

Supporting Information

Effect of pH, surfactant and temperature on mixed phase structure and band gap properties of BiNbO₄ nanoparticles prepared using different routes

Maram Bakiro^a, Salwa Hussein Ahmed^a and Ahmed Alzamly^{a}*

^a Department of Chemistry, UAE University, P.O. Box 15551, Al-Ain, UAE

*Corresponding author: ahmed.alzamly@uaeu.ac.ae

Equations used in calculation

In the BiNbO₄ orthorhombic structure, the plane spacing d is related to the lattice constants a , b , c and the Miller indices by the following relations

$$d_{(hkl)} = \frac{abc}{\sqrt{(h^2b^2c^2 + k^2a^2c^2 + l^2b^2a^2)}} \quad (1)$$

And the unit cell volume V , can be calculated from the following equation:

$$V = abc \quad (2)$$

However, in the BiNbO₄ triclinic structure, the plane spacing d is related to the lattice constants a , b , c and the Miller indices by the following relations:

$$\frac{1}{d_{(hkl)}} = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2klb^*c^* \cos \alpha^* + 2lhc^*a^* \cos \beta^* + 2kha^*b^* \cos \gamma^* \quad (3)$$

$$a^* = \frac{bc \sin \alpha}{V} \quad (4)$$

$$b^* = \frac{ca \sin \beta}{V} \quad (5)$$

$$c^* = \frac{ab \sin \gamma}{V} \quad (6)$$

$$\cos \alpha^* = \frac{\cos \beta \cos \gamma - \cos \alpha}{\sin \beta \sin \gamma} \quad (7)$$

$$\cos \beta^* = \frac{\cos \gamma \cos \alpha - \cos \beta}{\sin \gamma \sin \alpha} \quad (8)$$

$$\cos \gamma^* = \frac{\cos \alpha \cos \beta - \cos \gamma}{\sin \alpha \sin \beta} \quad (9)$$

$$V = 2bc \sqrt{\sin s \cdot \sin(s - \alpha) \sin(s - \beta) \cdot \sin(s - \gamma)} \quad (10)$$

Where $s = \frac{1}{2}(\alpha + \beta + \gamma)$

%Triclinic content.

Table S1. %Triclinic in Samples Prepared Using Co-Precipitation Method at 750 °C.

	CPT-pH=2	CPT-pH=7	CPT-pH=10
Mean	45.5625	86.4075	75.9500
Std. Deviation	4.18040	6.02874	9.54446
Std. Error of Mean	2.09020	3.01437	4.77223

Table S2. %Triclinic in Samples Prepared Using Hydrothermal Method at 750 °C.

	Hydrothermal-pH=2	Hydrothermal-pH=7	Hydrothermal-pH=10
Mean	60.1350	73.9228	92.2475
Std. Deviation	6.39166	8.06165	0.90644
Std. Error of Mean	3.19583	4.03083	0.45322

Table S3. %Triclinic in Samples Prepared Using Citrate Method at 750 °C.

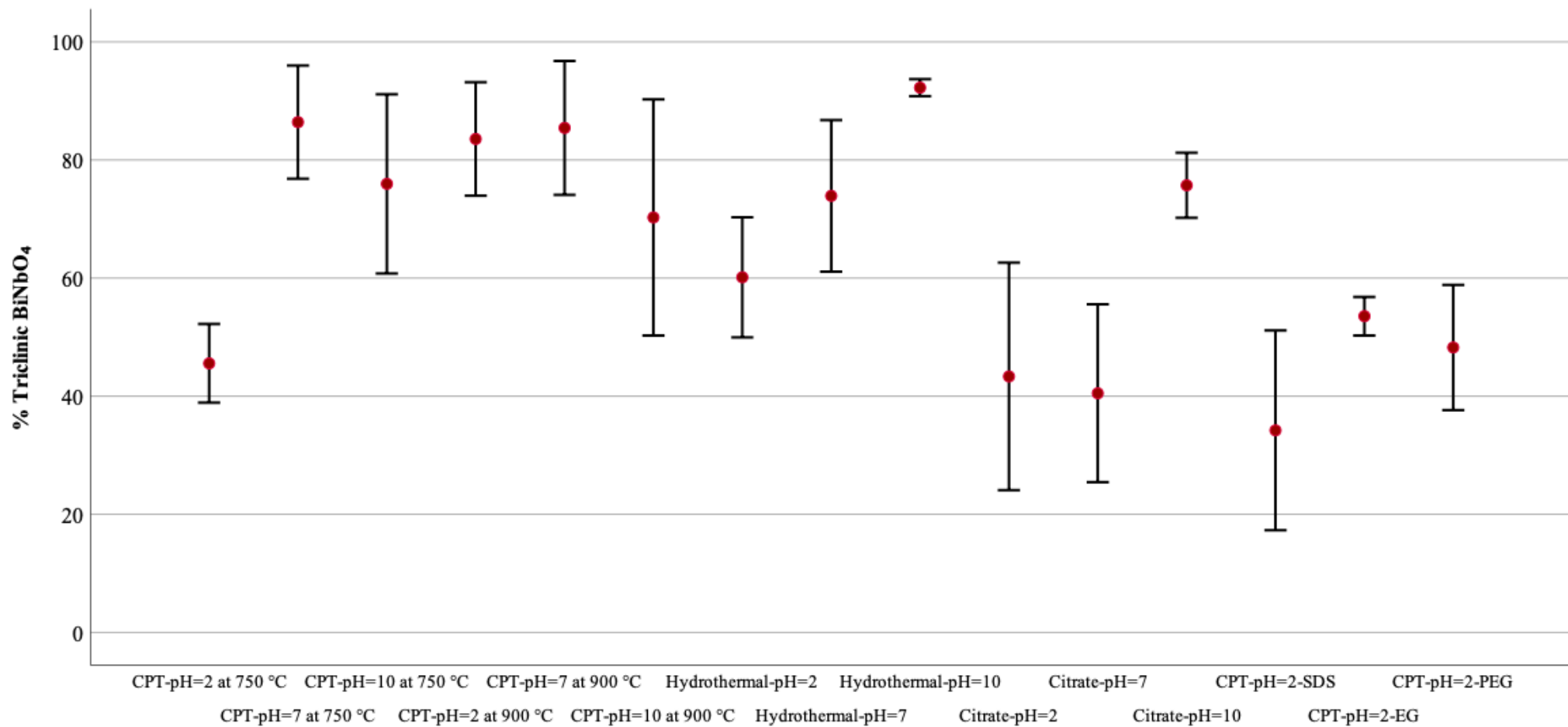
	Citrate-pH=2	Citrate-pH=7	Citrate-pH=10
Mean	43.3525	40.4950	75.7125
Std. Deviation	12.10862	9.46539	3.45900
Std. Error of Mean	6.05431	4.73270	1.72950

