

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

property: crystal structure of Ti_6O_{11} , Ti_7O_{13} , Ti_8O_{15} , Ti_9O_{17}

lattice parameters

(RT values)

a	5.566(2) Å	Ti_6O_{11}	space group $A\bar{1}$	63A, 71T, 82L
b	7.144(2) Å			
c	24.066(7) Å			
α	98.473(4)°			
β	120.802(8)°	Ti_7O_{13}	space group $C_i^1 - P\bar{1}$	
γ	108.520(6)°			
a	5.547(2) Å			
b	7.140(3) Å			
c	15.370(7) Å	Ti_8O_{15}	space group $C_i^1 - A\bar{1}$	
α	98.905(6)°			
β	125.457(9)°			
γ	108.517(6)°			
a	5.534(2) Å	Ti_9O_{17}	space group $C_i^1 - P\bar{1}$	
b	7.144(2) Å			
c	37.613(12) Å			
α	97.167(3)°			
β	128.384(6)°	Ti_9O_{17}	space group $C_i^1 - P\bar{1}$	
γ	108.470(4)°			
a	5.527(2) Å			
b	7.141(3) Å			
c	22.278(8) Å	Ti_9O_{17}	space group $C_i^1 - P\bar{1}$	
α	97.264(4)°			
β	131.338(7)°			
γ	108.499(4)°			

Estimated atomic positions [82L] show that in these shear phases the pseudo-rutile chains deviate considerably from the rutile axis, which allows the face-sharing Ti ions to move considerably further apart and reduce electron repulsion.

References:

- 63A Andersson, S., Jahnberg, L.: Arkiv Kemi 21 (1963) 413.
71T Teresaki, O., Watanabe, D.: Jpn. J. Appl. Phys. 10 (1971) 292.
82L Le Page, Y., Strobel, P.: J. Solid State Chem. 43 (1982) 314.