are in practice for their possible therapeutic potentials such as enhanced personal well-being and improved functional quality of life [18-20]. The living organisms are also able to exchange this energy from the environment for their health maintenance. Thus, a human can harness the energy from the environment or universe and can transmit the energy to any living or non-living object around this Universe. The object(s) always receive the energy and respond to useful way *via* biofield energy. This process is termed as biofield treatment. Mr. Trivedi's biofield treatment (The Trivedi Effect®) is well known and significantly studied in different fields such as microbiology [21-23], agriculture [24-26], and biotechnology [27, 28]. Recently, it was reported that biofield treatment changes the atomic, crystalline and powder characteristics as well as spectroscopic characters of different materials. Along with that, alteration in physical, thermal and chemical properties was also reported in materials like antimony, bismuth and ceramic oxide [29-31]. Hence, based on the results obtained after biofield treatment on different materials and considering the pharmaceutical applications of 2-CIBN, the present study was undertaken to evaluate the impact of biofield treatment on physical, thermal and spectroscopic characteristics of 2-CIBN.

2. Materials and Methods

2-Chlorobenzonitrile (2-CIBN) 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 sample 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 sample was returned in the similarly sealed condition for further characterization using XRD, surface area analyser, DSC, TGA, FT-IR and UV-Vis spectroscopic techniques.

2.1. 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:

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

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:

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

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

2.2. Surface Area Analysis

The surface area was measured by the Surface area analyser, Smart SORB 90 based on Brunauer–Emmett–Teller (BET). Percent changes in surface area were calculated using following equation:

$$\% \text{ change in surface area} = \frac{[S_{\text{Treated}} - S_{\text{Control}}]}{S_{\text{Control}}} \times 100$$

Where, S_{Control} and S_{Treated} are the surface area of control and treated samples, respectively.

2.3. Differential Scanning Calorimetry (DSC) Study

For studies related to melting temperature and latent heat of fusion of 2-CIBN, 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 temperature and latent heat of fusion were obtained from the DSC curve.

Percent change in latent heat of fusion was calculated using following equations:

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

Where, $\Delta H_{\text{Control}}$ and $\Delta H_{\text{Treated}}$ are the latent heat of fusion of control and treated samples, respectively. Similarly, percent change in melting point was also calculated to observe the difference in thermal properties of treated 2-CIBN sample as compared to control.

2.4. Thermogravimetric Analysis/ Derivative Thermogravimetry (TGA/DTG)

Thermal stability of control and treated sample of 2-CIBN

was analysed by using Mettler Toledo simultaneous thermogravimetric 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) were recorded.

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

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

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

Percent change in onset peak temperature was calculated using following equation:

$$\% \text{ change in onset peak temperature } T_{\text{onset}} = [(T_{\text{onset, treated}} - T_{\text{onset, control}}) / T_{\text{onset, control}}] \times 100$$

Where, $T_{\text{onset, control}}$ and $T_{\text{onset, treated}}$ are onset peak temperature in control and treated sample, respectively.

2.5. 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 2-CIBN sample.

2.5.1. FT-IR Spectroscopic Characterization

The samples were crushed into fine powder for analysis. The powdered sample was mixed in spectroscopic grade KBr in an agate mortar and pressed into pellets with a hydraulic press. FT-IR spectra were recorded on Shimadzu's Fourier transform infrared spectrometer (Japan) with a frequency range of 4000-500 cm^{-1} . The samples are prepared by grinding the dry blended powders of control and treated 2-CIBN with powdered KBr, and then compressed to form discs. The FT-IR spectroscopic analysis of 2-CIBN (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.* [32].

2.5.2. 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 the structural property of 2-CIBN sample. The UV-Vis spectroscopy gives the preliminary information related to the skeleton of chemical structure and possible arrangement of functional groups. With UV-Vis spectroscopy, it is possible to investigate electron transfers between orbitals or bands of atoms, ions and molecules existing in the gaseous, liquid and solid phase [32].

