

$\text{Sr}_5\text{Cu}[\text{VO}_4]_3\text{O}$	<i>hP44</i>	(176) $P6_3/m - ih^4fba$
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$\text{Sr}_5(\text{VO}_4)_3(\text{CuO})$ [1], apatite family; $\text{Sr}_{4.99}\text{Eu}_{0.01}(\text{PO}_4)_3\text{Br}_{0.5}\text{F}_{0.5}$ [2]

Structural features: Infinite columns of base-linked SrO_6O_3 tricapped trigonal prisms share atoms with VO_4 tetrahedra to form a 3D-framework; infinite linear -Cu-O- chains in columns of face-linked Sr_6 octahedra parallel to [001].

Carrillo Cabrera W., Von Schnering H.G. (1999) [1]

$\text{Cu}_{0.90}\text{O}_{12.95}\text{Sr}_5\text{V}_3$

$a = 1.0126$, $c = 0.7415$ nm, $c/a = 0.732$, $V = 0.6584$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.3449	0.094	0.0658		single atom V
O2	6 <i>h</i>	<i>m</i> ..	0.1609	0.4841	$\frac{1}{4}$		single atom V
Sr3	6 <i>h</i>	<i>m</i> ..	0.24992	0.25944	$\frac{1}{4}$		pentagonal bipyramid O ₇
V4	6 <i>h</i>	<i>m</i> ..	0.4003	0.0333	$\frac{1}{4}$		tetrahedron O ₄
O5	6 <i>h</i>	<i>m</i> ..	0.5961	0.1306	$\frac{1}{4}$		single atom V
Sr6	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0015		trigonal prism O ₆
Cu7	2 <i>b</i>	-3..	0	0	0	0.896	colinear O ₂
O8	2 <i>a</i>	-6..	0	0	$\frac{1}{4}$	0.95	colinear Cu ₂

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

Experimental: single crystal, diffractometer, X-rays, R = 0.043, T = 295 K

Remarks: In table 2 of [1] the *z*-coordinates of former sites V, O1 and O2 are misprinted as $\frac{1}{2}$ instead of $\frac{1}{4}$ (agreement with Wyckoff position 6*h*).

References: [1] Carrillo Cabrera W., Von Schnering H.G. (1999), Z. Anorg. Allg. Chem. 625, 183-185.
[2] Nötzold D., Wulff H. (2000), Phys. Status Solidi A 177, 281-292.