Preparation, Characterization and Structure Prediction of In$_2$SnO$_3$ and Spectroscopic (FT-IR, FT-Raman, NMR and UV-Visible) Study Using Computational Approach

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Unadulterated and scorch stage In$_2$SnO$_3$ nanopowder is effectively arranged with the doping proportion of 80–20% (In$_2$O$_3$–Sn) by simple sol–gel combustion direction. The material is characterized by XRD measurements and their geometrical parameters are compared with calculated values. The FT-IR and NMR spectra are recorded in both bulk and nanophase and FT-Raman spectrum is recorded in bulk phase and the fundamental frequencies are assigned. The optimized parameters and the frequencies are calculated using HF and DFT (B3LYP, B3PW91 and MPW1PW91) theory in bulk phase of In$_2$SnO$_3$ and are compared with its nanophase. The vibrational frequency pattern in nanophase gets realigned and the frequencies are shifted up and down little bit to the region of spectra when compared with bulk phase. The UV-visible spectrum is simulated and analyzed. The frontier molecular orbital analysis has been carried out and the values of the HOMO-LUMO bandgap (Kubo gap) explore the optical and electronic characteristics of the In$_2$SnO$_3$. Structural studies by XRD showed the crystallite sizes of the particles. The atomic arrangement in the grain boundary seems to be somewhat different from regular periodic arrangement whereas inside the grain there is a good periodic arrangement of atoms. Above 10 mol% Sn ions, 15 mol% Sn ions, 20 mol% Sn ions to 50 mol% Sn ions form correlated clusters, 20 mol% Sn ions which lead to broadening. These EPR spectra were formed to contain two different components, one from the single isolated ions and the other from the clusters. The transition is observed for different composition increase with decreasing grain size.

Keywords: FTIR, EPR, NMR, DFT, ITO.

1. INTRODUCTION

Rapid developments in today’s electronic devices including flat panel displays and touch panels are asking for highly sophisticated components, with an ever-increasing performance. The development of transparent conducting coatings as electrodes with customized characteristics like high electron work function, high electron mobility and high transparency, hence, is becoming more and more relevant. To meet these forthcoming requirements, however, novel materials or improved coating techniques must be developed. One of these approaches is focusing on a combination of several coating methods, as for example,
magnetron sputtering and sol–gel dip coating, to benefit from the advantages of both techniques. The properties; materials are fascinating and have formed the subject of intense research in recent years. These materials behave differently from bulk semiconductors. With decreasing particle size, the band structure of the semiconductor changes; the bandgap increases and the edges of the bands splits into discrete energy levels. These so-called quantum size effects occur. These quantum size effects have simulated great interest in both basic and applied research. Research in nanoscale materials is motivated by the possibility of processing and designing nanostructured materials with unique properties and important applications. Due to their finite small size and the high surface-to-volume ratio, nanostructured materials often exhibit novel, and sometimes unusual properties. The optical, electrical, magnetic, thermal, and chemical properties depend on the particle size and shape of these materials. Meanwhile the large number of surface and edge atoms provides active sites for catalyzing surface reactions.

In the areas of optoelectronic devices such as transparent semiconductor electrodes in liquid crystal displays, light emitting transport conductors and solar-electrical energy converters and chemical and gas sensitive semiconductor devices and nano electronics, the SnO2 and their composites are finding great interest and attention in recent years. It is well known that the optical, electrical and magnetic properties of nanophase SnO2 and In2O3 materials when both the material combined doped together, what will be the characteristics of the In2SnO3. In this route, it is attempted that the Sn is doped with In2O3 with the doping ratio of 80–20% (In2O3–Sn) by simple sol–gel combustion method. However, so far, no work has been reported on the study (comparison of bulk and nanophase) of preparation and characterization of pure and singe phase In2SnO3 nanopowder with HF and DFT computational calculation. In this work, the In2SnO3 nanopowder is successfully prepared by sol–gel combustion method and is investigated by FTIR, Laser Raman Spectroscopy, UV-vis, and Photoluminescence measurements. Moreover, FT-Raman, NMR and Visible spectra are recorded for bulk In2SnO3 for the comparison. The geometrical parameters and vibrational frequencies are calculated using HF and DFT theory and their results are compared with the experimental values.