3. Results and Discussion

3.1. X-ray Diffraction

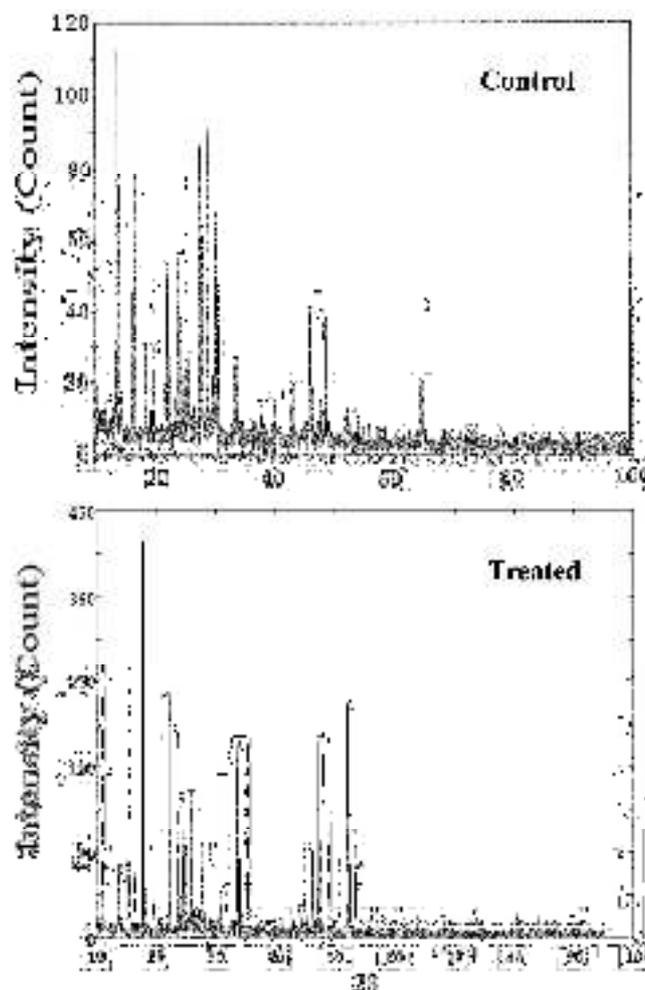


Fig. 1. XRD diffractogram of control and treated samples of 2-chlorobenzonitrile.

X-ray diffraction analysis was conducted to study the crystalline nature of the control and treated sample of 2-CIBN. XRD diffractogram of control and treated samples of 2-CIBN are shown in Fig. 1. The XRD diffractogram of control 2-CIBN showed intense crystalline peaks at 2θ equals to 13.67°, 16.62°, 27.74°, 28.87° and 30.28°. The intense peaks indicated the crystalline nature of 2-CIBN. However, the XRD diffractogram of treated 2-CIBN showed the crystalline peak at 2θ equals to 13.59°, 17.82°, 22.28°, 23.84°, 24.77°, 25.80°, 27.91°, and 33.65°. Most of the treated sample peaks showed high intensity as compared to the control, which indicated that crystallinity of treated 2-CIBN sample increased as compared to control. According to Britton D, 2-CIBN molecules involve Cl---N interactions as well as C-H---Cl and C-H---N hydrogen bonds, due to which they possess four crystallographic non-equivalent forms of molecules. These four crystallographic molecules differed from each other in terms of bond length and related by pseudosymmetry [33]. Besides, the molecules of 2-CIBN do not possess an organized structure as the molecular layers

are not perfectly overlapping with each other [34]. It is presumed that biofield energy may be absorbed by the treated 2-CIBN molecules that may lead to increasing the symmetry of 2-CIBN molecules by formation of a symmetrical crystalline long range pattern. Further, the molecular layers of 2-CIBN get more organized after biofield treatment hence, caused an increase in the intensity of peaks. Besides, the crystallite size was found to be 99.72 and 94.85 nm in control and treated 2-CIBN, respectively. The crystallite size was decreased by 4.88% in treated 2-CIBN as compared to control (Fig. 2). It may be due to biofield energy that probably induce strain in the lattice, and that possibly resulted in the fracturing of grains into subgrains and hence decreased crystallite size [29]. 2-CIBN is used as intermediate in the synthesis of many pharmaceutical compounds; hence, the decrease in crystallite size may lead to fasten the rate kinetics that ultimately enhances the percentage yield of end products [35].

