

# Structural and optical characterizations of BaSnO<sub>3</sub> nanopowder synthesized by aqueous sol-gel method

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## Abstract

Precursor gel for preparation of nanocrystalline  $BaSnO_3$  powder was synthesised by aqueous sol-gel method using  $Ba(OH)_2 \cdot 8H_2O$  and  $Na_2SnO_3 \cdot 3H_2O$  as raw materials. Thermogravimetric and differential scanning calorimetric analyses of the raw materials, precursor gel and a mechanical mixture of raw materials were carried out to understand the mechanisms involved in the formation of the single phase  $BaSnO_3$ . Based on the thermal analysis, the precursor gel was calcined at 400, 800 and 1400 °C for 4 h to obtain pure phase  $BaSnO_3$ powder. X-ray diffraction pattern of the powder calcined at 1400 °C was refined for atomic coordinate, lattice parameter (a = 4.1117(2)Å) and occupancies using Rietveld refinement analysis. The average crystallite size calculated from the Scherrer formula is ~35 nm. Transmission electron micrograph of the powders confirmed that particle sizes are in range of 20–40 nm. The phase purity of the powder calcined at 1400 °C was further examined by Fourier transform infrared spectroscopy. Optical properties of the  $BaSnO_3$  powder were studied by UV-visible absorption and photoluminescence (PL) spectra. The band gap energy (3.09 eV) obtained from the Tauc plot confirmed the semiconductor nature of the powder. The CIE coordinate corresponding to PL spectrum exhibited an intense emission in the visible region.

Keywords: BaSnO<sub>3</sub>, sol-gel, structural characterization, optical properties

## I. Introduction

In the last decade,  $BaSnO_3$  has drawn attention due to its properties, such as n-type semiconductivity [1], high electrical conductivity and optical transparency in visible region [2–4].  $BaSnO_3$  has been used as solid state gas sensor [5,6], an electrode material for the dyesensitized solar cell [7], anode material for lithium-ion battery [8], photocatalyst [9] and proton conductor for fuel cell [10]. The various methods were used to prepare barium stannate such as: high temperature solid state [11], sol-gel combustion [12,13], hydrothermal [14], polymeric precursor [15], lyothermal [16], wet chemical [17], chemical precipitation [18] and reverse micelles method [19]. Among the reported chemical methods, an aqueous sol-gel method is found to be a simple, costeffective and low-temperature chemical method for the synthesis of BaSnO<sub>3</sub>. For the same preparative method, the selection of reactants for the formation of BaSnO<sub>3</sub> plays a crucial role in quality control and hence properties of the powder. Efforts have been made to synthesize BaSnO<sub>2</sub> nanopowder at a lower temperature by using different Ba and Sn compounds [20]. Huang et al. [21] tried to use lower temperature by ball-milling a mixture of BaCO<sub>3</sub>-SnO<sub>2</sub> for prolonged period of 40 h in an air atmosphere and showed that the formation of BaSnO<sub>3</sub> was initiated at temperature 820 °C. Cerda et al. [12] synthesized BaSnO<sub>3</sub> at 1100 °C by an aqueous sol-gel method using  $Ba(OH)_2$  and  $K_2SnO_3$ . The used method seems to be a simple and cost-effective in terms of less number of steps involved in the preparation, but in this report details about the mechanism of the formation of BaSnO<sub>3</sub> powder have not been discussed. Therefore, in the present work, an attempt has been made to understand each and every step involved in the formation of phase pure nanocrystalline BaSnO<sub>3</sub> powder by an aqueous sol-gel method using Ba(OH)<sub>2</sub> and Na<sub>2</sub>SnO<sub>3</sub> as raw

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materials. The intension behind using  $Na_2SnO_3$  in place of  $K_2SnO_3$  used by earlier authors is that sodium is more reactive than potassium and hence it could more easily react with water and form NaOH which will accelerate reaction rate. Simultaneous thermogravimetric (TG) and differential scanning calorimetric (DSC) analysis and XRD techniques were used to understand the formation mechanism of BaSnO<sub>3</sub> nanocrystals. Structural and optical characterizations of the obtained phase pure BaSnO<sub>3</sub> powder were performed with different techniques.