Table S4. %Triclinic in Samples Prepared Using Co-Precipitation Method at 750 °C with Different Surfactants Added.

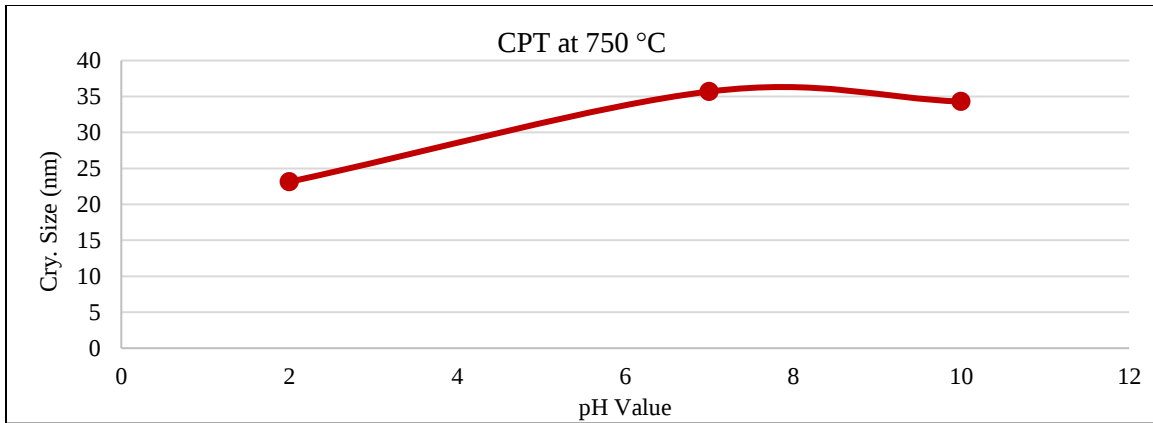
	CPT-pH=2	CPT-pH=2-SDS	CPT-pH=2-EG	CPT-pH=2-PEG
Mean	45.5625	34.2063	53.5500	48.2450
Std. Deviation	4.18040	10.63029	2.05115	6.66931
Std. Error of Mean	2.09020	5.31514	1.02557	3.33465

Table S5. %Triclinic in Samples Prepared Using Co-Precipitation Method at 750 °C and 900 °C.

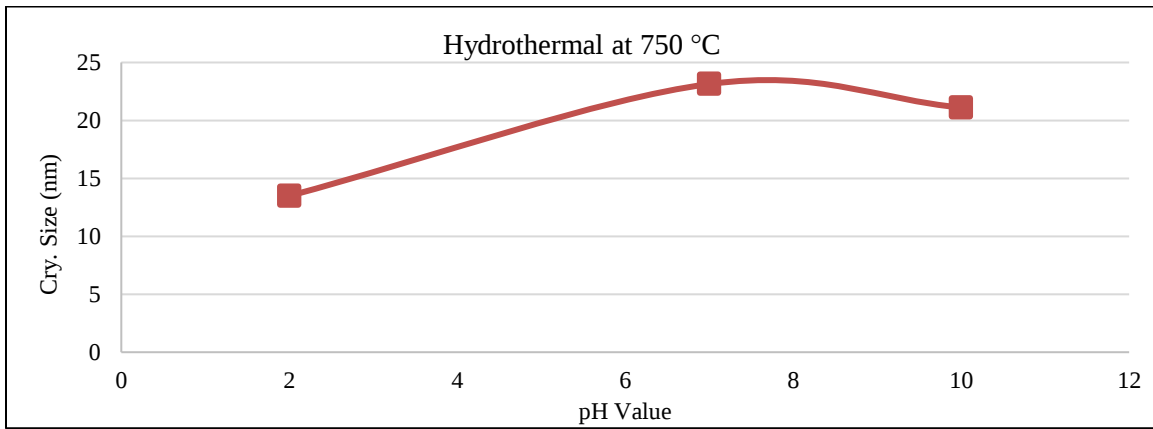
	CPT pH=2 at 750 °C	CPT pH=7 at 750 °C	CPT pH=10 at 750 °C	CPT pH=2 at 900 °C	CPT-pH=7 at 900 °C	CPT-pH=10 at 900 °C
Mean	45.5625	86.4075	75.9500	83.5580	85.4325	70.2675
Std. Deviation	4.18040	6.02874	9.54446	6.04369	7.12445	12.57059
Std. Error of Mean	2.09020	3.01437	4.77223	3.02184	3.56223	6.28529



