substance: CoO
property: phase diagram, crystal structure, lattice parameters

phase diagram: Fig. 1. The spinel Co_3O_4 is unstable at high temperatures and the monoxide shows a wide range of stoichiometry [64F].

phase boundaries

$\log_{10} a_{O_2}$	16.5 – 20300/T[K] for $Co_{1-\delta}O/Co_3O_4$ 7.2 – 24100/T[K] for $Co/Co_{1-\delta}O$	a_{O_2} is the oxygen activity	77D

crystal structure

$T > T_N$: NaCl cubic structure, space group O_h^5 – Fm3m, Z = 4 [53G].

T < T_N: Jahn-Teller distortion leading to an approximately tetragonal structure that preserves orbital angular momentum (Fig. 2) [53G], space group C_{2h}^3 – C2/m, Z = 2 [66S].

lattice parameters

a	4.2581(5) Å	high-	pressure dependence: Fig. 3	53G
	4.258 Å	temperature		66C
		phase, T = 295 K		
a	5.183 Å	low-	within the NaCl setting this can	66S
b	3.015 Å	temperature	be described as $a = b$ = 4.265 Å,	
c	3.017 Å	phase, T = 77 K	c = 4.217 Å, c/a = 0.9887,	
β	125º33'		$\alpha = \beta = \gamma$ = 89º58'	

References:

53G Greenwald, S.: Acta Crystallogr. 6 (1953) 396.
64F Fisher, B., Tannhauser, D. S.: J. Electrochem. Soc. 111 (1964) 1194.
66C Clendenen, R. L., Drickamer, H. G.: J. Chem. Phys. 44 (1966) 4223.
66S Saito, S., Nakahiyashi, K., Shinomura, Y.: J. Phys. Soc. Jpn. 21 (1966) 850.
77D Dieckmann, R.: Z. Phys. Chem. (N. F.) 107 (1977) 189.

Fig. 1.

Co – O. Phase diagram [77D]. a_{O_2}: oxygen activity.

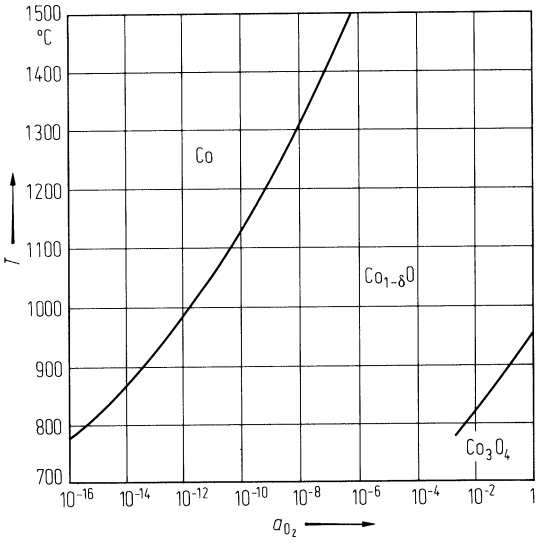

Fig. 2.

CoO. Unit cell dimensions above and below the transition temperature. The dashed vertical line shows the transition temperature as determined from magnetic measurements [53G].

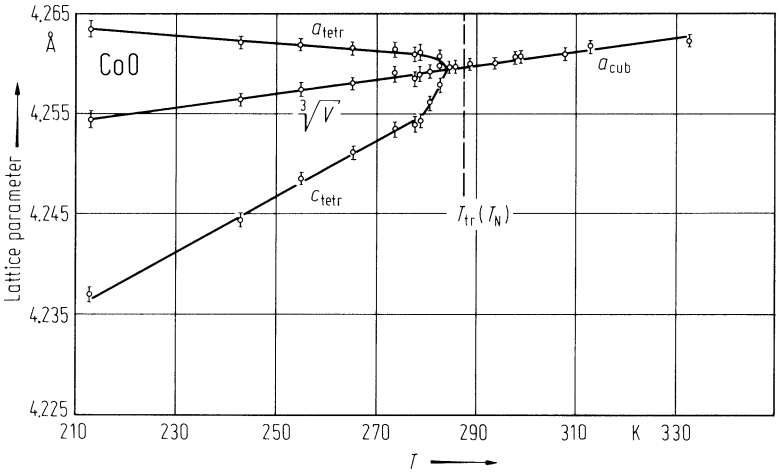

Fig. 3.

CoO. Unit cell length vs. pressure at RT [66C].