### **II. Experimental**

#### 2.1. Powder synthesis

The stoichiometric amounts of raw materials,  $Na_2SnO_3 \cdot 3H_2O$  (99% purity, Molychem) and  $Ba(OH)_2 \cdot 8H_2O$  (98% purity, Molychem), were dissolved separately in minimum quantities of distilled water. The solutions of barium hydroxide and sodium stannate were mixed homogeneously using a magnetic stirrer maintained at a constant rotation speed of 200 rpm for 3 h at 80 °C. pH of the solution was measured several times using a digital pH meter and found to be ~11. Thereafter, the solution was heated on a hot plate at 150 °C for several hours until formation of gel took place. The precursor gel was calcined at 400, 800 and 1400 °C for 4 h.

#### 2.2. Powder characterization

Thermal analysis of the raw materials, precursor gel and mechanical mixture of raw materials were carried out in the temperature range 25–1000 °C in a simultaneous TG/DSC setup (Mettler Toledo) with a heating rate 10 °C/min in a nitrogen gas atmosphere. Phase identification and structural characterization of the obtained powders were carried out using a Rigaku Mini Flex-II desktop X-ray diffractometer, with Ni-filtered Cu-K $\alpha$ (1.5405 Å) radiation at 30 kV and 20 mA. XRD patterns of the calcined powder were recorded over the angular range 20°  $\leq \theta \leq 80^\circ$  with step size 0.02° (2 $\theta$ ). Transmission electron micrographs (TEM) of the obtained powders were recorded using FEI Tecnai Model G2 series. The specimen was prepared by dispersing the powder in ethyl alcohol by ultra-sonication for 1 h. Thereafter, the solution was poured on a commercial carbon-coated copper grid and dried in a petri dish at 60 °C for 2 h in a hot air oven. Fourier transform infrared (FTIR) spectrum of the samples was recorded using Fourier transform infrared spectrometer (Shimadzu, Model DF 803) using KBr pellet method in the wave number range 400–4000 cm<sup>-1</sup>. The UV-visible spectrum of the synthesized BaSnO<sub>3</sub> nanopowder was recorded (Shimandzu, model UV-1700) using ethylene glycol as a suspension medium. The photoluminescence spectroscopy (PL) of the nanopowder was performed using Horiba photometry with Xe lamp as a source.

#### III. Results and discussion

#### 3.1. Thermal analysis

Figure 1a shows TGA-DSC curves of the raw material  $Ba(OH)_2 \cdot 8H_2O$ . TGA curve exhibits total weight loss of ~48% within the measured temperature range of 25–1000 °C in three steps. The first step weight loss (42.88%) in the temperature range of 30–150 °C accompanied by an endothermic peak around 90 °C is attributed to expulsion of physically absorbed water molecules according to the reaction (1):

$$Ba(OH)_2 \cdot 8H_2O \longrightarrow Ba(OH)_2 + 8H_2O$$
 (1)

However, the experimentally observed weight loss (42.88%) is slightly lower than the theoretical weight loss (~45%) calculated according to the reaction (1). This indicates that complete expulsion of water molecules (8 moles) is not taking place, may be due to the fast heating rate (10 °C/min) used during TGA data collection. The second step weight loss (~2%) accompanied by an endothermic peak around 384 °C is associated with removal of remaining water molecules. TGA curve of Ba(OH)<sub>2</sub> · 8 H<sub>2</sub>O observed in this work is in agreement with the TGA curve reported in the literature for this hydroxide [22]. The third step weight loss



Figure 1. The simultaneous TGA-DSC curves of starting materials: a) Ba(OH)<sub>2</sub> · 8 H<sub>2</sub>O and b) Na<sub>2</sub>SnO<sub>3</sub> · 3 H<sub>2</sub>O