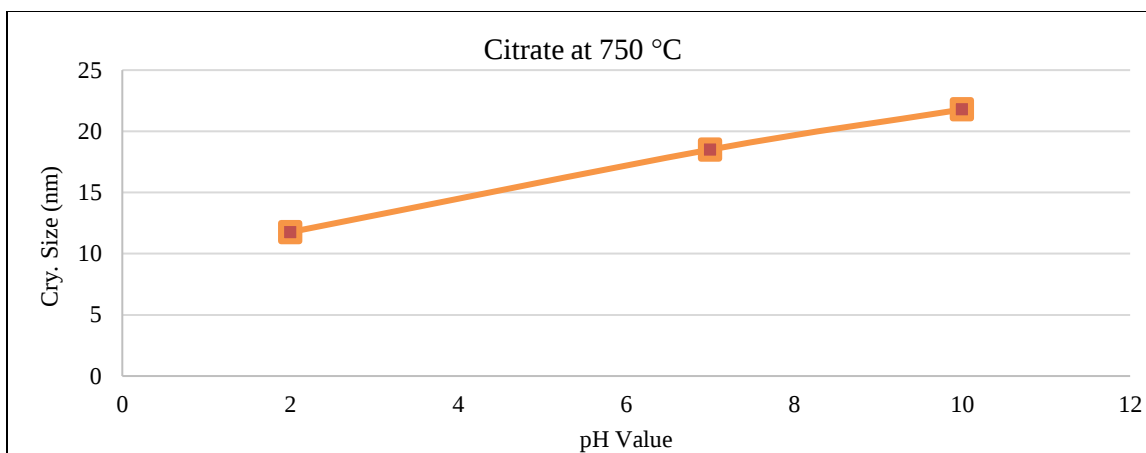
S6. %Triclinic in Samples Prepared Using Different Synthetic Approaches.



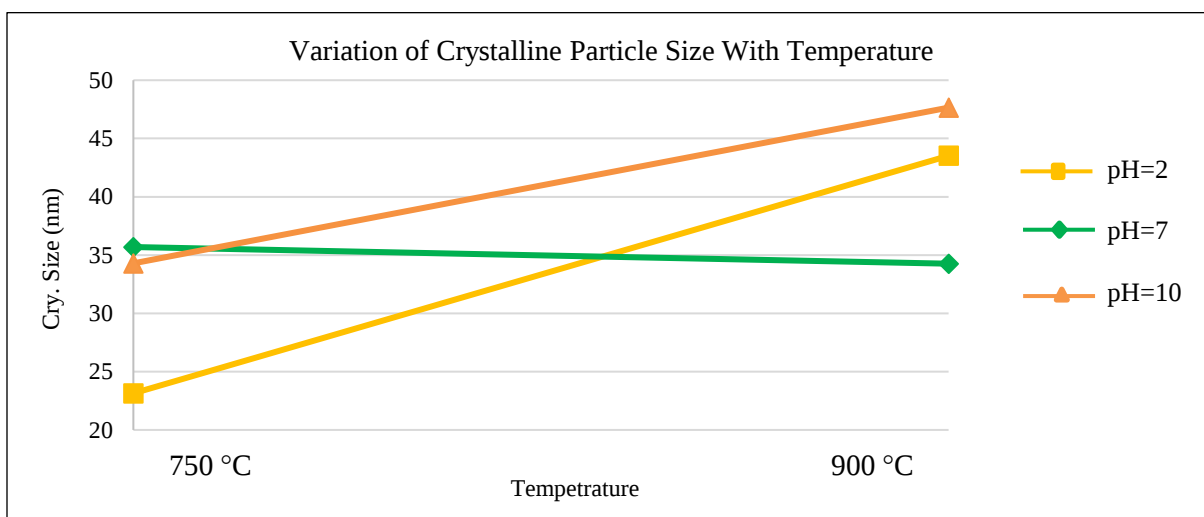
S7. Crystalline particle size vs. pH value of samples prepared using co-precipitation method calcined at 750 °C.



S8. Crystalline particle size vs. pH value of samples prepared using hydrothermal method and calcined at 750 °C.



S9. Crystalline particle size vs. pH value of samples prepared using citrate method and calcined at 750 °C.



S10. Crystalline particle size vs. calcination temperature of samples prepared using co-precipitation method at different pH values.

Energy-dispersive X-ray spectroscopy Figures:

Table S11. Weight and atomic percentage of BiNbO₄ prepared using co-precipitation method at pH=2

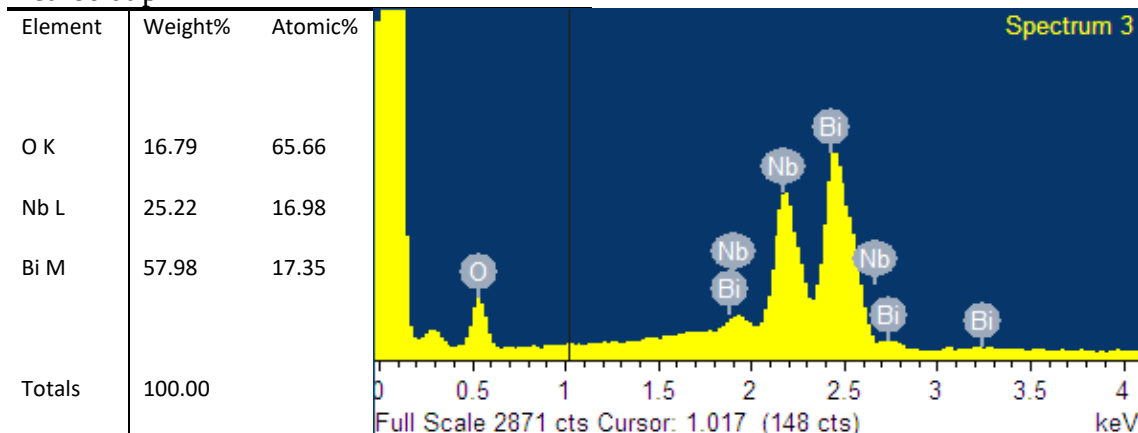


Table S12. Weight and atomic percentage of BiNbO₄ prepared using co-precipitation method at pH=7