3.2. Surface Area Analysis

The surface area of control and treated samples of 2-CIBN were investigated using BET method. The control sample showed a surface area of 0.764 m²/g; however, the treated sample of 2-CIBN showed a surface area of 0.271 m²/g. The decrease in surface area was 64.53% in the treated 2-CIBN sample as compared to control (Fig. 2). Murray *et al.* reported that increase in crystallinity might reduce the surface area as poorly crystallized sample possess more surface area than a well-crystallized sample [36]. As it was evident from XRD studies that after biofield treatment, the crystallinity of 2-CIBN sample increases, hence it could lead to decrease the surface area of treated sample as compared to control.

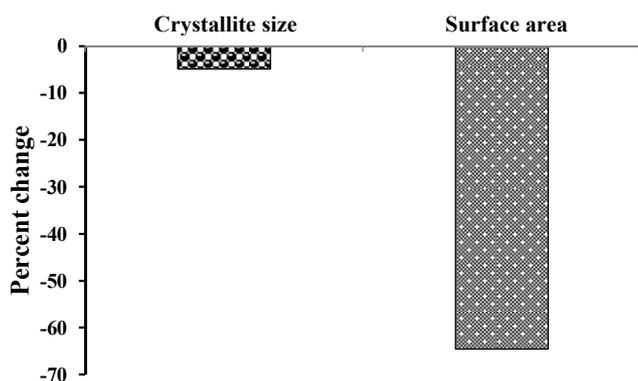


Fig. 2. Percent change in crystallite size and surface area of treated sample of 2-chlorobenzonitrile.

3.3. DSC Analysis

DSC was used to determine the latent heat of fusion (ΔH) and melting temperature in control and treated sample of 2-CIBN. The DSC analysis results of control and treated samples of 2-CIBN are presented in Table 1. In a solid, the amount of energy required to change the phase from solid to liquid is known as ΔH . The data showed that ΔH was

increased from 96.22 J/g (control) to 123.87 J/g in treated 2-CIBN. It indicates that ΔH was increased by 28.74% in treated sample as compared to control (Fig. 3). It was previously reported that 2-CIBN molecules possess CN---Cl intermolecular interactions but these interactions are weak in nature due to which 2-CIBN molecules possess lower enthalpy of sublimation as compared to other isomers [34]. It was hypothesized that biofield energy was absorbed by 2-CIBN molecules that possibly strengthened the intermolecular bonding between chlorine-cyano groups in 2-CIBN molecules. Hence, the treated 2-CIBN sample needs more energy in the form of ΔH to undergo the process of melting. Moreover, the melting temperature of treated 2-CIBN was increased from 45.78°C (control) to 46.72°C. Thus, data suggest that melting point was increased by 2.05% as compared to control (Fig. 3). The melting temperature is related to the kinetic energy of the atoms [37]. Previously, our group reported that biofield treatment has altered ΔH and melting point in lead and tin powder [38]. Besides, the increase of melting point in treated 2-CIBN suggests that kinetic energy and thermal vibrations of molecules probably altered after biofield treatment.

3.4. TGA/DTG Analysis

Thermogravimetric analysis/derivative thermogravimetry analysis (TGA/DTG) of control and biofield treated samples are summarized in Table 1. TGA thermogram (Fig. 4) showed that control 2-CIBN sample started losing weight around 132°C (onset) and stopped around 178°C (end set). However, the treated 2-CIBN started losing weight around 139°C (onset) and terminated around 176°C (end set). It indicates that onset temperature of treated 2-CIBN increased by 5.3% as compared to control (Fig. 3). Furthermore, in this process, control sample lost 61.05% and treated 2-CIBN sample lost 46.15% of its weight. Besides, DTG thermogram data showed T_{max} at 150.65°C in control, whereas, it was increased to 155.52°C in treated 2-CIBN (Table 1). It indicates that T_{max} was increased by 3.23% in treated 2-CIBN (Fig. 3). The increase in onset temperature can be related to increasing in thermal stability of treated 2-CIBN sample. As it was interpreted from DSC studies that ΔH increased by 28.74% which suggest that intermolecular bonding between Cl---CN group might strengthen after biofield treatment ultimately results to improve the stability of treated 2-CIBN sample against temperature. Furthermore, this hypothesis was also supported by the percent weight loss that is decreased by 15% in treated sample as compared to control. The result was also evident by T_{max} value that was increased by 3.23% in treated sample; hence suggest that the temperature at which maximum weight loss occurred was increased by 5°C in treated sample as compared to control.