(3.12%) in the temperature of 600–700 °C corresponds to the loss of water molecules produced during conversion of Ba(OH)<sub>2</sub> into BaO described with reaction (2):

$$Ba(OH)_2 \longrightarrow BaO + H_2O$$
 (2)

TGA-DSC curves of  $Na_2SnO_3 \cdot 3H_2O$  are shown in Fig. 1b. Total weight loss of 17.05% has been observed in the entire range of temperature measurement. The observed experimental weight loss is less than the theoretical weight loss (20%) calculated according to equation (3):

$$Na_2SnO_3 \cdot 3H_2O \longrightarrow Na_2SnO_3 + 3H_2O$$
 (3)

The weight loss of 17.05% occurs in two steps. The first step of weight loss (11.22%) was observed in the temperature range 27-300 °C and is assigned to the expulsion of water molecule according to reaction (4):

$$Na_2SnO_3 \cdot 3H_2O \longrightarrow Na_2SnO_3 \cdot H_2O + 2H_2O \quad (4)$$

In the literature, it is reported that dissociation of anhydrous  $Na_2SnO_3$  into  $Na_2O$  and  $SnO_2$  occurs at 900 °C. In our case  $Na_2SnO_3$  is in hydrated form, therefore, dissociation may take place at a temperature lower than 900 °C. Accordingly, the second step weight loss (6.05%) observed in the temperature range 300–1000 °C is accompanied by an exothermic peak around 750 °C assigned to the dissociation of hydrated sodium stannate into sodium and tin oxides and gradual loss of chemically adsorbed water molecule according to reaction (5):

$$Na_2SnO_3 \cdot H_2O \longrightarrow Na_2O + SnO_2 + H_2O$$
 (5)

The result obtained from the TGA-DSC analysis of  $Na_2SnO_3 \cdot 3H_2O$  is in agreement with earlier reports [23].

A stoichiometric mixture of the raw materials  $Ba(OH)_2 \cdot 8H_2O$  and  $Na_2SnO_3 \cdot 3H_2O$  for the formation of  $BaSnO_3$  by solid state ceramic route was prepared by their mechanical mixing in an agate mortar for 1 h using acetone as mixing media. The TGA-DSC curves of the

obtained mixture were shown in Fig. 2a. The curves display combined features of both components as shown in Fig. 1, i.e. Ba(OH)<sub>2</sub> converts into BaO (above 700 °C) and Na<sub>2</sub>SnO<sub>3</sub> into Na<sub>2</sub>O and SnO<sub>2</sub> (above 750 °C). In the measured temperature range, BaO, Na<sub>2</sub>O, and SnO<sub>2</sub> oxides are retaining their individuality, and no chemical reaction between them is taking place to form BaSnO<sub>3</sub> phase or any other phase up to 1000 °C. In other words, the formation of BaSnO<sub>3</sub> by solid state ceramic route using  $Ba(OH)_2 \cdot 8H_2O$  and  $Na_2SnO_3 \cdot 3H_2O$  may not take place before 1000 °C. In this work, the thermal analysis of a physical mixture of  $Ba(OH)_2 \cdot 8H_2O$  and  $Na_2SnO_3 \cdot 3H_2O$  was carried out just to show if the formation of BaSnO<sub>3</sub> is possible by solid state route or not. In order to understand the mechanism of the formation of BaSnO<sub>3</sub> using Ba(OH)<sub>2</sub>  $\cdot$  8 H<sub>2</sub>O and Na<sub>2</sub>SnO<sub>3</sub>  $\cdot$  3 H<sub>2</sub>O in a solid form more studies are required.