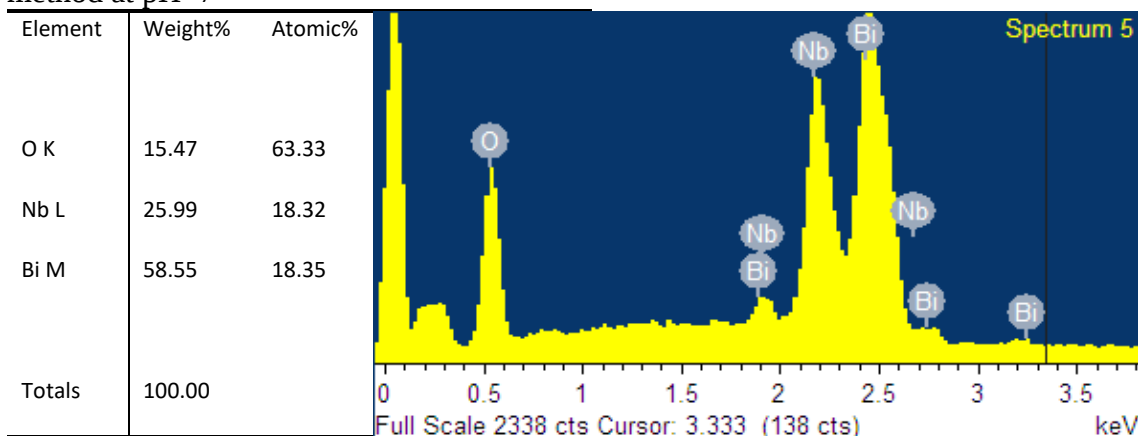


Table S13. Weight and atomic percentage of BiNbO₄ prepared using co-precipitation method at pH=10

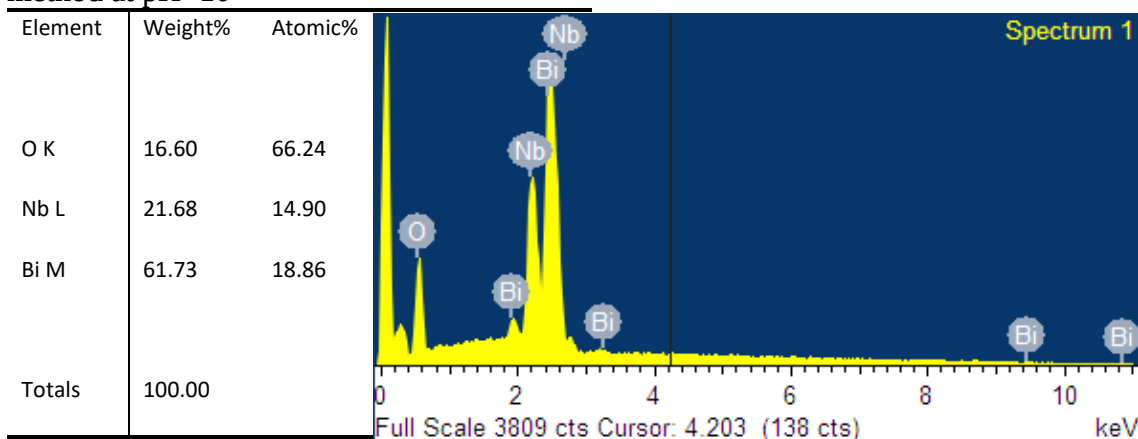


Table S14. Weight and atomic percentage of BiNbO₄ prepared using co-precipitation method at pH=2 with EG.

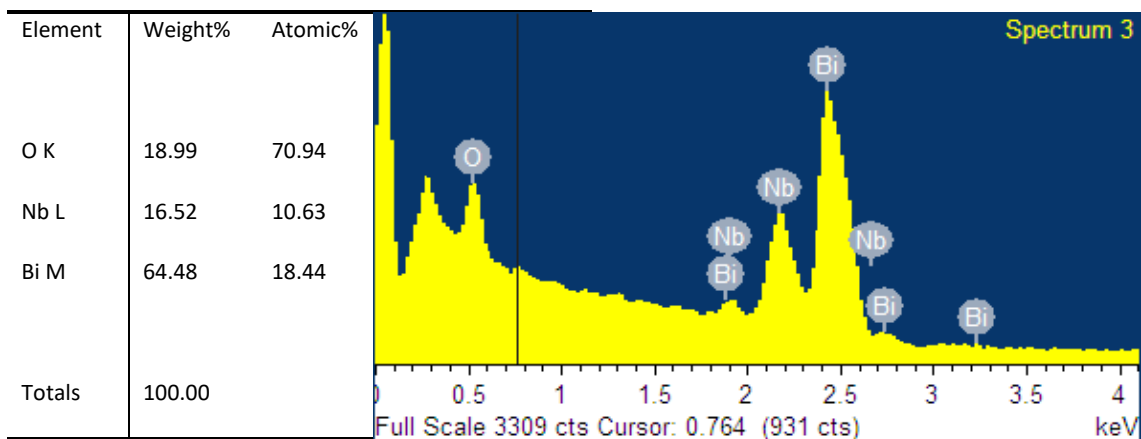


Table S15. Weight and atomic percentage of BiNbO₄ prepared using co-precipitation method at pH=2 with SDS.

