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RESEARCH ARTICLE

# Effect of Pressure on The Valency of Ytterbium in Ytterbium Monochalcogenides

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## Highlights

- Yb valence varies under pressure were derived from Birch–Murnaghan-based PV data
- Yb valency change is calculated using its linear dependency on lattice constant
- Pressure increases Yb valence, resulting a change from divalent to mixed-valence

## Abstract

*When pressure is applied then properties of material change due to the alteration of of valency. Several effects of pressure on the characteristics of material have been investigated. This study was focused at finding the change in valency as a function of pressure of Ytterbium Monochalcogenides YbX (X=S, Se and T). The change in valency of Ytterbium in Ytterbium monochalcogenides as functions of pressure have been calculated by using the modified data. For calculating the change in valency of Yb, the modified experimental pressure-volume relationships of YbS, YbSe and YbTe have been reproduced by using the Birch–Murnaghan equation. The equivalent pressure-volume relationships of these materials for stable divalent Ytterbium have also been calculated using the same equation. The change in valency is calculated by a method, that assumes the variation between the calculated and experimental lattice constants at separately pressure value of the assumed material.*

**Keywords:** *Birch-Murnaghan equation, ytterbium monochalcogenides, valency change, lattice constants*

## Introduction

Ytterbium monochalcogenides compounds show magnetic, optical, electronic, thermal and superconducting behaviour (Ansary et al., 2022). Ytterbium chalcogenides, characterized by their low band gap, stable thermodynamic properties, and exceptional optical behaviour (including negative dielectric effect in certain frequency ranges), show strong potential for use in photovoltaics, laser diodes, microwave circuits, optical switches, modulators, and diverse electronic applications(Eressa & Gerbi, 2024). Ytterbium sulfide (YbS) has gained considerable interest owing to its role in enhancing the performance of supercapacitors (Ubale et al., 2020). Moreover, it is utilized as an electrode component (Koshurnikova et al., 2013) and as a ternary magnetic material (Koshurnikova et al., 2013). Selenium-based nanoparticles exhibit notable biological activities, including anticancer, antioxidant, antibacterial, and antitumor effects (Vahdati & Moghadam, 2020). Ytterbium selenide (YbSe) nanoparticles show

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strong absorption in the near-infrared region and possess excellent photoluminescent properties. Similarly, ytterbium telluride (YbTe) is regarded as a promising candidate for the development of heterojunction diode lasers (Partin, 1983).When pressure is applied on the materials then electronic states of localized *f* electrons in the materials are accountable for changing the properties namely structural Phase transition (Petit et al., 2014).

When pressure is applied to samarium sulfide (SmS), its valence state changes and that induces the magic of transforming its cloudy appearance into a golden shine. While this alteration doesn't fulfil the ancient alchemist's vision, the changed material shows remarkably fascinating properties. The new characteristic is the rapid variation of samarium's valence between two distinct electronic states. In general, physical behaviour in materials holding lanthanoids can be influenced via correcting their valence states, either through pressure or chemical variation(Jayaraman, 1980). X-ray absorption and optical reflectivity studies tell that Yb ions in YbS and YbTe suffer continuous valence changes under pressure, with YbTe showing an earlier valence change due to stronger hybridization between its chalcogen p-bands and Yb 4f states compared to YbS (Schmiester et al., 1990). Divalent ytterbium monochalcogenides YbX (X=O, S, Se, and Te) are semiconductors whose lowermost electronic excitation includes a change from localized $4f^{14}$ states to 5d-like conduction bands, with excitation energies ranging from 1.1 to 1.8 eV in YbS to YbTe, and pressure lowers this energy threshold(Narayanamurti et al., 1974). A. Werner and his group studied how YbO responds to pressure up to 35 GPa. This is done with the help of energy-dispersive X-ray diffraction. Their study revealed a surprizing increase in compressibility above 8 GPa, telling a slow change in valency of ytterbium from +2 to +3. This change was visually confirmed by a visible colour change in the material from black to yellow when watched under reflected light. They also calculated the original bulk modulus of YbO to be around 130 ± 10 GPa (Werner et al., 1981). The outer electronic configuration of Yb in divalent state is $4f^{14}5d^{0}6s^{2}$. In the ytterbium monochalcogenides two s electrons fill the valence band resulting from the p positions of the anion. During the transition from divalent to trivalent state the outer electronic configuration of Yb changes from $4f^{14}5d^{0}6s^{2}$ to $4f^{(14-x)}5d^{x}6s^{2}$ resulting a semiconductor-to-metal transition (Chen et al., 2019). At zero pressure, YbO and YbS act as conventional band insulators due to localized 4f orbitals, but under high pressure, band broadening leads to 4f–5d inversion at the X point, driving an insulator-to-metal transition accompanied by a change in global band topology (Li & Zhang, 2015).