In the present work BaSnO<sub>3</sub> powder was synthesised using  $Ba(OH)_2 \cdot 8H_2O$  and  $Na_2SnO_3 \cdot 3H_2O$  by an aqueous sol-gel method and formation mechanism of BaSnO<sub>3</sub> has been studied in detail. The TGA-DSC curves of the dried precursor gel powder are shown in Fig. 2b. It is noticed that TGA-DSC curves of the precursor gel powder are entirely different from the TGA-DSC curves of a mechanical mixture of starting materials (Fig. 2a). TGA curve of the precursor gel shows total weight loss (2%) in three steps. The first step weight loss between 25-150 °C (0.22%) may be due to the dehydration of water, the second step weight loss (0.48%) in the temperature range of 600-720 °C is attributed to the decomposition of BaCO<sub>3</sub>. The third weight loss (1.30%) is accompanied by a small endothermic peak (at 800 °C) and attributed to the reaction between BaCO<sub>3</sub> and SnO<sub>2</sub> to form BaSnO<sub>3</sub>. Weight loss of only 1.3% in the third step indicates that precursor gel powder already contains more than 90% of BaSnO<sub>3</sub> phase. Remaining 10% of gel powder contains impurity phases BaCO<sub>3</sub> and SnO<sub>2</sub>. These impurity phases react with each other to form BaSnO<sub>3</sub> phase around 800 °C, which is evident from a small endothermic peak in DSC curve. Therefore, it is clear that formation of BaSnO<sub>3</sub> using  $Ba(OH)_2 \cdot 8H_2O$  and  $Na_2SnO_3 \cdot 3H_2O$  by an aque-



Figure 2. The simultaneous TGA-DSC curves of: a) mechanical mixture of raw materials and b) precursor powder gel

ous sol-gel method takes place at a lower temperature than solid state ceramic route. Based on the TGA-DSC results of precursor gel it is assumed that starting from the solution up to the formation of the gel, following possible reactions could take place:

$$Ba(OH)_2 \cdot 8 H_2O + H_2O \longrightarrow Ba^{2+} + 2 [OH]^- \quad (6)$$

$$Na_2SnO_3 + 3H_2O \longrightarrow 2Na^+ + [Sn(OH)_6]^{2-}$$
(7)

$$[Sn(OH)_6]^{2-} + Ba^{2+} \longrightarrow BaSn(OH)_6$$
(8)

$$2 \operatorname{Na}^{+} + 2 \operatorname{OH}^{-} \longrightarrow 2 \operatorname{NaOH}$$
(9)

$$BaSn(OH)_6 \longrightarrow BaSnO_3 + 3H_2O$$
(10)

 $Ba^{2+}$  ions react very easy with  $CO_2$ . Therefore, those  $Ba^{2+}$  ions which are present on the surface of the solution may react with the  $CO_2$  present in the atmosphere to form  $BaCO_3$  phase. Similarly,  $Sn^{4+}$  ions may also react with the  $O_2$  present in the ambient atmosphere and form  $SnO_2$  phase.

#### 3.2. XRD analyses

X-ray diffraction patterns of the precursor gel and the powders obtained after calcination of the precursor gel powder at 400, 800 and 1400 °C for 4 h are shown in Fig. 3. It can be noticed that XRD patterns of the precursor gel and powder calcined at 400 °C are similar and mainly amorphous in nature with some diffraction peaks of BaCO<sub>3</sub> and SnO<sub>2</sub> phases, which are well matched to the JCPDS file no 05-0378 and 41-1445, respectively. Therefore, the formation of BaCO<sub>3</sub> and SnO<sub>2</sub> phases



Figure 3. X-ray diffraction pattern BaSnO<sub>3</sub> of powder calcined at different temperatures

have taken place by reaction of  $Ba^{2+}/Sn^{4+}$  ions (from  $Ba(OH)_2 \cdot 8 H_2O$  and  $Na_2SnO_3 \cdot 3 H_2O$ ) present in the water solutions with  $CO_2/O_2$  gasses present in the atmosphere as discussed in TGA-DSC section.