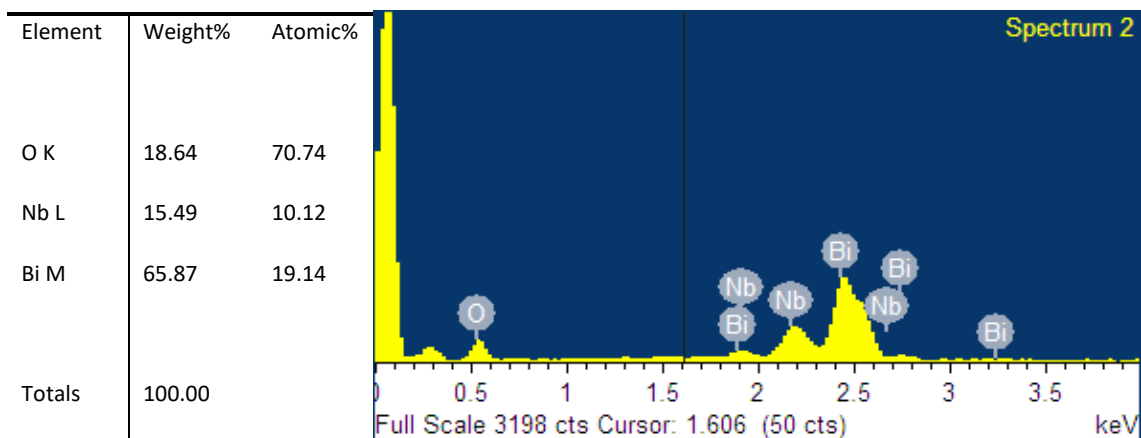


Table S16. Weight and atomic percentage of BiNbO₄ prepared using co-precipitation method at pH=2 with PEG.

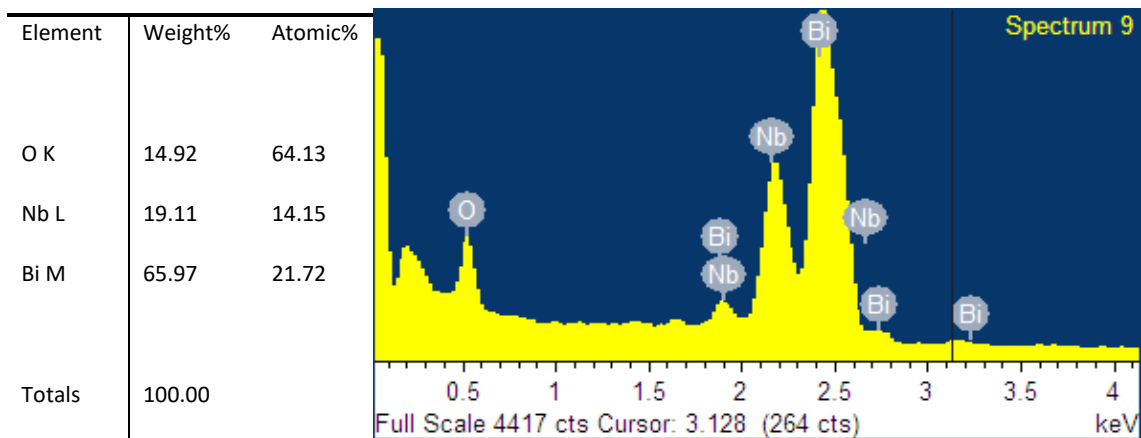


Table S17. Weight and atomic percentage of BiNbO₄ prepared using citrate method at pH=2

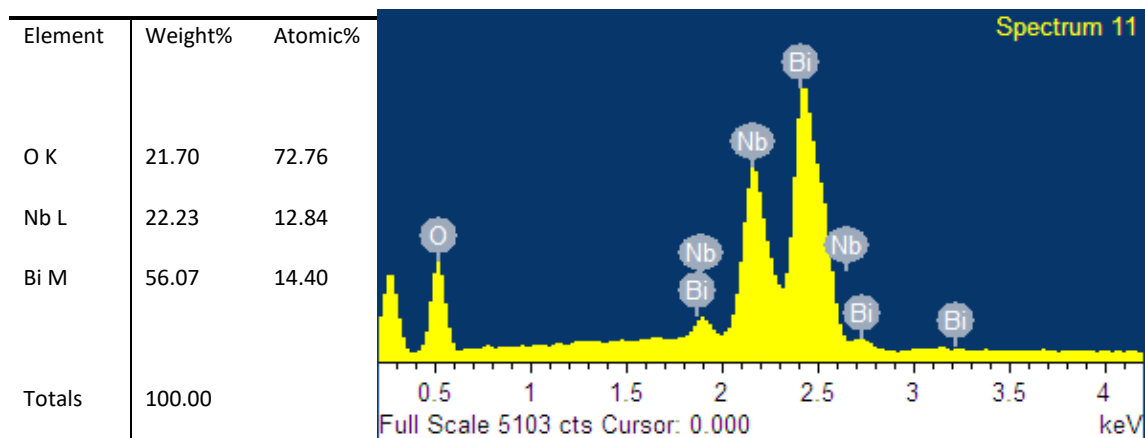


Table S18. Weight and atomic percentage of BiNbO₄ prepared using citrate method at pH=7.