In this study, the change in valency of Ytterbium in Ytterbium monochalcogenides as functions of pressure have been calculated by using the modified data. For calculating the change in valency of Yb, the modified experimental pressure-volume relationships of YbS, YbSe and YbTe have been reproduced by using the Birch–Murnaghan equation of state (Birch, 1947) along with suitable parameters in the equation. Same work has already been published (Islam et al., 2022) for cerium monochalcogenides and cerium monopnictides. Let us discuss about experimentally observed (Jayaraman et al., 1974) pressure volume relationship of YbX (X=S, Se and Te). Ytterbium monochalcogenides show rare compressibility within the pressure range 15–20 GPa but they retain the $B_1$ type crystal structure through the given pressure range. This irregular behaviour is ascribed to a pressure-driven change in the valence of Yb, from the divalent ($2^{+}$) state toward the trivalent ($3^{+}$) state.

## Theoretical Methodology and Calculation

To find the change in valency of Ytterbium in ytterbium monochalcogenides YbX (X=S, Se and Te) due to change in pressure, we have used the concepts that, experimentally measured pressure–volume (*P–V*) behaviour of these compounds was effectively modelled with the help of Birch equation (Birch, 1947; Mito et al., 2007),

$$P(Z) = 1.5B_0\{(Y)^{-7/3} - (Y)^{-5/3}\}[1 - 0.75(B' - 4)(1 - (Y)^{-2/3})] \quad (1)$$

where P(Z) is pressure which is function of relative volume ($Y=V/V_0$). Where, ($B_0$) is bulk modulus of elasticiyy and ($B'$) is its first pressure derivative that facilitated as adjustinging constraints. Beside this, the *P–V* relations corresponding to stable divalent ytterbium ions were found through the same Birch formalism, employing suitable values of $B_0$ and $B'$. These results evidently establish how pressure effects the valence state of ytterbium in the studied compounds.

### Reproduction of experimental relative volume

The experimental pressure-volume relationship, as reported by (Jayaraman et al., 1974) can be fitted using the Birch equation of state i.e. equation (1). The reproduced experimental relative volumes for YbS, YbSe and YbTe are shown in figure 1, figure 2 and figure 3 respectively by orange dots. The experimental data has been reproduced perfectly in the pressure range:

0 to 30 GPa, using the parameters $B_0$ = 33 GPa and $B'$ = 6.17 for YbS, 0 to 25 GPa, using the parameters $B_0$ = 51.9 GPa and $B'$ =

3.1 for YbSe and 0 to 30 GPa, using the parameters $B_0$ = 34.85 GPa and $B'$ = 4.39 for YbTe.

