TlTaSe$_3$ was prepared from a fused mixture of Tl$_4$Ta$_2$Se$_{11}$, Ta and Se in the molar ratio 1:2:1. The compound shows dimorphism with H-TlTaSe$_3$, hexagonal, space group $P6_3/mmc$, $a = 7.2436(6)$ Å, $c = 5.9736(6)$ Å, $c/a = 1.213$ and O-TlTaSe$_3$, orthorhombic, space group $Pnma$, $a = 9.554(13)$ Å, $b = 3.6244(6)$ Å, $c = 14.7271(17)$ Å. The crystal structure of H-TlTaSe$_3$ is isotypic to BaVSe$_3$ whereas that of O-TlTaSe$_3$ is closely related to the NH$_4$CdCl$_3$-type. Characteristic features of the structures are: $1\infty [TaSe_3^{2-}]$ chains of regular octahedra sharing faces along [001] for the hexagonal form and columns of double edge-sharing octahedra $1\infty [Ta_2Se_6^{2-}]$ running along [010] for O-TlTaSe$_3$. The columns are each separated by Tl$^+$ ions with the coordination number CN = 12 and CN = 8 respectively. The structures are compared and discussed in context with other isotypic structures of chalcogenides. The orthorhombic modification O-TlTaSe$_3$ is a semiconductor while H-TlTaSe$_3$ shows conventional metallic behaviour. The electronic structures of both modifications are discussed on the base of band structure calculations performed within the framework of density functional theory.

Key words: Thallium Tantalum Selenide, Crystal Structure, Dimorphic, Properties, Electronic Band Structure