

**substance:**  $\text{Ti}_n\text{O}_{2n-1}$  ( $n \geq 3$ )

**property:** crystal structure of high-temperature phase ( $T > T_{\text{tr}}$ ) of  $\text{Ti}_3\text{O}_5$

**crystal structure:** monoclinic, space group  $\text{C}_{2h}^3 - \text{C}2/m$ ,  $Z = 4$ . Similar to anasovite or monoclinically deformed pseudobrookite in which all Ti atoms are equivalent [59A]. Structurally related to rutile [69I].

**lattice parameters**

$a$	9.82 Å	$T = 393\text{K}$		59A
$b$	3.78 Å			
$c$	9.97 Å			
$\beta$	91.0°		$\beta \rightarrow 90^\circ$ with increasing temperature	
$a$	9.828 Å	RT	apparently a RT metastable form	69I
$b$	3.776 Å		of the high-temperature	
$c$	9.898 Å		modification reported by [59A]	
$\beta$	91°19'			

**density**

$d_{\text{calc}}$	4.11 g cm <sup>-3</sup>	RT		69I
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**transition temperature**

$T_{\text{tr}}$	393 K			59A
	450 K		from DTA and XRD measurements	71R,
			( $\Delta H_{\text{tr}} = 1.5(4)$ kcal mol <sup>-1</sup> )	77R
	460 K		from discontinuities in electric	71R
			and magnetic properties	

Unit cell volume and  $c$ -parameter change abruptly at 450 K, see Fig. 1.

**References:**

- 59A Asbrink, S., Magnéli, A.: Acta Crystallogr. 12 (1959) 575.  
69I Iwasaki, H., Bright, N. F. H., Rowland, J. F.: J. Less-Common Met. 17 (1969) 99.  
71R Rao, C. N. R., Randes, S., Loehman, R. E., Honig, J. M.: J. Solid State Chem. 3 (1971) 83.  
77R Rao, C. N. R., Rao, G. R.: Phys. Lett. A61 (1977) 247.

**Fig. 1.**

$\text{Ti}_3\text{O}_5$ . Unit cell volume and  $c$ -parameter vs. temperature [77R].

