

V_4P_2C	$hP21$	(189) $P-62m - jg^3fda$
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V_4P_2C [1]; Ca_2IrO_4 [2]; $K_{1.71}DyI_4$ [3]

Structural features: Infinite chains of edge-linked CV_6 octahedra share edges and vertices with PV_6 trigonal prisms (in part monocapped) to form a 3D-framework.

Boller H. (1973) [1]

CP_2V_4

$a = 0.956$, $c = 0.316$ nm, $c/a = 0.331$, $V = 0.2501$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
V1	$6j$	$m..$	0.24	0.45	0		square pyramid CP_4
V2	$3g$	$m2m$	0.19	0	$\frac{1}{2}$		octahedron C_2P_4
V3	$3g$	$m2m$	0.47	0	$\frac{1}{2}$		coplanar triangle C_2P
P4	$3g$	$m2m$	0.715	0	$\frac{1}{2}$		monocapped trigonal prism V_7
C5	$3f$	$m2m$	0.33	0	0		octahedron V_6
P6	$2d$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		trigonal prism V_6
P7	$1a$	$-62m$	0	0	0		trigonal prism V_6

Transformation from published data: $-x, -y, -z$; origin shift $0\ 0\ \frac{1}{2}$

Experimental: powder, diffractometer, X-rays

Remarks: In table 3 of [1] the x -coordinate of the C site is misprinted as 0.33 instead of 0.67 (checked on the drawing in fig. 2).

References: [1] Boller H. (1973), Monatsh. Chem. 104, 48-56. [2] Babel D., Rüdorff W., Tschöpp R. (1966), Z. Anorg. Allg. Chem. 347, 282-288. [3] Hohnstedt C., Meyer G. (1991), Naturwissenschaften 78, 462-463.