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Effect of the In by Bi substitution in the Sm_2InTaO_7 system for the photocatalytic splitting of water PABLO DE LA MORA, MELISSA MENDEZ GALVAN, Facultad de Ciencias, GUSTAVO TAVIZON, Facultad de Quimica, Universidad Nacional Autonoma de Mexico, JUAN RAMIREZ DE AREL-LANO, Tecnologico de Monterrey, Campus Ciudad de Mexico — Tantalum oxidebased photocatalysts with octahedrally coordinated d¹⁰ configuration, represent promising semiconductor systems to develop photocatalysts with visible-light response in the photochemical splitting of water. Several Indium oxide-based compounds have shown acceptable activity in water photolysis. Recently, the pyrochlore Sm₂InTaO₇ (a 4f-d¹⁰-d⁰ system) was reported as a visible-light photocatalyst for water splitting. In the present work, by solid state reaction, we have obtained and structurally characterized compounds of the $\text{Sm}_2\text{In}_{1-x}\text{Bi}_x\text{TaO}_7$ system. In these systems we have found that the optical band gap value depends on the Bi content; this value is 2.7, 2.52 and 2,1eV for x=0, 0.15 and 0.30 respectively. The specific surface area values we have found are typical of solid state reaction products, $0.5-1.2 \text{ m}^2/\text{g}$. To understand the effect of the In substitution by Bi, the compounds were studied with first principles calculations using the WIEN2k package and the gap was evaluated using the mBJ potential

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