

pH-regulated hydrothermal synthesis, characterization of $\text{Sb}_4\text{O}_5\text{X}_2$ (X=Br / Cl) and its use for the dye degradation of methyl orange both with and without light illumination

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Table S1. Bond Valence Sum Calculations for $\text{Sb}_4\text{O}_5\text{Cl}_2$ and $\text{Sb}_4\text{O}_5\text{Br}_2$ employing $R_0(\text{Sb}-\text{O}) = 1.973\text{Å}$, $R_0(\text{Sb}-\text{Br}) = 2.50\text{Å}$, $R_0(\text{Sb}-\text{Cl}) = 2.35\text{Å}$

ATOMS	BVS	ATOMS	BVS
Sb1	2.5	Sb1	2.6
Sb2	2.9	Sb2	2.7
Br	0.7	Cl	0.6

Table S2: λ_{max} (nm) and band gap(eV) at different pH in aqueous solution:

pH	λ_{max} for $\text{Sb}_4\text{O}_5\text{Cl}_2$ (nm)	λ_{max} for $\text{Sb}_4\text{O}_5\text{Br}_2$ (nm)	E_g for $\text{Sb}_4\text{O}_5\text{Cl}_2$ (eV)	E_g for $\text{Sb}_4\text{O}_5\text{Br}_2$ (eV)
2	322	274.7	3.48	3.39
3	322	269.7	3.4	3.47
4	322	262.3	3.4	3.47
5	322	274.0	3.4	3.46
6	322	269.0	3.45	3.47

Table S3: λ_{\max} (nm) and band gap (eV) at different pH in dye solution :

pH	λ_{\max} for $\text{Sb}_4\text{O}_5\text{Cl}_2$ (nm)	λ_{\max} for $\text{Sb}_4\text{O}_5\text{Br}_2$ (nm)	E_g for $\text{Sb}_4\text{O}_5\text{Cl}_2$ (eV)	E_g for $\text{Sb}_4\text{O}_5\text{Br}_2$ (eV)
2	496	462.9	2.215	2.37
3	462.4	489.5	2.356	2.30
4	476	471	2.247	2.20
5	500	462.5	2.198	2.376
6	496	502.7	2.215	2.22

Table S4: Shape and size of antimony oxybromide and antimony oxychloride :

pH	For $\text{Sb}_4\text{O}_5\text{Br}_2$		For $\text{Sb}_4\text{O}_5\text{Cl}_2$	
	Shape	Area (μm^2)	Shape	Area (μm^2)
2	Needle shaped	6.95×0.8	3D Sheet	24.75×15.40
3	Needle shaped	6.34×10.504	3D Sheet	14.375×6.075
4	Both needle and hexagonal shaped cluster	8.078× 7.09	3D Sheet	20.83×10.74
5	Hexagonal shaped cluster	4.669×3.748	3D Sheet	15.98×7.114
6	Hexagonal shaped cluster	17.244×0.458	3D Sheet	6.005×4.922

