

ZrTaNO	<i>hP4</i>	(187) <i>P-6m2</i> – edba
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ZrTaNO [1]

Structural features: Close-packed Zr and Ta layers in h stacking; O in trigonal voids in Zr layers, N in trigonal voids in Ta layers. O(Zr₃Ta₂) trigonal bipyramids share vertices to form a 3D-framework; N in trigonal (Ta₃) voids.

Schönberg N. (1954) [1]

NOTaZr

$a = 0.3645$, $c = 0.3881$ nm, $c/a = 1.065$, $V = 0.0447$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zr1	1 <i>e</i>	-6 <i>m2</i>	$\frac{2}{3}$	$\frac{1}{3}$	0		coplanar triangle O ₃
N2	1 <i>d</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		coplanar triangle Ta ₃
Ta3	1 <i>b</i>	-6 <i>m2</i>	0	0	$\frac{1}{2}$		trigonal bipyramid O ₂ N ₃
O4	1 <i>a</i>	-6 <i>m2</i>	0	0	0		trigonal bipyramid Ta ₂ Zr ₃

Transformation from published data: origin shift $\frac{1}{3} \frac{2}{3} 0$

Experimental: powder, film, X-rays

References: [1] Schönberg N. (1954), Acta Chem. Scand. 8, 627-629.