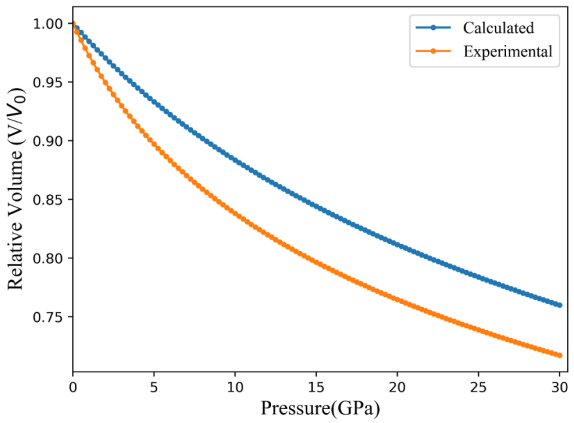


**Fig. 1.** Relative volume versus pressure curves for YbS.

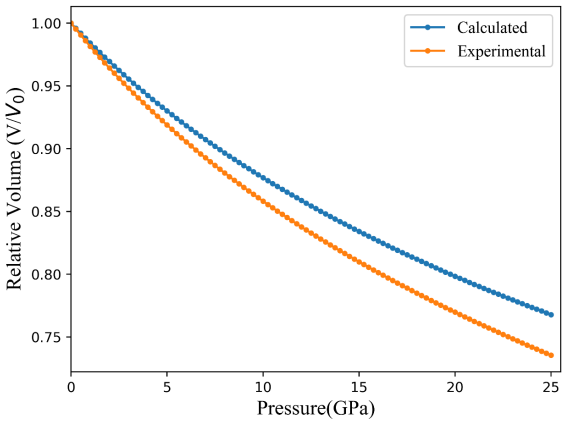


**Fig. 2.** Relative volume versus pressure curves for YbSe.

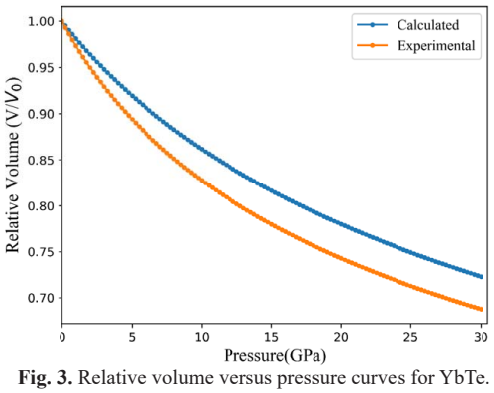


**Fig. 3.** Relative volume versus pressure curves for YbTe.

## Theoretically calculated relative volume for stable divalent ytterbium

Three compounds, YbS, YbSe and YbTe, from the group of ytterbium monochalcogenides have been designated. For divalent stable ytterbium in respective compounds the parameters $B_0$ and B' are 63 GPa and 4, 61 GPa and 3.4 and 51 GPa and 3.7. With the help of these parameters in equation (1), the relative volumes of respective compounds as a function of pressure have been calculated and are presented in Figure 1, 2 and 3 above by blue dots.

## Calculation of Valence Change of Yb

It is found that, the valence of Yb in YbX (X=S, Se and Te) varies linearly with lattice constant 'a'(Leger, 1993).Using this concept, valence change is unity1 when change in lattice constant is $\{a_{P_0}^{2+}(\text{cal}) - a_{P_0}^{3+}(\text{cal})\}$. Here $a_{P_0}^{2+}(\text{cal})$ and $a_{P_0}^{3+}(\text{exp})$ are calculaed lattice constant of ytterbium atom at zero pressure having valency 2 and 3 respectively. If $a_P^{2+}(\text{cal})$and$a_P^{2+x}(\text{exp})$ are calculated and experimentally observed lattice constant at pressure P having valency 2 and 2+x respectively then the valency x can be determined by using formula

$$x = \frac{\{a_P^{2+}(\text{cal}) - a_P^{2+x}(\text{exp})\}}{\{a_{P_0}^{2+}(\text{cal}) - a_{P_0}^{3+}(\text{cal})\}} \qquad (2)$$