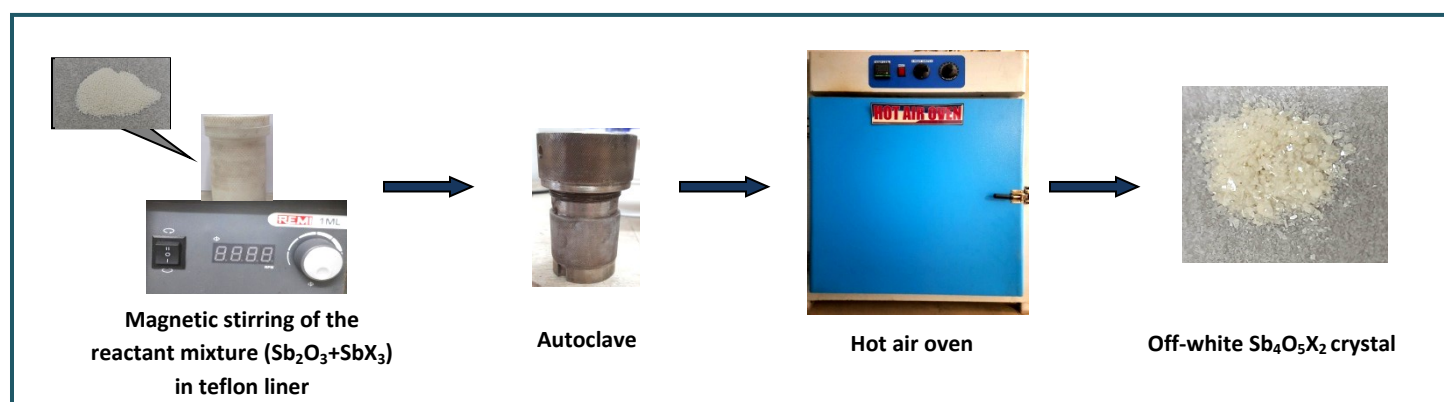


Fig S1: Schematic representation of experimental procedure of $\text{Sb}_4\text{O}_5\text{X}_2$ compounds