2. EXPERIMENTAL DETAILS

2.1. Synthesis of In2SnO3
Calculated amount of In(NO3)3 [5.0 M], dissolved in minimum volume of water was added to the aqueous [5.0 M] to [0.5 M] solution of Sn(NO3)2 obtained by stirring the In-metal ingots with concentrated HNO3 for 40 hrs at 100 °C. The volume of In(NO3)3 solution and the weight of Sn(NO3)2 were taken by maintaining the In/Sn atomic ratio 50:50, 85:15, 80:20 and 90:10. The mixture was diluted with water and the resultant solution was stirred magnetically for 2 hr. Urea was added to the above mixture till a gel of hydrated indium tin oxide appeared. It was stirred for additional 1 hr at an ambient temperature. The pH of the above solution was maintained in the range 6.5–7.2 at this stage. The solution was stirred again for 1/2 h to ensure the complete precipitation. The precipitation was placed in a hot plate at 100 °C for 20 min until it turned as gel. For In/Sn = 80:20, which also shifted to lower temperature with increase in Sn content, (Among the proportion of In/Sn = 50:50, 70:30, 80:20, and 90:10) we get the result good for 80/20 proportion which was here reported.

2.2. Oxidation Behavior of InSn Alloy
The forms a solid solution in indium up to 50% with variation in bond length and lattice parameter. In the present work 5 at% Sn to 0.5 at% Sn has been added and fired in a furnace to get nanocrystalline alloy. It has been studied for its oxidation behavior with various compositions. Figure 1 shows the XRD patterns for as-prepared with seven different compositions. XRD studies of the as-prepared material show the presence of tetragonal In lines indicating that Sn has gone to the substitutional position forming solid solution. XRD shows complete oxidation of the alloy giving mainly cubic phase of In2O3.

2.3. Spectral Information
Bulk In2SnO3 is prepared by above said method. The FT-IR spectra of the compound in both phases are recorded in Bruker IFS 66 V spectrometer in the range of 1000 cm−1–50 cm−1. The spectral resolution is ±2 cm−1. FT-Raman spectra of same compound is also recorded in the same instrument with FRA 106 Raman module equipped with Nd:YAG laser source operating at 1.064 μm line widths with 200 mW power. The spectra are recorded in the range

Figure 1. Molecular structure of In2SnO3 with α velocity.
of 1000 cm$^{-1}$–50 cm$^{-1}$ with scanning speed of 30 min$^{-1}$ of spectral width 2 cm$^{-1}$. The frequencies of all sharp bands are accurate, i.e., ±1 cm$^{-1}$.

3. COMPUTATIONAL METHODS

In the present work, HF and some of the hybrid methods; B3LYP, B3PW91 and MPW1PW91 are carried out using the basis set 3-21G(d, p). All these calculations are performed using GAUSSIAN 09W$^{13}$ program package on Pentium IV processor in personal computer. In DFT methods; Becke’s three parameter hybrids function combined with the Lee-Yang-Parr correlation function (B3LYP)$^{14,15}$ Becke’s three parameter exact exchange-function (B3)$^{16}$ combined with gradient-corrected correlational functional of Lee, Yang and Parr et al., (LYP)$^{17–18}$ and Perdew and Wang (PW91)$^{19,20}$ predict the best results for molecular geometry and vibrational frequencies for moderately larger molecules. The calculated frequencies are scaled down by suitable scaling factors to yield the coherent with the observed frequencies. The optimized molecular structure of the molecule is obtained from Gaussian 09 and GaussView program and is shown in Figure 1. The comparative optimized structural parameters such as bond length, bond angle and dihedral angle are presented in Table I.

The observed (FT-IR and FT-Raman) and calculated vibrational frequencies, vibrational assignments and the total energy distribution (TED) for B3PW91 of In$_2$SnO$_3$ are presented in Table II. Experimental and simulated spectra of IR and Raman in both phases are presented in the Figures 2 and 3 respectively. The total energy distribution (TED) calculations show the relative contributions of the redundant internal coordinates to each normal vibrational mode of the molecule which enable numerically to describe the character of each mode and are carried out by SQM method$^{21,22}$ using the output files created at the end of the frequency calculations. The TED calculations are performed by using FP8 program.$^{25}$

4. RESULTS AND DISCUSSION

4.1. Molecular Geometry

In$_2$SnO$_3$ possess a ring molecular structure and belong to C$_{2v}$ point group symmetry. The optimized structure of the molecule is obtained from Gaussian 09 and GaussView program and is shown in Figure 1 with electron density surface map. The structure optimization and zero point vibrational energy of the compound in HF and DFT with 3-21G(d, p) are 6.43, 5.70, 5.80 and 5.90 kCal/mol, respectively. The present molecule is constructed by O–Sn–O and In–O–In bonds which are connected as loop. The shape of the molecular structure is changed in nanophase from bulk. So, the present molecule SnO$_2$ has attained a higher coordination and satisfied bonds in nanophase. The O$_3$ atom is symmetrically surrounded by In$_1$ and In$_2$ and separated by an angle 120.72° whereas the Sn atom is surrounded by O$_2$ and O$_3$ at an angle 88.41°. This view only by the attractive force difference between O and In/Sn.

