

substance: titanium oxide (TiO₂)

property: crystal structure, lattice parameters and related parameters of anatase

crystal structure: tetragonal, space group $D_{4h}^{19} - I4_1/amd$, $Z = 4$ [70R, 72H]. The structure may be derived from the B1 structure of NaCl by ordering Ti^{4+} ions and Ti-vacancies as shown in Fig. 1; the bridging oxygens are displaced towards one another to produce shorter O – O distances.

lattice parameters

<i>a</i>	3.7845 Å	$T = 28^{\circ}C$	70R
<i>c</i>	9.5143 Å		
<i>a</i>	3.7855 Å	$T = 84^{\circ}C$	
<i>c</i>	9.5185 Å		
<i>a</i>	3.7866 Å	$T = 161^{\circ}C$	
<i>c</i>	9.5248 Å		
<i>a</i>	3.7875 Å	$T = 210^{\circ}C$	
<i>c</i>	9.5294 Å		
<i>a</i>	3.7884 Å	$T = 258^{\circ}C$	
<i>c</i>	9.5342 Å		
<i>a</i>	3.7894 Å	$T = 306^{\circ}C$	
<i>c</i>	9.5374 Å		
<i>a</i>	3.7907 Å	$T = 354^{\circ}C$	
<i>c</i>	9.5432 Å		
<i>a</i>	3.7923 Å	$T = 449^{\circ}C$	
<i>c</i>	9.5548 Å		
<i>a</i>	3.7939 Å	$T = 497^{\circ}C$	
<i>c</i>	9.5595 Å		
<i>a</i>	3.7948 Å	$T = 534^{\circ}C$	
<i>c</i>	9.5669 Å		
<i>a</i>	3.7962 Å	$T = 571^{\circ}C$	
<i>c</i>	9.5754 Å		
<i>a</i>	3.7970 Å	$T = 608^{\circ}C$	
<i>c</i>	9.5794 Å		
<i>a</i>	3.7989 Å	$T = 645^{\circ}C$	
<i>c</i>	9.5872 Å		
<i>a</i>	3.7998 Å	$T = 679^{\circ}C$	
<i>c</i>	9.5933 Å		
<i>a</i>	3.8009 Å	$T = 712^{\circ}C$	
<i>c</i>	9.5975 Å		

density

d_{calc}	3.894 g cm ⁻³	$T = 298 K$	70R
------------	--------------------------	-------------	-----

interatomic distances and angles

(from [72H]) (see also Fig. 2)

	$T = 25^{\circ}\text{C}$	$T = 300^{\circ}\text{C}$	$T = 600^{\circ}\text{C}$	$T = 900^{\circ}\text{C}$	
$d(\text{Ti}-\text{O})$	1.9338(5) Å	1.9365(5) Å	1.9410(5) Å	1.9452(7) Å	(s) shared edge
$d(\text{Ti}-\text{O} \parallel [001])$	1.9797(23) Å	1.9831(22) Å	1.9909(23) Å	1.9957(31) Å	
$d(\text{O}-\text{O})$ (s)	2.4658(29) Å	2.4681(29) Å	2.4745(30) Å	2.4777(39) Å	
$d(\text{O}-\text{O})$	2.7924(13) Å	2.7968(13) Å	2.8037(14) Å	2.8108(18) Å	
angle O-Ti-O	101.90(7) $^{\circ}$	101.96(7) $^{\circ}$	102.01(7) $^{\circ}$	102.10(9) $^{\circ}$	

coefficient of linear thermal expansion

α_{\parallel}	$7.380 \cdot 10^{-6} + 6.620 \cdot 10^{-9}(T-273) + 1.771 \cdot 10^{-11}(T-273)^2$	see Fig. 3	70R
α_{\perp}	$3.533 \cdot 10^{-6} + 5.610 \cdot 10^{-9}(T-273) + 4.315 \cdot 10^{-12}(T-273)^2$		

References:

- 70R Rao, K. V. K., Nagender Naidu, S. V., Iyengar, L.: J. Am. Ceram. Soc. 53 (1970) 124.
72H Horn, M., Schwertfeger, C. F., Meagher, E. P.: Z. Kristallogr. 136 (1972) 273.
75W Wells, A. F.: Structural Inorganic Chemistry O. U. P. 1975.

Fig. 1.

TiO_2 , anatase. Relationship of anatase to NaCl. Metal ions removed from the NaCl structure are shown as dotted circles [75W].

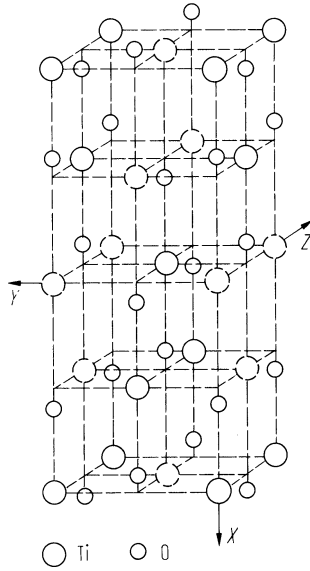


Fig. 2.

TiO₂, anatase. Upper and lower bounds to the two nearest Ti–O bond lengths vs. temperature [72H].

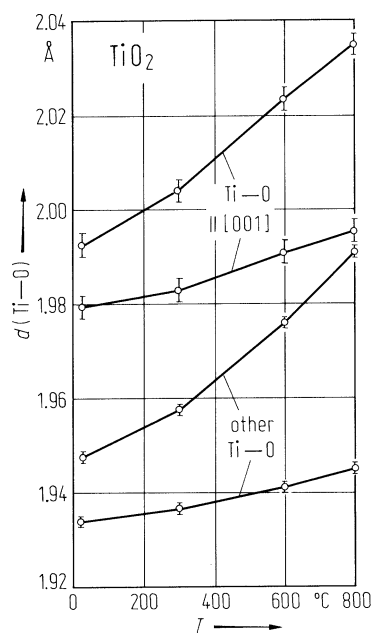


Fig. 3.

TiO₂, anatase and rutile. Thermal expansion coefficients vs. temperature [70R].