Ytterbium monochalcogenides exhibit fcc (NaCl) structures and each ytterbium ion has coordination number 6.At ambient pressure, the radii of $Yb^{2+}$ and $Yb^{3+}$ ions are $r_{P_0}^{2+}(\text{Yb}) = 1.02\text{Å}$ and $r_{P_0}^{3+}(\text{Yb}) = 0.868\text{Å}$ respectively (Shannon, 1976). Now,

$$\{a_{P_0}^{2+}(\text{cal}) - a_{P_0}^{3+}(\text{cal})\} = \{2r_{P_0}^{2+}(\text{Yb}) + 2r_{P_0}(\text{X})\} - \{2r_{P_0}^{3+}(\text{Yb}) + 2r_{P_0}(\text{X})\} = \{2r_{P_0}^{2+}(\text{Yb}) - 2r_{P_0}^{3+}(\text{Yb})\}$$

where, $r_{P_0}(\text{X})$ is ionic radius of anion X. The calculated value of $\{a_{P_0}^{2+}(\text{cal}) - a_{P_0}^{3+}(\text{cal})\}$ is 0.304 Å. Hence equation (1) becomes

$$x = \frac{a_{P_0}^{2+}\left\{\frac{a_P^{2+}(cal)}{a_{P_0}^{2+}} - \frac{a_P^{2+x}(exp)}{a_{P_0}^{2+}}\right\}}{0.304} \quad (3)$$

For simple cubic crystal volume of unit cell is $V=a^3$ and hence $a=V^{1/3}$. So that equation (3) can be written as

$$x = \frac{a_{P_0}^{2+}\left[\left\{\frac{V_P(cal)}{V_{P_0}}\right\}^{1/3} - \left\{\frac{V_P(exp)}{V_{P_0}}\right\}^{1/3}\right]}{0.304} \quad (4)$$

where, $V_{P_0}$ , $V_P(cal)$, and $V_P(exp)$ are calculated volume of unit cell at zero pressure for $Yb^{2+}$ ion, calculated volume of unit cell at pressure P for $Yb^{2+}$ ion and experimentally determined volume of unit cell at pressure P for $Yb^{2+x}$ ion respectively.

Again, $a_{P_0}^{2+} = 2r_{P_0}^{2+}(Yb) + 2r_{P_0}(X) = 2\{r_{P_0}^{2+}(Yb) + r_{P_0}(X)\}$ (5)

For YbS, $a_{P_0}^{2+}$=2(1.02+1.84) =5.72 Å

For YbSe, $a_{P_0}^{2+}$=2(1.02+1.98) =6 Å

For YbTe, $a_{P_0}^{2+}$=2(1.02+2.21) =6.46 Å (Shannon, 1976)

Finally, new valency of ytterbium is (v) = $2+\frac{a_{P_0}^{2+}\left[\left\{\frac{V_P(cal)}{V_{P_0}}\right\}^{1/3} - \left\{\frac{V_P(exp)}{V_{P_0}}\right\}^{1/3}\right]}{0.304}$ (6)

## Results and Discussion

The pressure dependence of the Ytterbium valence in YbS, YbSe, and YbTe was calculated using the pressure–volume relationships derived from the Birch–Murnaghan equation of state. Figure 4 illustrates the variation of the Yb valence with pressure in these compounds. At ambient pressure, ytterbium in all three materials remains essentially divalent (2+). However, with increasing external pressure, a systematic and continuous rise in the average valence is observed, indicating a transition from a pure divalent state to a mixed-valence configuration. This behaviour originates from pressure-induced modifications in the electronic structure, particularly the enhanced hybridization between the localized 4f orbitals of Yb and the conduction band states. The gradual deviation from bivalency highlights the sensitivity of these compounds to external compression and underscores the role of electronic correlations under pressure.