Table I. Optimized geometrical parameters for In$_2$SnO$_3$ computed at HF and DFT [B3LYP; B3PW91 and MPW1PW91] methods with 3-21G(d, p) basis sets.

<table>
<thead>
<tr>
<th>Geometrical parameters</th>
<th>HF/ 3-21G(d, p)</th>
<th>B3LYP/ 3-21G(d, p)</th>
<th>B3PW91/ 3-21G(d, p)</th>
<th>MPW1PW91/ 3-21G(d, p)</th>
</tr>
</thead>
<tbody>
<tr>
<td>In$_1$–O$_1$</td>
<td>1.998</td>
<td>2.010</td>
<td>2.001</td>
<td>1.997</td>
</tr>
<tr>
<td>In$_1$–O$_2$</td>
<td>1.948</td>
<td>1.982</td>
<td>1.974</td>
<td>1.968</td>
</tr>
<tr>
<td>In$_1$–O$_3$</td>
<td>1.998</td>
<td>2.010</td>
<td>2.001</td>
<td>1.997</td>
</tr>
<tr>
<td>In$_2$–O$_1$</td>
<td>1.948</td>
<td>1.982</td>
<td>1.974</td>
<td>1.968</td>
</tr>
<tr>
<td>In$_2$–O$_2$</td>
<td>1.948</td>
<td>1.982</td>
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<tr>
<td>O$_3$–Sn$_2$</td>
<td>1.935</td>
<td>1.976</td>
<td>1.968</td>
<td>1.962</td>
</tr>
<tr>
<td>O$_3$–Sn$_3$</td>
<td>1.935</td>
<td>1.976</td>
<td>1.968</td>
<td>1.962</td>
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<tr>
<td>Bond angle (°)</td>
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<td></td>
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<tr>
<td>O$_3$–In$_1$–O$_3$</td>
<td>107.11</td>
<td>108.38</td>
<td>108.90</td>
<td>108.52</td>
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<tr>
<td>O$_3$–In$_2$–O$_3$</td>
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<td>108.38</td>
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<td>120.72</td>
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<td>In$_1$–O$_1$–Sn$_2$</td>
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<td>147.03</td>
<td>146.52</td>
<td>146.49</td>
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<td>In$_1$–O$_1$–Sn$_3$</td>
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<td>147.03</td>
<td>146.52</td>
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<td>Sn$_2$–O$_3$–O$_3$</td>
<td>89.25</td>
<td>87.96</td>
<td>88.41</td>
<td>88.50</td>
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<tr>
<td>Dihedral angle (°)</td>
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<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>O$_3$–Sn$_2$–O$_3$–Sn$_2$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>O$_3$–Sn$_2$–O$_3$–In$_3$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>O$_3$–Sn$_3$–O$_3$–O$_3$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>In$_1$–O$_1$–Sn$_2$–O$_3$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

4.2. Vibrational Assignments

The molecule In$_2$SnO$_3$ belongs to C$_{2v}$ point group symmetry which consists of 6 atoms, so it has 12 normal vibrational modes. Out of 12 fundamental vibrations of the molecule can be distributed as four stretching $B_2$ and $A_1$ symmetric and $A_2$ and $B_1$ asymmetric vibrations, i.e., $\Gamma_{\text{vib}} = 4A_1 + 4B_2 + 2A_2 + 2B_1$. The harmonic vibrational frequencies (un-scaled and scaled) calculated at HF and DFT levels using the double split valence basis set along with the diffuse and polarization functions, 3-21G(d, p) and observed FT-IR and FT-Raman frequencies for various modes of vibrations have been presented in Table II.

