

$\text{Hf}_6(\text{Ni}_{0.76}\text{Sb}_{0.24})\text{Sb}_2$ $hP12$ (189) $P\text{-}62m - \text{ifda}$ **Hf₆Ni_{0.76}Sb_{2.24}** [1]

Structural features: Infinite columns of base-linked SbHf_6 trigonal prisms share edges to form a 3D-framework; single columns of base-linked $(\text{Ni,Sb})\text{Hf}_6$ trigonal prisms in channels parallel to $[001]$. Variant of $\beta_1\text{-K}_2\text{UF}_6$ with splitting of one of the Hf sites.

Kleinke H. (1998) [1]

 $\text{Hf}_6\text{Ni}_{0.76}\text{Sb}_{2.24}$ $a = 0.7605$, $c = 0.3724$ nm, $c/a = 0.490$, $V = 0.1865$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Hf1	$6i$	$..m$	0.2433	0	0.455	0.5	
Hf2	$3f$	$m2m$	0.5973	0	0		
Sb3	$2d$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		
M4	$1a$	$-62m$	0	0	0		

 $\text{M4} = 0.76\text{Ni} + 0.24\text{Sb}$ Transformation from published data: $-x, -y, -z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.041$, $T = 295$ K

Remarks: Homogeneity range $\text{Hf}_6\text{Ni}_{1-x}\text{Sb}_{2+x}$, $-0.25 < x < 0.24$. Short interatomic distances for partly occupied site(s). In table 3 of [1] the Wyckoff positions of former Hf2, Ni and Sb are misprinted as $3g$, $1b$ and $2c$ instead of $6i$, $1a$ and $2d$, respectively.

References: [1] Kleinke H. (1998), J. Alloys Compd. 270, 136-141.