

ZrO_{0.37}*hP*12(182) *P*6₃22 – gdcb**ZrO_x** [1]; Mn₂N_{0.86} [3]

Structural features: Close-packed Zr layers in h stacking; O in octahedral voids (partial order).

Yamaguchi S. (1968) [1]

O_{0.37}Zr $a = 0.5631$, $c = 0.5191$ nm, $c/a = 0.922$, $V = 0.1425$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zr1	6 <i>g</i>	.2.	0.3333	0	0		trigonal prism O ₆
O2	2 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.07	octahedron Zr ₆
O3	2 <i>c</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.82	octahedron Zr ₆
O4	2 <i>b</i>	3.2	0	0	$\frac{1}{4}$	0.22	octahedron Zr ₆

Experimental: single crystal, photographs, X-rays

Remarks: Homogeneity range ZrO_x, $0.343 < x < 0.368$. The structure was studied jointly on X-ray, neutron and electron diffraction data. A report on ζ-Mn₂N with ε-Fe₂N type structure [2] is superseded in [3]. The description of *lt*-Mn₂N_{0.86} in space group (36) *Cmc*2₁ in [4] does not take into consideration all symmetry elements of the proposed model.

References: [1] Yamaguchi S. (1968), J. Phys. Soc. Jpn. 24, 855-868. [2] Hägg G. (1929), Z. Phys. Chem., Abt. B 4, 346-370. [3] Nasr Eddine M., Bertaut E.F., Maunaye M. (1977), Acta Crystallogr. B 33, 2696-2698. [4] Nasr Eddine M., Bertaut E.F. (1977), Solid State Commun. 23, 147-150.