4.2.1. Sn–O Vibrations

Many simple metal oxides with more than one oxygen atom bound to a single metal atom usually absorb in the region 1020 cm$^{-1}$–970 cm$^{-1}$. Owing to the nano size effect, the Sn–O stretching vibrations are found in the region 800 cm$^{-1}$–300 cm$^{-1}$. The Sn–O stretching is usually observed around 670 cm$^{-1}$ and 560 cm$^{-1}$. In this present case, the Sn–O asymmetric and symmetric stretching vibrations appeared with very strong and
strong intensity at 840 cm\(^{-1}\) and 760 cm\(^{-1}\) respectively in bulk phase whereas the same are observed with strong and weak intensity at 832 cm\(^{-1}\) and 754 cm\(^{-1}\) respectively in nanophase as shown in Figure 3. The Sn–O in plane bending is identified at 400 cm\(^{-1}\) and 315 cm\(^{-1}\) in bulk and 493 cm\(^{-1}\) and 458 cm\(^{-1}\) in nanophase. The Sn–O out of plane bending is found at 150 cm\(^{-1}\) and 120 cm\(^{-1}\). But in nanophase, the out-of-plane bending is observed 220 cm\(^{-1}\) and 150 cm\(^{-1}\). When compared with bulk, there is no change in Sn–O stretching vibrations. But in the case of bending vibrations, the wavenumbers are shifted up to higher region of the spectra which is purely due to the change of bulk Sn–O to pseudo (super atoms) Sn–O.\(^{29}\) In addition to that, this view of change in bending vibrations and the presence of Raman bands ensure that the optical properties of nanomaterial are enhanced.\(^{38–41}\) The In–O stretching vibrations are observed with strong intensity at 570 cm\(^{-1}\) and 460 cm\(^{-1}\) in bulk phase whereas in nano phase the vibrations are at 604 cm\(^{-1}\) and 567 cm\(^{-1}\).

The In–O in plane bending is identified with medium and weak intensity at 190 cm\(^{-1}\) and 170 cm\(^{-1}\) in bulk and 427 cm\(^{-1}\) and 320 cm\(^{-1}\) in nanophase. The In–O out-of-plane bending is found at 110 cm\(^{-1}\) and 100 cm\(^{-1}\). But in nanophase, the out of plane bending is observed 110 cm\(^{-1}\) and 105 cm\(^{-1}\). In this case, the stretching and bending vibrations are moved up to higher region of the spectra which is also purely due to the change of bulk In–O to pseudo (super atoms) In–O.

### 4.2.2. Electronic Properties (HOMO-LUMO Analysis)

The calculations of the electronic structure of In\(_2\)SnO\(_3\) are optimized in singlet state. The low energy electronic excited states of molecule are calculated at the B3LYP/3-21G\(d,p\) level using the TD-DFT approach on the previously optimized ground-state geometry of the molecule. The calculations are performed with gas phase, DMSO.
and chloroform solvent effect. The calculated excitation energies, oscillator strength \( f \) and wavelength \( \lambda \) and spectral assignments are given in Table V. The major contributions of the transitions are designated with the aid of swizard program.\(^{34}\) TD-DFT calculations predict three transitions in the near ultraviolet region for the molecule under study. The strong transitions at 5045 nm with an oscillator strength \( f = 0.0037 \) in gas phase, the 5544 nm with an oscillator strength \( f = 0.0032 \) in ethanol and 5172 nm with an oscillator strength \( f = 0.0037 \) in DMSO are calculated and assigned to an \( n \rightarrow \pi^* \) transition. As can be seen, the calculations performed at Gas and ethanol is very close to each other when compared with DMSO phase. In view of calculated absorption spectra, the maximum absorption wavelength corresponds to the electronic transition from the HOMO to LUMO with 25% and from the HOMO to LUMO + 1 with 75% contribution.

The other wavelength, excitation energies, oscillator strength and calculated counterparts with major contributions are obtained in Table V. In nano phase, the strong transitions at 1984 nm with an oscillator strength \( f = 0.013 \) in gas phase. In nano phase the transition is shifted down due to the large Kubo gap \( \delta \) (bandgap). The frontier molecular orbitals play an important role in the electric and optical properties.\(^{42-45}\) The HOMO represents the ability to donate an electron, LUMO as an electron acceptor.

