

$\text{ZrIr}_3\text{B}_{3.75}$  $hP16$  $(176) P6_3/m - h^2db$ **ZrIr<sub>3</sub>B<sub>3.75</sub>** [1]

Structural features: Infinite columns of face-linked  $\text{BIr}_6$  octahedra (parallel to  $[001]$ ) and  $\text{B}(\text{Zr}_3\text{Ir}_3)\text{Ir}$  monocapped trigonal prisms (prism axes perpendicular to  $[001]$ ) share atoms to form a dense framework. Linear -B- chains (partial vacancies ignored) and single B atoms.

Rogl P. (1978) [1]

 $\text{B}_{3.76}\text{Ir}_3\text{Zr}$  $a = 0.756$ ,  $c = 0.3512$  nm,  $c/a = 0.465$ ,  $V = 0.1738$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
B1	$6h$	$m..$	0.044	0.439	$\frac{1}{4}$		tricapped trigonal prism $\text{Ir}_4\text{B}_2\text{Zr}_3$
Ir2	$6h$	$m..$	0.2551	0.3285	$\frac{1}{4}$		pentagonal pyramid $\text{B}_6$
Zr3	$2d$	$-6..$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		pseudo Frank-Kasper $\text{B}_9\text{Ir}_9\text{Zr}_2$
B4	$2b$	$-3..$	0	0	0	0.76	colinear $\text{B}_2$

Transformation from published data:  $y, x, -z$ Experimental: single crystal, diffractometer, X-rays,  $R = 0.038$ 

References: [1] Rogl P. (1978), Acta Crystallogr. B 34, 721-724.