The overall thermal studies suggest that thermal stability of treated 2-CIBN sample increased which might be advantageous for this compound regarding its wide application.

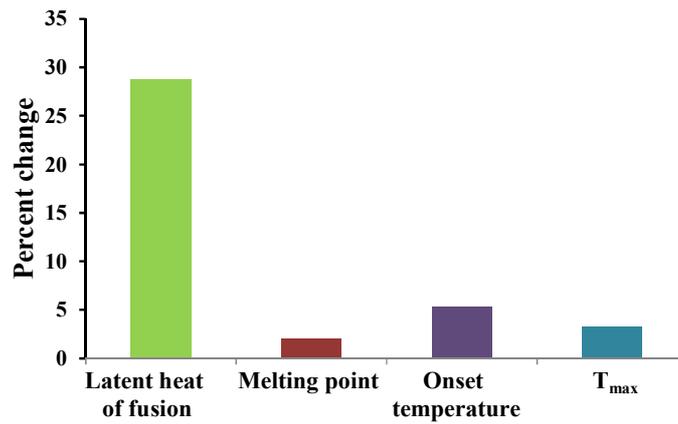


Fig. 3. Percent change in latent heat of fusion, melting point, onset temperature and T_{max} in biofield treated 2-chlorobenzonitrile with respect to control.