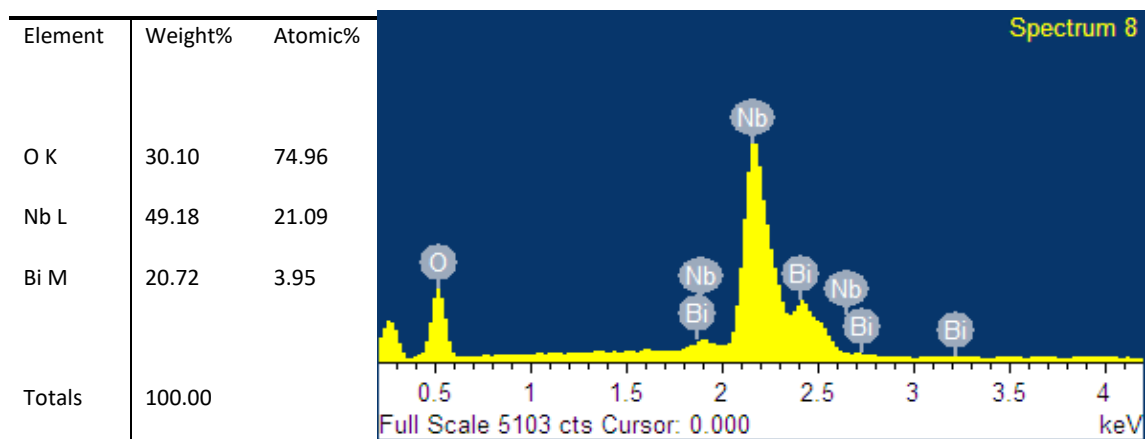


Table S19. Weight and atomic percentage of BiNbO₄ prepared using citrate method at pH=10.

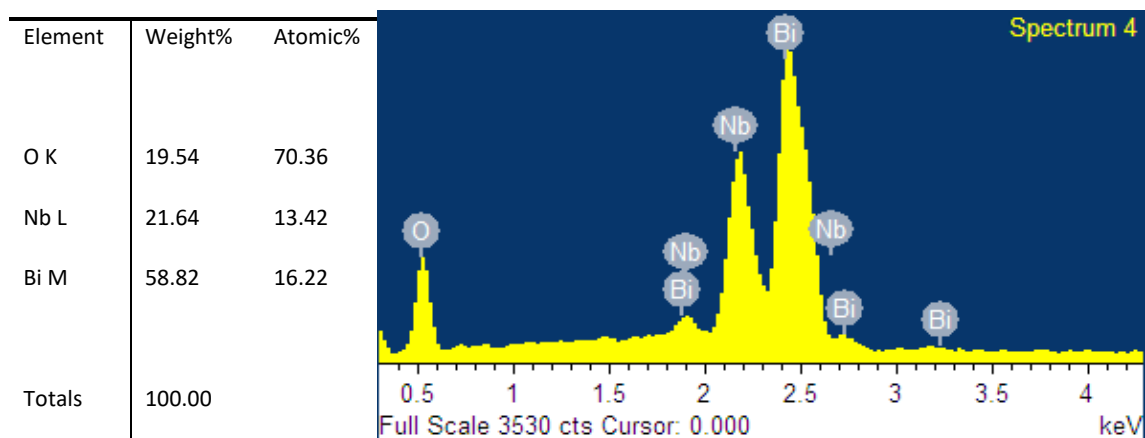


Table S20. Weight and atomic percentage of BiNbO₄ prepared using hydrothermal method at pH=2.

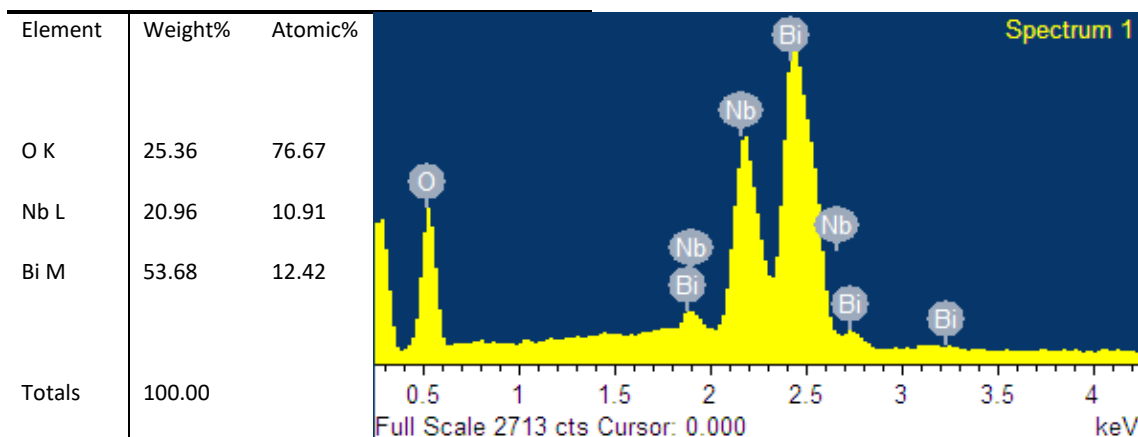


Table S21. Weight and atomic percentage of BiNbO₄ prepared using hydrothermal method at pH=7.

