Nb_9PdAs_7	*hP*51	(174) *P*-6 – k^8j^8eda

Nb_9PdAs_7 [1]
Structural features: $AsNb_6Pd_3$ tricapped, $As(Nb_4Pd_2)Nb_2$ and $AsNb_6(NbPd)$ bicapped, $AsNb_6Nb$ monocapped and $AsNb_6$ trigonal prisms share atoms to form a 3D-framework with WC-type columns (10 As-centered prisms in the triangular cross-section).

Wang M., Mar A. (2001) [1]
As_7Nb_9Pd
a = 1.66955, c = 0.35582 nm, c/a = 0.213, V = 0.8589 nm^3, Z = 3

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
As1	3*k*	*m*..	0.0728	0.27065	$^1/_2$		square antiprism Pd_2Nb_6
As2	3*k*	*m*..	0.11474	0.48934	$^1/_2$		monocapped trigonal prism Nb_7
Nb3	3*k*	*m*..	0.12059	0.13091	$^1/_2$		7-capped pentagonal prism $As_5Pd_4Nb_8$
As4	3*k*	*m*..	0.28996	0.4467	$^1/_2$		monocapped trigonal prism Nb_7
Nb5	3*k*	*m*..	0.31844	0.11658	$^1/_2$		15-vertex Frank-Kasper $As_5Pd_2Nb_8$
Nb6	3*k*	*m*..	0.35451	0.32442	$^1/_2$		15-vertex Frank-Kasper As_5Nb_{10}
Nb7	3*k*	*m*..	0.49636	0.07269	$^1/_2$		15-vertex polyhedron As_5Nb_{10}
Nb8	3*k*	*m*..	0.53367	0.28785	$^1/_2$		14-vertex polyhedron As_6Nb_8
Nb9	3*j*	*m*..	0.02973	0.35787	0		15-vertex Frank-Kasper As_5Nb_9Pd
Nb10	3*j*	*m*..	0.07225	0.57828	0		15-vertex polyhedron As_5Nb_{10}
Pd11	3*j*	*m*..	0.15826	0.01025	0		bicapped hexagonal prism $As_4Nb_8Pd_2$
Nb12	3*j*	*m*..	0.20192	0.31536	0		15-vertex Frank-Kasper As_5Nb_9Pd
Nb13	3*j*	*m*..	0.24556	0.53364	0		14-vertex polyhedron As_6Nb_8
As14	3*j*	*m*..	0.2614	0.19388	0		square antiprism Nb_7Pd
As15	3*j*	*m*..	0.44785	0.15675	0		pseudo Frank-Kasper Nb_7As_6
As16	3*j*	*m*..	0.48689	0.37261	0		monocapped trigonal prism Nb_7
As17	1*e*	-6..	$^2/_3$	$^1/_3$	0		trigonal prism Nb_6
As18	1*d*	-6..	$^1/_3$	$^2/_3$	$^1/_2$		trigonal prism Nb_6
As19	1*a*	-6..	0	0	0		tricapped trigonal prism Pd_3Nb_6

Transformation from published data: *y*,*x*,*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.033, T = 295 K

References: [1] Wang M., Mar A. (2001), Inorg. Chem. 40, 5365-5370.