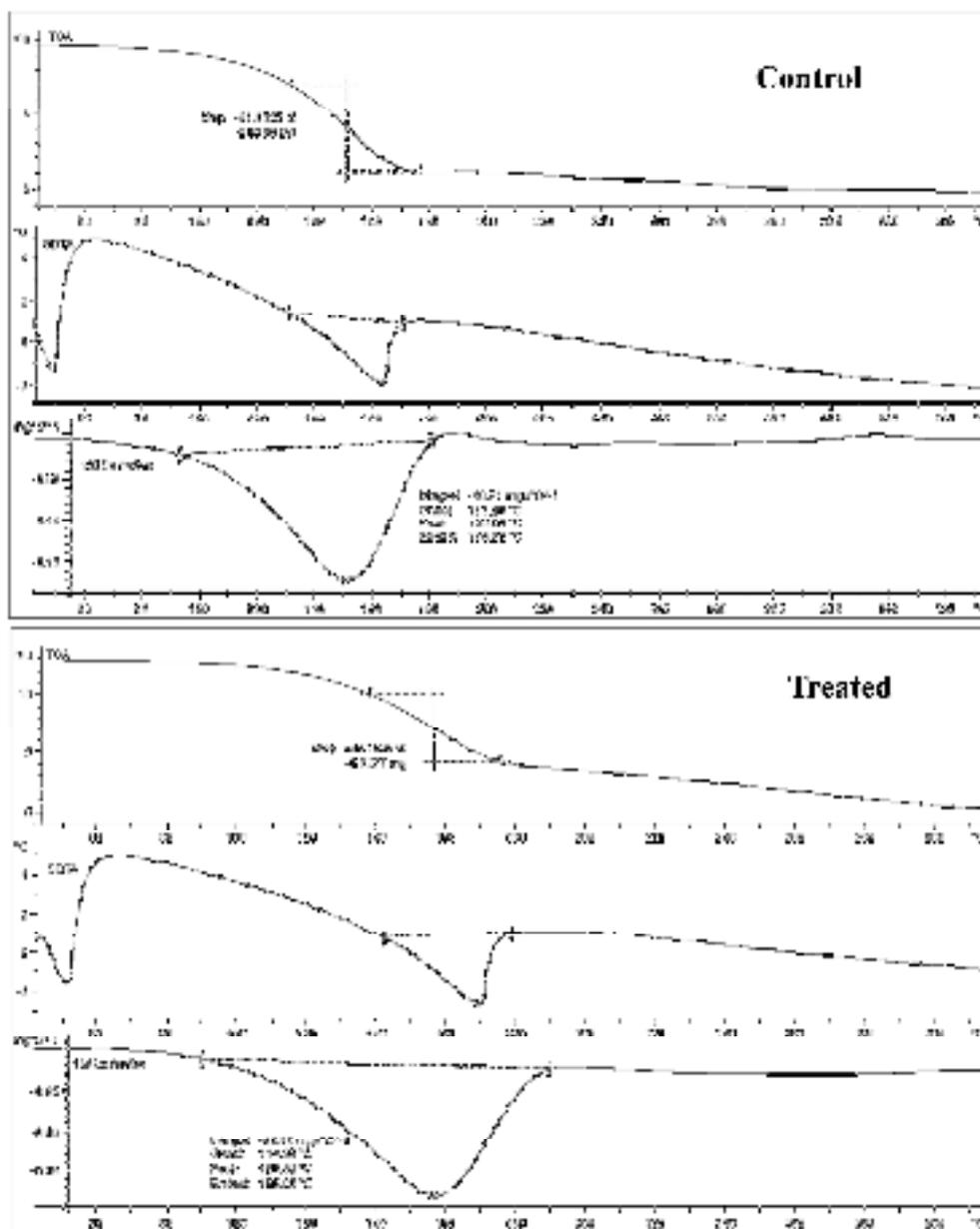


Fig. 4. TGA thermograms of control and treated samples of 2-chlorobenzonitrile.

Table 1. Thermal analysis of control and treated samples of 2-chlorobenzonitrile.

Parameter	Control	Treated
Latent heat of fusion ΔH (J/g)	96.22	123.87
Melting point ($^{\circ}\text{C}$)	45.78	46.72
Onset temperature ($^{\circ}\text{C}$)	132	139
T_{max} ($^{\circ}\text{C}$)	150.65	155.52
Weight loss (%)	61.05	46.15

T_{max} : temperature at which maximum weight loss occur

3.5. Spectroscopic Studies

3.5.1. FT-IR Analysis

FT-IR spectra of control, T1 and T2 samples of 2-CIBN are shown in Fig. 5. It showed similar distribution patterns for both control and treated (T1 and T2) samples of 2-CIBN. The C-H stretching (aromatic) peak was appeared at 3066 cm^{-1} in control 2-CIBN. In treated samples, C-H stretching (aromatic) peak was

appeared at same frequency *i.e.* 3066 cm^{-1} in T1 and T2 sample. The peak due to overtone (in ring) was appeared at 2341 , 2339 and 2341 cm^{-1} in control, T1 and T2 sample respectively. The $\text{C}\equiv\text{N}$ stretching peak was appeared at 2229 cm^{-1} in control and T1 and 2231 cm^{-1} in T2 sample. The peak due to C-C stretching (in ring) was appeared at 1591 cm^{-1} in all three samples *i.e.* control, T1 and T2. Similarly, C-H in plane bending was found at 1134 cm^{-1} in all three samples *i.e.* control, T1 and T2. The peaks due to C-Cl stretching were also appeared at same frequencies in control and treated (T1 and T2) samples *i.e.* at 557 and 459 cm^{-1} . The peak due to C-H out of plane bending was appeared at 759 cm^{-1} in control and T1 sample whereas, at 758 cm^{-1} in T2 sample. C-C \equiv N stretching peak was appeared at 1203 cm^{-1} in all three samples *i.e.* control, T1 and T2. The peak due to C-Cl in plane bending was found at 386 cm^{-1} in control whereas, at 370 cm^{-1} in T1 and 385 cm^{-1} in T2 sample of 2-CIBN. The FT-IR spectra were well supported by reference data [39].

