$Zr_3Pb_{0.04}O_{2.08}F_{7.92}$	*hP*70	(186) $P6_3mc$ – dc^8b^5

$Pb_{0.04}Zr_3O_{2.08}F_{7.92}$ [1]
Structural features: Units of six edge-linked $Zr(F,O)_8$ square antiprisms (an empty central cube) share vertices to form a 3D-framework; Pb in tetrahedral voids.

Papiernik R., Frit B. (1984) [1]
$F_{7.92}O_{2.08}Pb_{0.04}Zr_3$
$a = 0.7671$, $c = 1.249$ nm, $c/a = 1.628$, $V = 0.6365$ nm^3, $Z = 4$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
M1	12*d*	1	0.341	0.005	0.449		non-colinear Zr_2
F2	6*c*	.*m*.	0.161	0.839	0.259	0.68	
Zr3	6*c*	.*m*.	0.1789	0.8211	0.0797		square antiprism O_4F_4
O4	6*c*	.*m*.	0.204	0.796	0.241	0.32	
O5	6*c*	.*m*.	0.464	0.536	0.147	0.58	
Zr6	6*c*	.*m*.	0.4878	0.5122	0.31		square antiprism O_4F_4
F7	6*c*	.*m*.	0.505	0.495	0.132	0.42	
M8	6*c*	.*m*.	0.7768	0.2232	0.279		non-colinear Zr_2
M9	6*c*	.*m*.	0.8914	0.1086	0.107		non-colinear Zr_2
F10	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0	0.65	
O11	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.042	0.35	
O12	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.348	0.595	
F13	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.395	0.405	
Pb14	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.5604	0.085	tetrahedron F_4

M1 = 0.957F + 0.043O; M8 = 0.957F + 0.043O; M9 = 0.957F + 0.043O
Transformation from published data: origin shift 0 0 0.18
Experimental: single crystal, diffractometer, X-rays, R = 0.031

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Papiernik R., Frit B. (1984), Rev. Chim. Miner. 21, 321-334.