

$\text{Ba}_{0.4}\text{Hf}_6\text{As}_{8.85}$ *hP40* $(176) P6_3/m - h^6e$ **Ba_{0.8}Hf₁₂As_{17.7}** [1]

Structural features: Infinite columns of base-linked HfAs₆As₃ tricapped and HfAs₆As₂ bicapped trigonal prisms (partial vacancies ignored) share atoms to form a 3D-framework with WC-type columns (5 prisms in the dented triangular cross-section); Ba in channels of hexagonal cross-section parallel to [001] (partial disorder). Infinite square-mesh As ribbons (6-atom wide; partial vacancies).

Lam R., Mar A. (1998) [1]

 $\text{As}_{8.85}\text{Ba}_{0.42}\text{Hf}_6$ $a = 1.4997$, $c = 0.35526$ nm, $c/a = 0.237$, $V = 0.6920$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
As1	6 <i>h</i>	<i>m</i> ..	0.0142	0.45	$\frac{1}{4}$	0.56	8-vertex polyhedron As ₄ Hf ₄
As2	6 <i>h</i>	<i>m</i> ..	0.0718	0.2384	$\frac{1}{4}$		non-colinear As ₂
As3	6 <i>h</i>	<i>m</i> ..	0.285	0.5099	$\frac{1}{4}$		trigonal prism Hf ₆
As4	6 <i>h</i>	<i>m</i> ..	0.3422	0.2965	$\frac{1}{4}$	0.39	8-vertex polyhedron As ₄ Hf ₄
Hf5	6 <i>h</i>	<i>m</i> ..	0.35495	0.11892	$\frac{1}{4}$		tricapped trigonal prism As ₉
Hf6	6 <i>h</i>	<i>m</i> ..	0.61802	0.1772	$\frac{1}{4}$		square antiprism As ₈
Ba7	4 <i>e</i>	3..	0	0	0.137	0.209	

Experimental: single crystal, diffractometer, X-rays, wR = 0.118, T = 295 K

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

References: [1] Lam R., Mar A. (1998), Inorg. Chem. 37, 5364-5368.