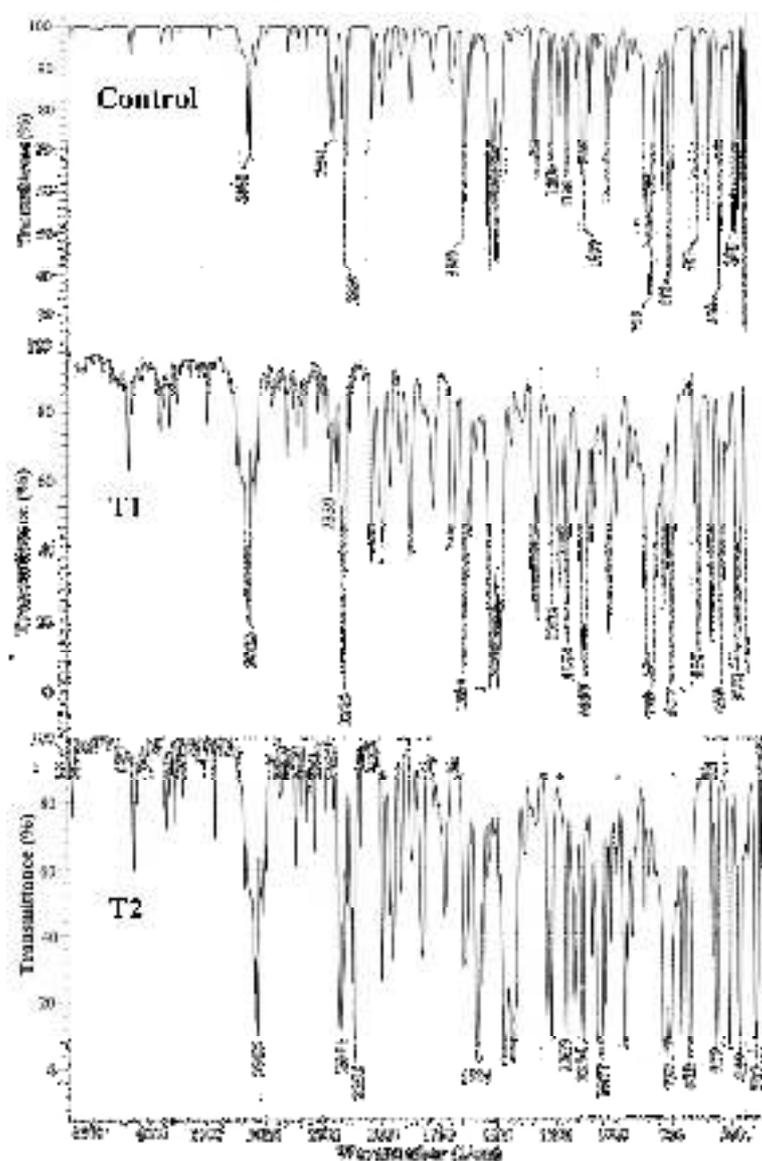


Fig. 5. FT-IR spectra of control and treated samples of 2-chlorobenzonitrile.

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

3.5.2. UV-Vis Spectroscopic Analysis

The UV spectra of control and treated samples (T1 and T2) of 2-CIBN are shown in Fig. 6. The UV spectrum of control sample showed characteristic absorption peaks at 206 and 229 nm which were also observed in T1 sample at 209 and 229 nm; however, in case of T2 sample, the peak near to 210 nm get merged with the next peak due to increase in intensity and form one broad peak at 228 nm. Also, the peak at 229 nm in

T1 sample showed increase intensity as compared to control. Other two absorption peaks were observed at 279 and 287 nm in the control sample that were evident in T1 and T2 at the same position however some change in intensity was observed in T2 sample as compared to control. It was reported previously that intensity of peak might increase due to intermolecular bonding between molecules of the sample [40]. Hence, it is hypothesized that due to biofield treatment, the strength and extent of intermolecular bonding between CN---Cl group increased, which results in increased intensity of peaks in treated samples as compared to control. The UV spectrum of control 2-CIBN was well supported by literature data [39].

