

UMo₁₃P₉

hP23

(187) *P-6m2* – $1k^4_{jea}$

UMo₁₃P₉ [1]

Structural features: Infinite columns of base-linked PMo₆Mo monocapped, PMo₆Mo₂ and P(U₂Mo₄)Mo₂ bicapped trigonal prisms share atoms to form a 3D-framework with two kinds of WC-type column (3 and 6 prisms in the triangular cross-section, respectively).

Le Sénéchal C. et al. (2001) [1]

Mo₁₃P₉U_{0.88}

$a = 1.08061$, $c = 0.33138$ nm, $c/a = 0.307$, $V = 0.3351$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mo1	<i>6l</i>	<i>m.</i>	0.2844	0.0046	0		square pyramid P ₅
P2	<i>3k</i>	<i>mm2</i>	0.0979	0.9021	$\frac{1}{2}$		monocapped trigonal prism Mo ₇
Mo3	<i>3k</i>	<i>mm2</i>	0.2409	0.7591	$\frac{1}{2}$		square pyramid P ₅
Mo4	<i>3k</i>	<i>mm2</i>	0.5268	0.4732	$\frac{1}{2}$		tetrahedron P ₄
P5	<i>3k</i>	<i>mm2</i>	0.7942	0.2058	$\frac{1}{2}$		trigonal prism Mo ₆
P6	<i>3j</i>	<i>mm2</i>	0.4356	0.5644	0		square antiprism Mo ₈
U7	<i>1e</i>	<i>-6m2</i>	$\frac{2}{3}$	$\frac{1}{3}$	0	0.88	bicapped hexagonal prism P ₆ Mo ₆ U ₂
Mo8	<i>1a</i>	<i>-6m2</i>	0	0	0		trigonal prism P ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.046, T = 293 K

References: [1] Le Sénéchal C., Babizhets'kii V.S., Députier S., Pivan J.Y., Guérin R. (2001), Z. Anorg. Allg. Chem. 627, 1325-1333.