The 3D plots of the frontier orbitals, HOMO and LUMO for molecule are in gas, shown in Figure 4. According to Figure 4, LUMO is mainly localized over the O and Sn atoms and however HOMO is characterized by a charge distribution on O atoms jointly and In and Sn atom separately. In the case of LUMO-1, the \( P_i \) orbital lobes of In and O are overlapped. The HOMO \( \rightarrow \) LUMO transition implies an electron density transfer from Sn and In atom to O atom. The HOMO and LUMO energy is \(-1.0784 \text{ eV}\) in gas phase (bulk). Energy difference between HOMO and LUMO orbital is called as Kubo gap \( (\delta)\) that is an important stability for structures. The calculated energy gaps 1.0784 eV, but in nano phase Kubo gap is 4.079 eV. The increment of Kubo gap ensures the enhanced semiconductor property of the molecule.

### 4.2.3. NMR Analysis

NMR spectroscopy is currently used for structure of organic molecules as well as metal. The combined use of experimental and computer simulation methods offers a powerful way to interpret and predict the structure of large molecules. The optimized structure of In\(_2\)SnO\(_3\) is used to calculate the NMR spectra at the HF and DFT methods with \(3-21G(d,p)\) level using the GIAO method. The theoretical NMR chemical shifts of In\(_2\)SnO\(_3\) have been compared with the experimental data as shown in Table IV.

#### Table IV. Experimental and calculated NMR chemical shifts (ppm) of SnO\(_2\).

<table>
<thead>
<tr>
<th>Atom position</th>
<th>HF/3-21G(d,p) (ppm)</th>
<th>HF/6-31G(d)GIAO (ppm)</th>
<th>Shift (ppm)</th>
<th>B3LYP/3-21G(d,p) (ppm)</th>
<th>B3LYP/6-311+G(2d,p)GIAO (ppm)</th>
<th>Shift (ppm)</th>
<th>Nano phase (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>In(_{i})</td>
<td>-1922.51</td>
<td></td>
<td></td>
<td>819.57</td>
<td>-</td>
<td></td>
<td>-</td>
</tr>
<tr>
<td>In(_{0})</td>
<td>-1922.51</td>
<td></td>
<td></td>
<td>819.57</td>
<td>-</td>
<td></td>
<td>-</td>
</tr>
<tr>
<td>Sn(_{i})</td>
<td>-3208.39</td>
<td></td>
<td></td>
<td>263.68</td>
<td>-</td>
<td></td>
<td>-</td>
</tr>
<tr>
<td>O(_{i})</td>
<td>4054.39</td>
<td>-3731.29</td>
<td>323.10</td>
<td>3566.2</td>
<td>3246.20</td>
<td>320.0</td>
<td>63.51</td>
</tr>
<tr>
<td>O(_{0})</td>
<td>2412.11</td>
<td>-2089.01</td>
<td>323.10</td>
<td>1670.18</td>
<td>1350.18</td>
<td>320.0</td>
<td>-</td>
</tr>
<tr>
<td>O(_{i})</td>
<td>2412.11</td>
<td>-2089.01</td>
<td>323.10</td>
<td>1670.18</td>
<td>1350.18</td>
<td>320.0</td>
<td>-</td>
</tr>
</tbody>
</table>
Chemical shifts are reported in ppm relative to TMS for NMR spectra. Considering that the range of NMR chemical shifts for analogous metal-organic molecules usually is >100 ppm. The accuracy ensures reliable interpretation of spectroscopic parameters. In the present work, NMR chemical shifts in the SnO2 are 323.10 and 320.0 ppm, for HF/6-311 + G(2d, p)GIAO and B3LYP/6-311 + G(2d, p)GIAO respectively from TMS as in the Table IV. Sn and In atoms have the less electronegative property than oxygen atom. The Sn and In atoms are bonded to oxygen atom which shows high chemical shifts. The values of the chemical shift of HF and DFT are nearly same. The calculated chemical shift of the molecule in bulk phase is 323.10 and 320.0 ppm whereas in Nano phase 63.512 ppm as in the Table IV. From this observation, the diamagnetic shielding of In2SnO3 is also increased in nano phase which results change in magnetic property of the compound.

### 4.2.4. Molecular Electrostatic Potential (MEP) Maps

Molecular electrostatic potential is calculated at the B3LYP/3-21G(d, p) optimized geometry. The different values of the electrostatic potential at the surface are represented by different colors. Potential increases in the order red < orange < yellow < green < blue. The color code of these maps is in the range between −0.865 a.u. (deepest red) to 0.865 a.u. (deepest blue) in compound. The positive (blue) regions of MEP are related to electrophilic reactivity and the negative (green) regions to nucleophilic reactivity shown in Figure 5. As can be seen from the MEP map of the title molecule, the negative regions are mainly localized on the Oxygen atoms. A maximum positive region is localized on Indium and Sn atoms indicating a possible site for nucleophilic attack. The MEP map is shows that the negative potential sites are on electronegative atoms (O atom) as well as the positive potential sites are around the Indium atom. From these results, it is clear that the In atoms indicate the strongest attraction and O atom indicates the strongest repulsion.