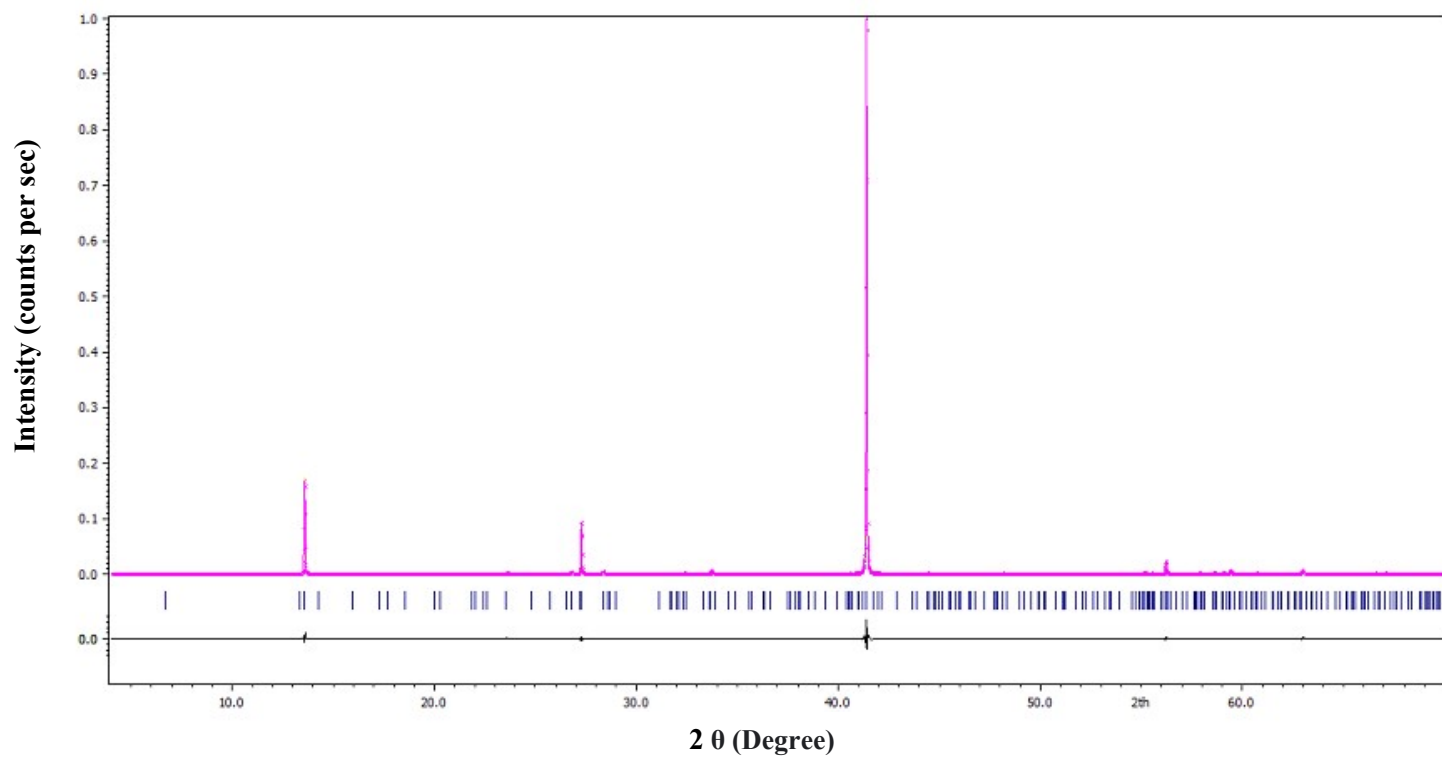


Fig S2: PXRD graph for $\text{Sb}_4\text{O}_5\text{Br}_2$

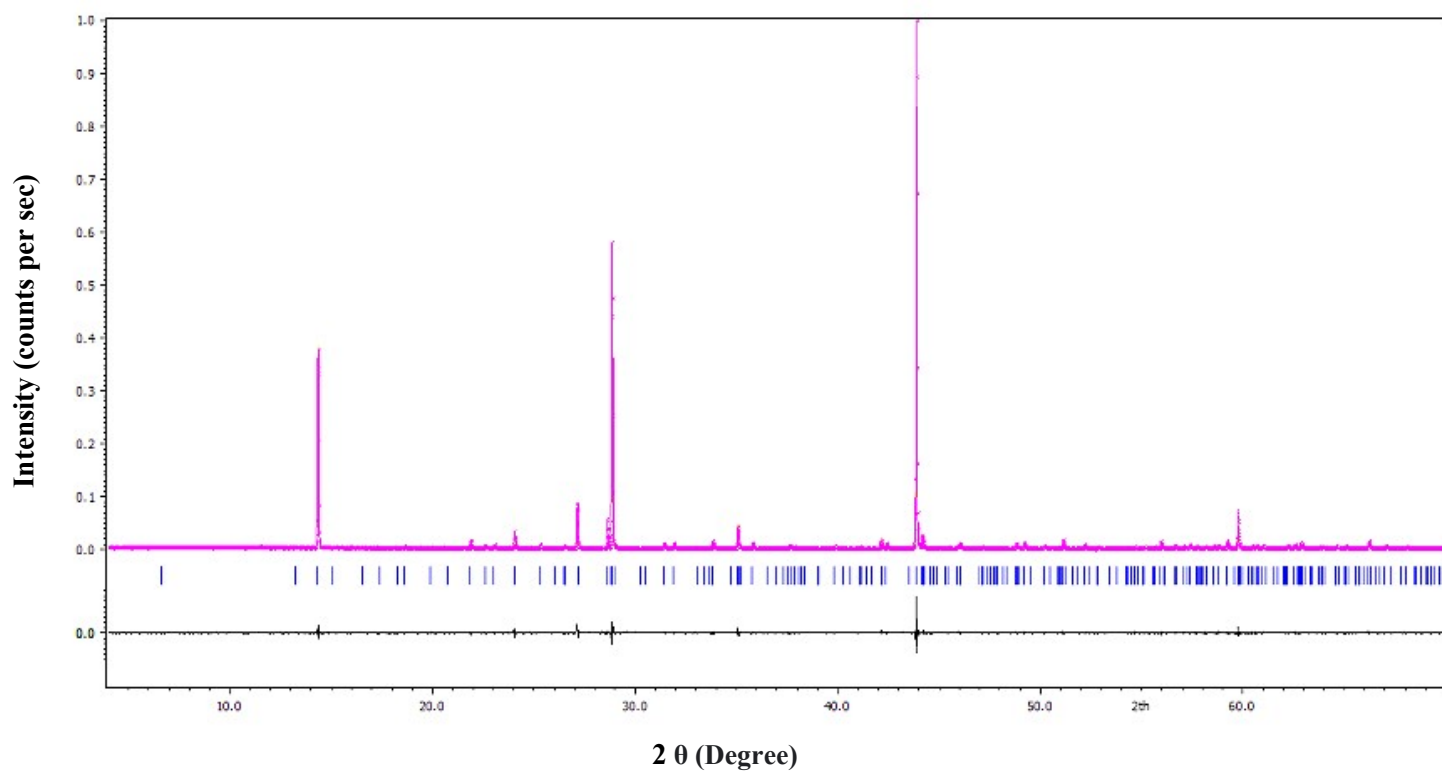


Fig S3: PXRD graph for $\text{Sb}_4\text{O}_5\text{Cl}_2$