XRD pattern of the powder calcined at 800 °C contains mainly diffraction peaks of BaSnO<sub>3</sub> phase (JCPDS file no. 15-0780) except for a weak XRD peak (~23.8°) of BaCO<sub>3</sub> phase. It was reported in the literature [24] that formation of BaSnO<sub>3</sub> using commercially available BaCO<sub>3</sub> and SnO<sub>2</sub> by conventional solid state ceramic method requires temperature  $\geq 1000$  °C. In this work, the thermal analysis of a mechanical mixture of  $Ba(OH)_2 \cdot 8H_2O$  and  $Na_2SnO_3 \cdot 3H_2O$  also confirmed that formation of BaSnO<sub>3</sub> by solid state ceramic route will take place at temperatures >1000 °C. In XRD pattern of the powder calcined at 1400 °C only peaks of  $BaSnO_2$  phase are present which shows that the powder obtained at this temperature is devoid of any impurity phase. Reitveld refinement of the XRD data of the powder calcined at 1400 °C was performed using software Full Proof and it is shown in Fig. 4. Based on the Rietveld analysis the structure of the synthesized BaSnO<sub>3</sub> powder was found to be cubic perovskite structure with space group Pm3m and its crystal structure is shown as the inset in Fig. 4. The lattice parameters obtained by the Rietveld refinement ( $a = 4.11172 \pm 0.0015$  Å, unit cell volume  $V = 69.38 \text{ Å}^3$  and theoretical density  $\rho =$  $7.277 \text{ g/cm}^3$ ) are in good agreement with the values re-



Figure 4. X-ray Rietveld refinement of BaSnO<sub>3</sub> powder calcined at 1400 °C (Yobs, Ycal, Yobs-Ycal and Bragg's positions represent the experimental data, calculated data, the difference between the two and Bragg's positions, respectively)

Table 1. Atomic coordinates and occupancies of elements of  ${\rm BaSnO}_3$ 

Atom	Site	x	у	Ζ	В	Occ.
Sn	1a	0	0	0	1.02	1
Ba	1b	0.5	0.5	0.5	0.89	1
0	3d	0.5	0	0	0.56	3

No.	Plane	2θ [°]	Powder calcined at 800 °C		Powder calcined at 1400 °C		
			β[°]	<i>D</i> [nm]	β[°]	<i>D</i> [nm]	
1	(110)	30.62	0.2833	29.08	0.2099	39.20	
2	(111)	37.82	0.3048	30.92	0.2166	38.80	
3	(200)	44.92	0.1466	37.31	0.2521	34.00	
4	(211)	54.44	0.3277	27.27	0.2942	30.40	
5	(220)	63.85	0.4196	22.31	0.3427	28.35	
6	(310)	72.41	0.4477	22.00	0.3955	33.45	
			Average size is 28.14		Average size is 34.80		

Table 2. Plane, diffraction angle (2 $\theta$ ), full width at half maximum ( $\beta$ ) and crystallite size (D) of powders obtained after heat treatment at 800 °C and 1400 °C

ported in the literature [25]. Atomic coordinates and occupancies are given in Table 1. The fitting parameters obtained after the refinement are  $\chi^2 = 5.90$ ,  $R_p = 8.8\%$ ,  $R_{wp} = 8.18$ .

The crystallite sizes *D* were calculated using Scherrer's formula:

$$D = \frac{0.9\lambda}{\beta \cdot \cos \theta_{max}} \tag{11}$$

where  $\lambda$  is wavelength of X-rays,  $\beta$  is the full width at half maximum of the particular (*h k l*) plane in radians and  $\theta_{max}$  is the corresponding incident angle. The value of crystallite size of powders obtained after calcination at 800 °C and 1400 °C are given in Table 2. The average crystallite size of the powders obtained after calcination at 800 and 1400 °C is ~28 nm and 35 nm, respectively.