#### 4.2.5. XRD Analysis

XRD shows complete oxidation of the alloy giving mainly cubic phase of In2O3 nanophase as shown in Figure 6. In the present study, the main aim was to get core shell structure of Indium and tin metallic alloy nano-powder. If the desired nanostructure is obtained having different molar ratio with 12 to 20 nm grain size, electron confinement is expected and one can look for single electron conduction through ITO nano-powder without the formation of a depletion region in the semiconductor region. The XRD data of the compound is presented in Table VI. If the desired core–shell structure is obtained having InSn alloy with 12 to 20 nm grain size as a core, electron confinement is expected and one can look for single electron conduction.
through ITO without the formation of a depletion region in the semiconductor region.\textsuperscript{46, 47} However, because of crystal structure difference, tetragonal for the alloy and either cubic (or orthorhombic) for the oxide, such a core–shell structure is not formed in our case.\textsuperscript{48} The alloy is partially oxidized with approximately 50% cubic phase and 50% orthorhombic phase as can be observed on TEM pictures.\textsuperscript{49}

We have studied the surface chemistry of ITO and we have found that several metal alkoxides can react with surface hydroxyl/(OH) groups to give well defined surface bound complexes of fixed stoichiometry.\textsuperscript{31–33}

4.2.6. EPR Studies

If (g) factor experimental and calculated values are equal the $e^{-n}$ around the orbit are free $e^{-n}$ spin, in orbital are explained in the Figure 7. EPR studies showed the concentration dependence of monitoring the In$^{3+}$ environment only lowers concentration of Sn$^{4+}$ in ITO particle monitor the cation site by getting substituted in it. Above 0.5 mol% Sn ions form correlated clusters, which lead to broadening. These EPR spectra were found to contain two different components, one from single isolated ions and the other from the clusters. Samples with 0.05 mol% Sn ions dopant (lower content) showed sextet due to single ion, also sharp line at $g = 1.5$ electronic.\textsuperscript{34} Electron Paramagnetic resonance spectra were measured on a Varian spectrometer with 100 kcs/s field modulation and operating at about 9.2 Gc/s. The signal enhancing runs were carried out using an analog digital converter, counting equipment and a 512-channel analysis (Webster and Jones, to be published). The sweep was triggered either by a sample of DPPH or by the strong control line (ml = 0) of the F centre.\textsuperscript{35} The $g$ values were measured using DPPH taking $g = 2.0036$, in all spectra shown the magnetic field increases from left to right. The line-width quoted corresponds to the distance between the points of maximum slope of the absorption curve. The analysis has been carried out for ITO crystalline samples with different proportion. The 'g' factor of ITO.

$$g = 1 + \frac{S(S + 1) + J(J + 1) - I(I + 1)}{2J(J + 1)}$$

Where $J = l \pm s$ where sand $l$ are spin orbital angular quantum number. When $L = 0$ $S = J = 2.00$. Atomic number of in is 49 electronic configurations is [Kr] 4 d10 5s2 5p1.\textsuperscript{36–37}

5. CONCLUSION

In this work, pure and singe phase In$_2$SnO$_3$ nanopowder is successfully prepared with the doping ratio of 80–20% (In$_2$O$_3$–Sn) by simple sol–gel combustion direction. The material is characterized by XRD measurements and their geometrical parameters are compared with calculated values. The FT-IR and NMR spectra are recorded in both bulk and nanophas e and FT-Raman spectrum is recorded in bulk phase and the fundamental frequencies are assigned. The optimized parameters and the frequencies are calculated using HF and DFT (B3LYP, B3PW91 and MPW1PW91) theory in bulk phase of In$_2$SnO$_3$ and are compared with its nanophase. The vibrational frequency pattern in nanophase gets realigned and the frequencies are shifted up and down little bit to the region of spectra when compared with bulk phase. The UV-visible spectrum is simulated and analyzed. The frontier molecular orbital analysis

**Table VI.** XRD analysis of for In$_2$SnO$_3$.

<table>
<thead>
<tr>
<th>Atom</th>
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References and Notes

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