substance: Co_3O_4
property: crystal structure, lattice parameters, Debye temperature

crystal structure: spinel, space group O_h^7 – Fd3m. The tetragonal 8(a) sites are occupied by Co^{2+}, and the octahedral 16(d) sites by Co^{3+}. The 32 O^{2-} ions occupy 32(e) sites.

position parameter of the (e)-sites

u	0.3881		64R
	0.392		73S
	0.3887		68K

lattice parameter

a	8.084 Å	lattice parameters of Ni- and Zn-doped samples: Figs. 1, 2	73S
	8.065 Å		64R
	8.0835 Å		68K
	8.080 Å		78A, 79G

interatomic distances

$d(Co^{2+}–O)$	1.93 Å	tetrahedral site	64R
	1.99 Å		73S
	1.946 Å		68K
$d(Co^{3+}–O)$	1.92 Å	octahedral site	64R
	1.89 Å		73S
	1.915 Å		68K

low-temperature crystal structure

At low temperatures, magnetic ordering gives space group $T_d^2 - F\bar{4}3m$ [64R]. This structure has 4 Co^{2+} on the 4(a) sites (f.c. + 0 0 0), 4 Co^{2+} on the 4(c) sites (f.c. + 1/4 1/4 1/4), 16 Co^{3+} on 16(e) sites (x = 5/8), 16 O^{2-}on 16(e) sites ($x = u$) and 16 O^{2-} on 16(e) sites ($x = 4 – u$).

Debye temperature

Θ_D	525 K	RT	from neutron scattering temperature factor	64R

References:

64R Roth, W. L.: J. Phys. Chem. Solids 25 (1964)1.

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73S Smith, W. L., Hobson, A. D.: Acta Crystallogr. B29 (1975) 362.

78A Appandairajan, N. K., Gopalakrishnan, J.: Proc. Indian Acad. Sci. Sect. A 87 (1978) 115.

79G Gopalakrishnan. J., Appandairajan, N. K., Viswanathan, B.: Proc. Indian Acad. Sci. Sect. A 88 (1979) 217.

Fig. 1.

$Co(Ni_xCo_{2-x})O_4$. Lattice parameter vs. composition [78A].

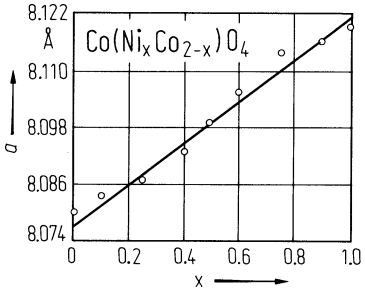

Fig. 2.

$(Co_{1-x}Zn_x)Co_2O_4$. Lattice parameter vs. composition [79G].