#### 3.3. Transmission electron microscopy analyses

Transmission electron micrograph (TEM) of the precursor gel calcined at temperature 1400 °C for 4 h is shown in Fig. 5a. According to the TEM results it is clear that particles have sizes in the range from 10 to 40 nm and cubic shape similar to their unit cell. Histogram of the particle size distribution, obtained using software ImageJ, is shown in Fig. 5b. From the particle size distribution fitted by Gaussian function the average grain size was calculated to be 25 nm, which is slightly lower than the crystallite size ~35 nm (Table 1) calculated using Scherrer's formula. Selected area electron diffraction (SAED) pattern of the powder, presented in Fig. 5c, shows sparser ring pattern typically exhibited by poly-crystalline materials [26]. It is verified that diffraction spots present in the SEAD pattern belong to BaSnO<sub>3</sub>. The Miller indices (*h k l*) of diffracting planes were calculated using values of inter planar spacing, *d*, obtained from the pattern. These values are 1.475, 1.861, 2.359 and 1.646 Å and corresponding Miller indices of planes are (220), (102), (111) and (112). The average value of the lattice parameter calculated using SAED is 4.11204 Å which is consistent with value (4.11172 Å) obtained from the Rietveld refinement of X-ray diffraction data.

#### 3.4. Fourier transform infrared spectroscopy

Fourier transform infrared (FTIR) spectra of the synthesized powders were recorded to check the presence of BaCO<sub>3</sub>, the most commonly found impurity phase detected in the preparation of BaSnO<sub>3</sub>. According to the reported literature [27], FTIR was found to be the most sensitive technique for the detection of  $BaCO_3$  (down to 0.6%). FTIR spectra of the BaSnO<sub>3</sub> powders calcined at 800 and 1400 °C are shown in Fig. 6. The distinct feature of the FTIR spectra is a band around 640 cm<sup>-1</sup> characteristic for stretching mode of Sn-O bonds [28]. The presence of this band confirms the formation of BaSnO<sub>3</sub> phase. The width of this band is particle size dependent. Therefore, the width of the band is broad for the powder calcined at 1400 °C as compared to the powder calcined at 800 °C. Moreover, FTIR spectrum of the powder calcined at 800 °C has a few more bands. The weak absorption bands around 850, 1050 and 1430 cm<sup>-1</sup>



Figure 5. TEM image (a), Gaussian distribution plot (b) and selected area electron diffraction pattern (c) of prepared BaSnO<sub>3</sub> sample calcined at temperature 1400 °C



Figure 6. FTIR spectra of BaSnO<sub>3</sub> powder calcined at two different temperatures

in the FTIR spectrum of the powder calcined at 800 °C indicate the presence of impurity  $BaCO_3$  phase [29]. In the FTIR spectra of the powder at 800 °C there is also a wide band of –OH group observed at 3200 cm<sup>-1</sup>. On the other hand, all observed bands in the spectrum of the powder calcined at 1400 °C match with bands present in the FTIR spectrum of the pure phase  $BaSnO_3$  reported in the literature [30].

#### 3.5. UV-visible spectroscopy

The absorption spectrum of the powder calcined at 1400 °C was recorded in the wavelength range 200–800 nm by dispersing powder in ethylene glycol and it is shown in Fig. 7a. The absorption spectrum of  $BaSnO_3$  powder synthesized in this work is similar to the spectrum exhibited by wide band gap semiconductor oxide [31]. The spectrum shows an absorption band around 445 nm which is due to the electron transfer from the top of the valance band to the bottom of the conduction band [32]. The band gap energy is the energy difference between the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO) and

is termed as  $E_g$ . A better estimation of the band gap energy ( $E_g$ ) was also obtained using Tauc's relation. According to this relation, the absorption coefficient for a direct band gap material is given by:

$$\alpha \cdot h \cdot \nu = B \cdot \left(h \cdot \nu - E_g\right)^m \tag{12}$$

where B is a constant independent of energy,  $E_g$  optical band gap energy, h is Planck's constant, v is frequency of the incident photon and *m* is an index which depends on the nature of electronic transition responsible for the optical transition ( $m = \frac{1}{2}$  for direct transition and m = 2for non-direct transition). Tauc's plot (using data shown in Fig. 7a) for band gap energy calculation was generated and shown in Fig. 7b. The direct energy band gap can be obtained from the intercept of the resulting linear region with the energy axis at  $(\alpha \cdot h \cdot \nu)^2 = 0$ . The band gap was calculated and found to be 3.09 eV, which is in agreement with value reported in the literature [31,32]. Slight difference in the value of energy band gap obtained from Fig. 7 may be due to the quantum size effect described by Koferstein and Yakuphanoglu [33], i.e. as the particle size of the system decreases the gap between the conduction band and the valance band also known as band gap of the material increases.