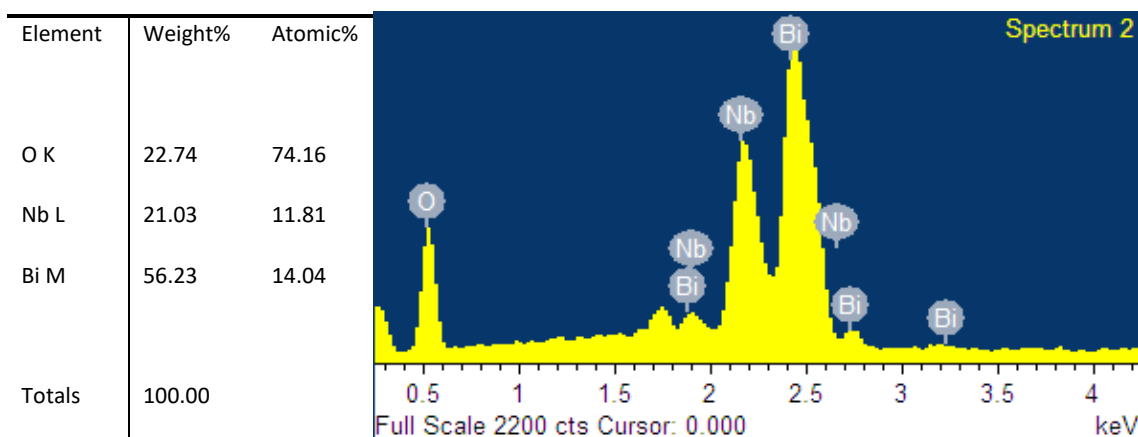
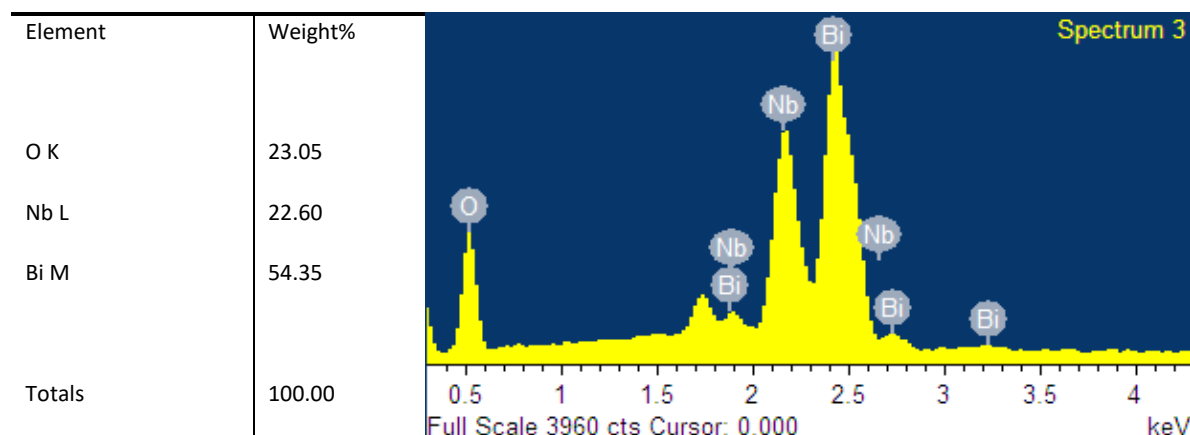
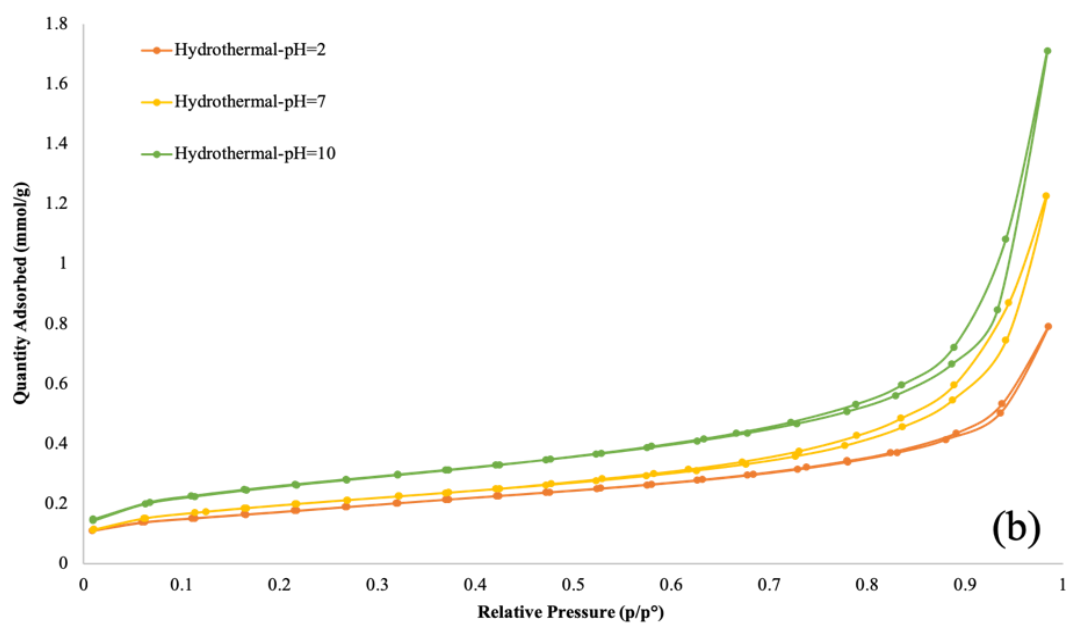
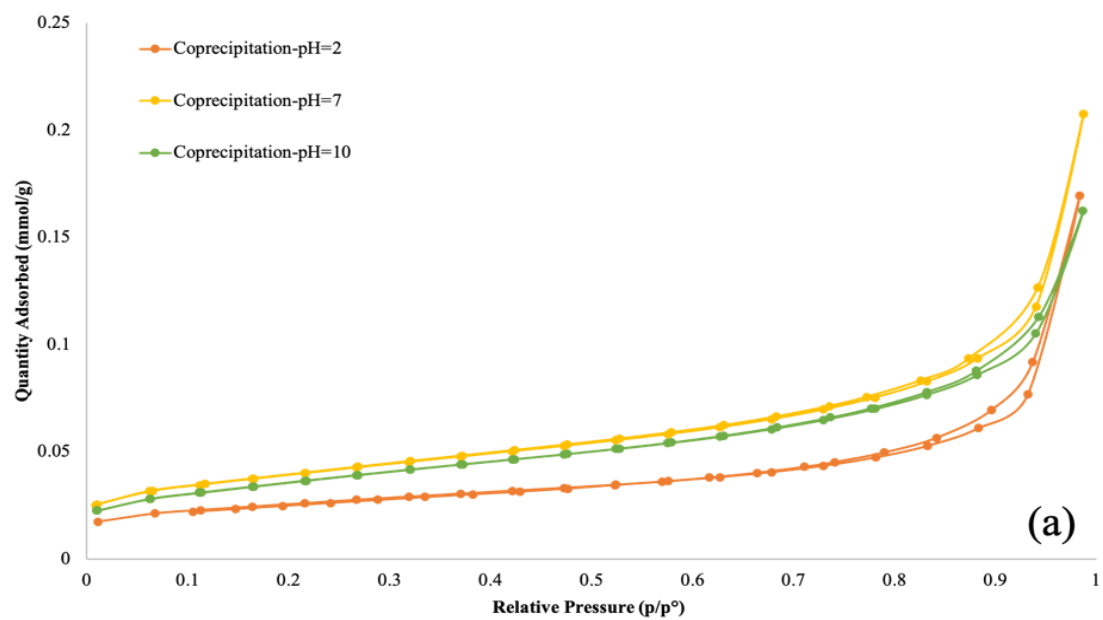
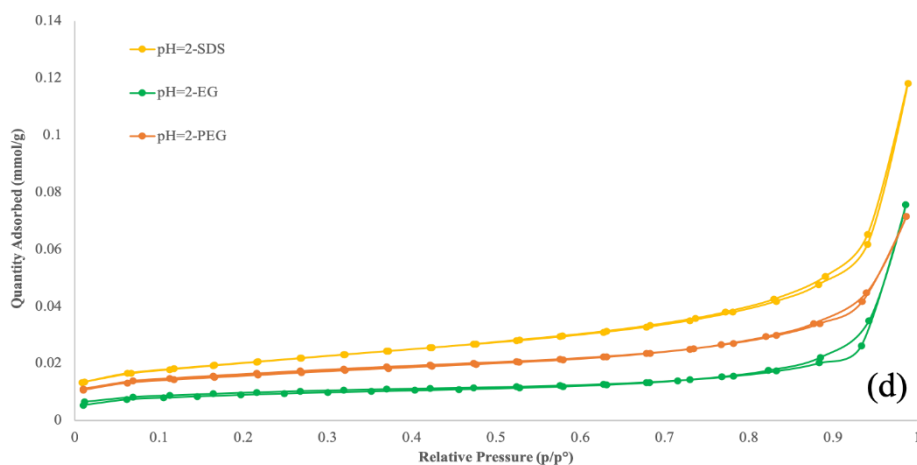
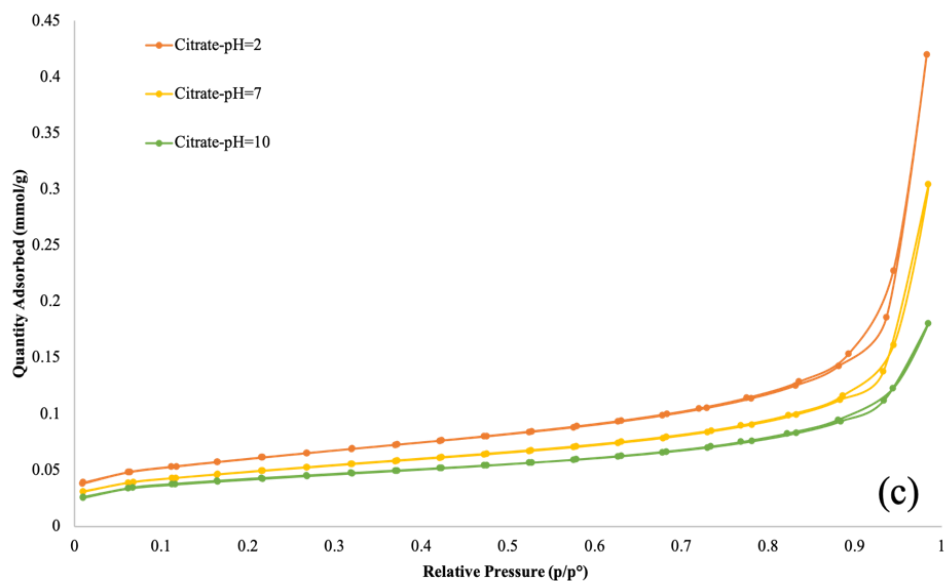


Table S22. Weight and atomic percentage of BiNbO₄ prepared using hydrothermal method at pH=10.







S23. BET analyses of BiNbO_4 calcined at 750°C and synthesized using different synthetic approaches at different pH values; (a) co-precipitation, (b) hydrothermal, (c) citrate precursor method, (d) different surfactant added