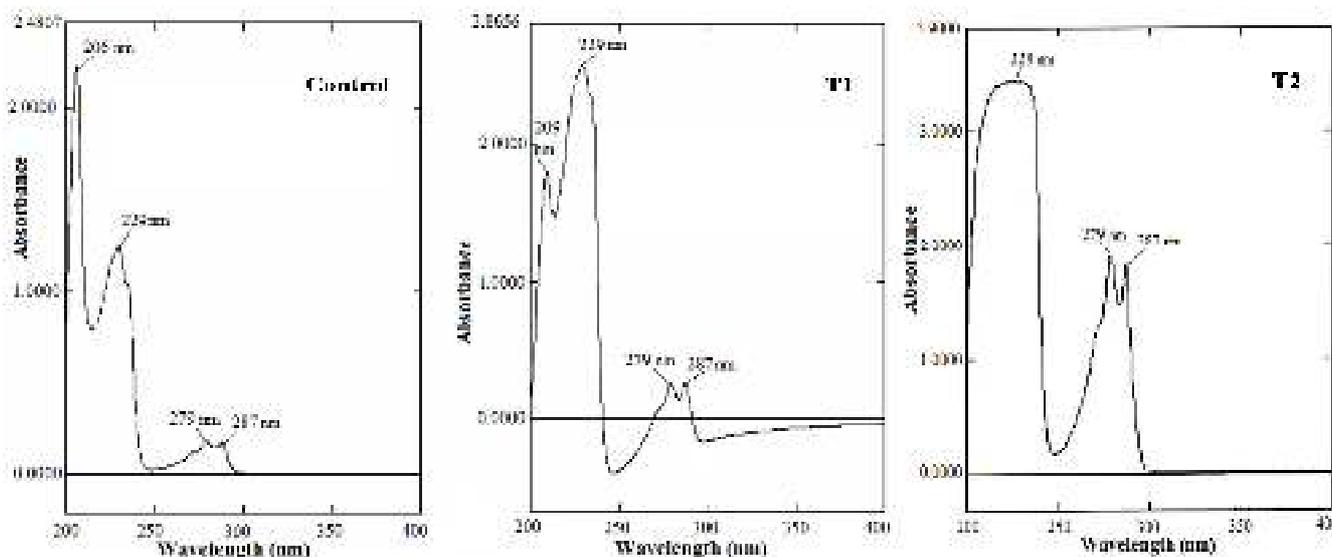


Fig. 6. UV-Vis spectra of control and treated samples of 2-chlorobenzonitrile.

4. Conclusions

The overall study showed the influence of biofield treatment on physical, thermal and spectroscopic properties of 2-CIBN. XRD results showed that crystallite size was decreased by 4.88% in treated 2-CIBN samples as compared to control, which might be due to fracturing of grains into subgrains caused by lattice strain produced *via* biofield energy. The increase in the intensity of peaks suggests the increased crystallinity of treated sample due to the formation of symmetrical and organised molecular layers caused *via* biofield treatment. The reduced crystallite size and increased crystallinity may lead to increasing the reaction kinetics as well as the stability of 2-CIBN, which could make it more useful as an intermediate compound. The surface area analysis showed 64.53% decrease in surface area of the treated 2-CIBN sample as compared to the control that might result due to increase in crystallinity and formation of a well-crystallised sample after biofield treatment. DSC analysis data revealed that latent heat of fusion as well as melting temperature were increased by 28.74% and 2.05% respectively in treated 2-CIBN as compared to control. TGA/DTG studies showed

that onset temperature and T_{max} were increased by 5.3% and 3.23% respectively in treated 2-CIBN samples. On the basis of thermal analysis data, it is hypothesized that thermal stability of treated 2-CIBN sample increased which may affect its shelf life and efficacy when used in various chemical reactions. The UV-Vis spectra showed alteration in the intensity of peaks that might happen due to increase in intermolecular bonding in 2-CIBN molecules after biofield treatment. This increase in intermolecular bonding can further relate to increased thermal stability of treated sample as compared to control. Therefore, it is assumed that biofield treated 2-CIBN could be more useful in the production of various pharmaceutical products.

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