Among the studied systems, YbS exhibits the most pronounced valence change with pressure. The valence increases rapidly, reaching nearly 2.35 at around 15–20 GPa, after which the growth begins to saturate. This steep rise suggests that YbS experiences stronger f–d hybridization at relatively lower pressures compared to YbSe and YbTe. The smaller ionic radius of sulfur contributes to enhanced orbital overlap, thereby favouring an earlier onset of intermediate valence states. In contrast, YbSe shows a much weaker response to applied pressure, with the valence remaining below 2.25 even at 25 GPa. This indicates that significantly higher external pressures are required to induce substantial charge transfer in YbSe, pointing to a relatively more stable divalent state in this compound. YbTe displays intermediate characteristics, where the valence gradually increases with pressure, reaching approximately 2.34 at 25–30 GPa, and shows clear signs of near-saturation at higher pressures.

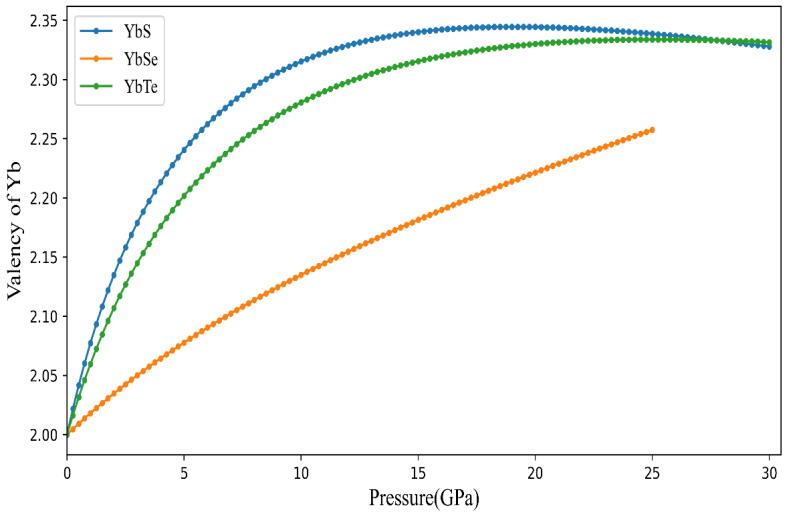


**Fig. 4.** Calculated valence of Yb as a function of pressure in YbX (X=S, Se and Te)

The comparative analysis of these compounds establishes a clear trend in the rate of valence enhancement: YbS > YbTe > YbSe. This ordering can be rationalized by considering the chemical pressure effect, which is directly linked to the size of the chalcogen anions. The reduced ionic size of sulfide ($S^{2-}$) leads to stronger orbital overlap between the Yb 4f states and conduction band, thereby promoting faster charge transfer under compression. Conversely, the larger telluride ($Te^{2-}$) and selenide ($Se^{2-}$) ions reduce the extent of orbital overlap, thereby slowing down the pressure-driven valence transition. These findings confirm that external pressure acts as an efficient tuning parameter for driving mixed-valence behaviour in ytterbium monochalcogenides, with the effectiveness of the transition strongly dependent on the chemical identity of the anion.

## Conclusions

The pressure–volume behavior of YbS, YbSe, and YbTe was successfully analyzed using the Birch–Murnaghan equation of state, and the pressure-induced valence changes of ytterbium were determined. The results demonstrate that applied pressure has a significant influence on the electronic configuration of ytterbium, driving a transition from a divalent to a mixed-valence state. The extent and rate of this transition were found to vary across the compounds, following the order YbS>YbTe>YbSe. These findings indicate that the local chemical environment, particularly the size of the chalcogen anion, plays a decisive role in governing the pressure-driven valence transition. Therefore, external pressure can be considered an effective control parameter for tuning the mixed-valence behavior in ytterbium monochalcogenides, with potential implications for their electronic, optical, and thermoelectric applications under extreme conditions.

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## Authors contribution

First author Shiva Prasad Baral contributed the pressure-induced evolution of Yb valence, derived from Birch–Murnaghan P–V data and its linear dependence on lattice constant, calculating and computing transition from divalent to mixed-valence state under pressure.

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## Conflict of interest

There is no conflict of interest.

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