## 3.6. Photoluminescence (PL) spectroscopy

The photoluminescence spectrum (PL) of the powder calcined at 1400 °C (Fig. 8a) was recorded by exciting the powder using a source with the wavelength of 380 nm. The transitions between energy levels of constituent elements barium (Ba) and tin (Sn) of the compound BaSnO<sub>3</sub> cause emissions. The emission peaks exhibited by the synthesized powder are identified using data prepared by Sansonetti and Martin [34] and given in Table 3. This result indicates that the material has luminescence properties and it gives the intense emission in the visible region due to the transfer of charge between Sn<sup>2+</sup>-O<sup>2-</sup> levels [35]. Besides this strong intensity emission, spectrum also exhibits few emissions of weak intensity. The weak intensity emissions may



Figure 7. Absorption spectra of BaSnO<sub>3</sub> powder (a) and plot of  $(\alpha \cdot h \cdot v)^2$  vs. photon energy (b)



Figure 8. Photoluminescence (PL) spectra of BaSnO<sub>3</sub> powder calcined at 1400 °C (a) and CIE plot of photoluminescence spectrum of calcined powder (b)

No.	Wavelength [nm]	Barium (Ba)	Tin (Sn)
1	415	${}^{2}\mathrm{P}_{1/2}^{0}-{}^{2}\mathrm{D}_{3/2}$	
2	443		${}^{1}S_{0} - {}^{1}P_{1}^{0}$
3	464	${}^{2}S_{1/2} - {}^{2}P_{3/2}^{0}$	
4	499	${}^{2}S_{1/2} - {}^{2}P_{1/2}^{0}$	
5	514		${}^{2}P_{1/2}^{0} - {}^{2}D_{3/2}$
6	622	${}^{3}D_{3} - {}^{3}D_{3}^{0}$	

Table 3. Wavelength corresponding to different transitions

be attributed to the presence of defects in the material. The commission international del'Eclairage (CIE) coordinate has been calculated from the photoluminescence spectrum and indexed in CIE graph as shown in Fig. 8b. The CIE coordinate for BaSnO<sub>3</sub> obtained at 1400 °C is found to be x = 0.40, y = 0.35, which indicates that the emission has the contribution of red, blue and green (RBG). Therefore, the synthesized BaSnO<sub>3</sub> having emission in the visible region can find various applications in optical devices application like other phosphor materials [36].

#### **IV.** Conclusions

Thermal analysis of a stoichiometric mechanical mixture of  $Ba(OH)_2$  and  $Na_2SnO_3$  raw materials confirmed that no reaction between these starting materials takes place up to 1000 °C. However, when an aqueous solution of these starting materials was mixed and heated at 150 °C, amorphous phase of  $BaSnO_3$  along with minor amounts of impurity phases  $BaCO_3$  and  $SnO_2$  occurred at 150 °C and crystallization of  $BaSnO_3$  phase appeared at 800 °C. The phase pure  $BaSnO_3$  powder was obtained after calcination at 1400 °C for 4 h. FTIR also confirmed that the  $BaSnO_3$  powder obtained at 800 °C is contaminated with a trace amount of  $BaCO_3$ , whereas the powder obtained at 1400 °C is devoid of any impurity phase. TEM studies confirmed that the powder calcined at 1400 °C has cubical shape

particles of ~25 nm in size, whereas XRD and Rietveld refinement showed that the powder has cubic structure with the lattice parameter a = 4.1117(2) Å. The band gap determined from the UV-visible absorption spectrum of the phase pure BaSnO<sub>3</sub> powder is 3.09 eV which confirmed its semiconductor nature. PL spectra recorded in emission mode exhibited few intense peaks in the visible range. The corresponding CIE plot shows that the emission spectra of BaSnO<sub>3</sub> have the equal contributions of red, blue, and green which makes this material a promising candidate for the luminescence applications.

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