

**substance: PdO**

**property: crystal structure, lattice parameters, thermal expansion**

**crystal structure:** tetragonal, space group,  $D_{4h}^9 - P4_1/mmc$ ,  $Z = 2$  [71R].

Each Pd is surrounded by a slightly distorted square of oxygen atoms at 2.02369 Å.

The four oxygens are actually in the form of a rectangle with sides 3.0434 and 2.682 Å. Coordinates in the unit cell: 2Pd atoms at 0, 0, 0; 1/2, 1/2, 1; 2O atoms at 1/2, 0, 1/4; 1/2, 0, 3/4 [71R].

**lattice parameters**

$a$	3.03 Å	53W
	3.0434 Å	68M
	3.0434(2) Å	71R
$c$	5.33 Å	53W
	5.337 Å	68M
	5.3363(4) Å	71R

variation with temperature

$a$	3.0475 Å	$T = 20\text{ }^{\circ}\text{C}$	74B
$c$	5.3430 Å		
$a$	3.0525 Å	$T = 220\text{ }^{\circ}\text{C}$	
$c$	5.3516 Å		
$a$	3.0557 Å	$T = 420\text{ }^{\circ}\text{C}$	
$c$	5.3582 Å		
$a$	3.0593 Å	$T = 620\text{ }^{\circ}\text{C}$	
$c$	5.3662 Å		
$a$	3.0625 Å	$T = 750\text{ }^{\circ}\text{C}$	
$c$	5.3731 Å		

**linear thermal expansion coefficients**

$\alpha_a$	$6.7(5) \cdot 10^{-6}\text{ K}^{-1}$	$T = 20 \dots 750^{\circ}\text{C}$	in $a$ -direction	74B
$\alpha_c$	$7.7(7) \cdot 10^{-6}\text{ K}^{-1}$	$T = 20 \dots 750^{\circ}\text{C}$	in $c$ -direction	

PdO dissociates at high temperature.

## References:

- 53W Waser, J., Levy, H. A., Peterson, S. W.: Acta Crystallogr. 6 (1953) 661.  
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71R Rogers, D. B., Shannon, R. D., Gillson, J. L.: J. Solid State Chem. 3 (1971) 314.  
74B Bayer G., Wiedmann, H. G.: Thermal Anal. Proc. Int. Conf. 4th. H. Buzas (ed.) London: Heiden, 1975, p. 763.