Synthesis, Structure and Photocatalysis in $LiBi_4Ta_3O_{14}$ and $LiBi_4Nb_3O_{14}$

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The application of photocatalytic materials in wastewater treatment, control of toxic air contaminants and remediation of hazardous wastes has been of interest. Several materials like TiO2, pyrochlores and bismuth tantalates have been extensively studied. In search of novel structural types with enhanced photo-catalytic activities, a series of new compounds, LiBi₄Ta₃O₁₄ and LiBi₄Nb₃O₁₄ in the Li₂O-Bi₂O₃-(Nb/Ta)₂O₅ system have been isolated for the first time in the hitherto unknown lithium bismuth niobates and tantalates. Both the compounds crystallize in the monoclinic space group, C2/c with a = 13.115(2) Å, b = 7.583(1) Å, c = 12.226(2) Å, β = $101.477(3)^{\circ}$, V = 1182.6(5) Å³ and Z = 4; a = 13.035(3) Å, b = 7.647(2) Å, c = 12.217(3) Å, β = 101.512(4)°, V = 1193.4(5) Å³ and Z = 4 for LiBi₄Ta₃O₁₄ and LiBi₄Nb₃O₁₄ respectively. The structures were solved by direct methods and refined to R of 0.057 and 0.078. The crystal structure consists of layers of $[Bi_2O_2]^{2+}$ units separated by layers of LiO₄ tetrahedra and (Nb/Ta)O₆ octahedra hence depicting a new structural type.

The UV-Visible diffuse reflectance spectra suggest a band gap of 3.4 eV and 3.2 eV for $\text{LiBi}_4 \text{Ta}_3 \text{O}_{14}$ and $\text{LiBi}_4 \text{Nb}_3 \text{O}_{14}$ respectively. Photo-catalytic degradation of a wide range of dyes was studied.

Keywords: crystal structures, photocatalysis, dyes