

K_2ReH_9	$hP36$	(189) $P-62m - lkigf^2da$
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K_2ReH_9 [2]

Structural features: Single ReH_6H_3 tricapped trigonal prisms. Filled-up derivative of Fe_2P with H in tetrahedral (K_3Re) and square pyramidal (K_4Re) voids.

Bronger W. et al. (1999) [1]

H_9K_2Re

$a = 0.9599$, $c = 0.5549$ nm, $c/a = 0.578$, $V = 0.4428$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
H1	12l	1	0.2237	0.5321	0.2805		single atom Re
H2	6k	$m..$	0.3686	0.5127	$\frac{1}{2}$		single atom Re
H3	6i	$..m$	0.8712	0	0.2077		single atom Re
K4	3g	$m2m$	0.2626	0	$\frac{1}{2}$		square prism (cube) H_8
H5	3f	$m2m$	0.1749	0	0		single atom Re
K6	3f	$m2m$	0.5876	0	0		14-vertex polyhedron H_{14}
Re7	2d	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism H_9
Re8	1a	$-62m$	0	0	0		tricapped trigonal prism H_9

Experimental: single crystal, diffractometer, neutrons, $R = 0.042$

Remarks: Identical to the phase called K_2ReH_8 in [4]. The data from [2] are also reported in [3].

References: [1] Bronger W., A Brassard L., Müller P., Lebech B., Schultz T. (1999), Z. Anorg. Allg. Chem. 625, 1143-1146. [2] Abrahams S.C., Ginsberg A.P., Knox K. (1964), Inorg. Chem. 3, 558-567. [3] Abrahams S.C., Knox K. (1964), J. Phys. (Paris) 25, 461-462. [4] Ginsberg A.P., Miller J.M., Koubek E. (1961), J. Am. Chem. Soc. 83, 4909-4915.