

substance: VO₂

property: crystal structure, low temperature phase

This oxide exists in a narrow stoichiometry range VO_{2-δ} (δ < 0.006) [75B]. Below this stoichiometry, (121)CS planes have been identified [780]. Intergrowths of V₈O₁₅, or, more rarely, V₉O₁₇, have been observed in slightly reduced material; no phase V_nO_{2n-1} with n > 10 has been found [78G]. Values of δ < 0 have also been reported [70K, 74K, 79M].

At ca. 340 K, VO₂ exhibits a metal-semiconductor transition, which is accompanied by a discontinuous transition in other physical properties. Detailed structure: Fig. 1.

crystal structure: monoclinic, space group C_{2h}⁵ – P2₁/c, Z = 4

lattice parameters

<i>a</i>	5.743 Å	<i>T</i> = 298 K	56A
<i>b</i>	4.517 Å		
<i>c</i>	5.375 Å		
<i>β</i>	121.61°		
<i>a</i>	5.7517 ₃₀ Å	<i>T</i> = 298 K	70L
<i>b</i>	4.5378 ₂₅ Å		
<i>c</i>	5.3825 ₂₅ Å		
<i>β</i>	122.646 ₉₆ °		
<i>a</i>	5.75173 Å	<i>T</i> = 298 K	79K
<i>b</i>	4.52596 Å		
<i>c</i>	5.38326 Å		
<i>β</i>	122.6148°		

References:

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Fig. 1.

VO₂. Structure and unit cell of (a) monoclinic VO₂, (b) tetragonal VO₂ [78P].

