

Thermostructural properties of β and γ polymorphs of lead orthovanadate ($\text{Pb}_3\text{V}_2\text{O}_8$) in a broad temperature range (298 K-973 K): An X-ray diffraction study

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Lead orthovanadate, $\text{Pb}_3\text{V}_2\text{O}_8$, is known to exhibit polymorphism, the three reported phases are α (monoclinic), stable below 273 K, β (monoclinic) and γ (rhombohedral). For temperatures exceeding the room temperatures, the transition from β to γ has been observed, at 373 K [1-3]. Thermal expansion of the polymorphs has been reported in a limited temperature range 90- 550 K [1]. In the present work we extend the knowledge on the system by studying the broad temperature range (298-973 K) and by investigating the structure details as function of temperature. The atomic positions, interatomic distances, interbond angles, polyhedron distortions are determined. The β phase unit-cell parameters a and c show an increase with temperature i.e. 0.21% for a and 0.58% for c but the parameter b decreases by 0.68%. The increase in angle β is 0.11% and unit-cell volume of β phase increases by about 0.12%. In case of the γ phase, the unit-cell parameters increase by about 0.88% along a and 1.11% along c - direction having about 2.87% increase in unit-cell volume. The thermal expansion coefficient (TEC) tensor calculated shows expansion anisotropy for β phase and follows order $\alpha_c > \alpha_a > \alpha_b$. For the γ phase, TEC also shows expansion anisotropy that follows order $\alpha_c > \alpha_a = \alpha_b$. The evolution of lattice parameters of β and γ phases is in line literature data [1] referring to temperature ranging to 550 K.

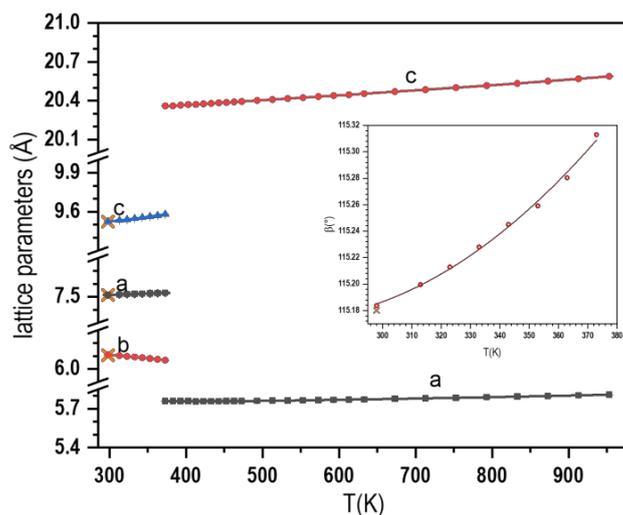


Figure 1. Evolution of lattice parameters of β and γ phases. In inset the evolution of angle β with temperature in β phase is shown. The room temperature values for beta phase from ref [1] are displayed as crosses for comparison.

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References

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