

UNiAlH<sub>2.2</sub>*hP27*(189) *P-62m* – jhg<sup>2</sup>f<sup>2</sup>eca**UNiAlH<sub>2.2</sub>** [1]

Structural features: Filled-up derivative of ZrNiAl with H in tetrahedral (U<sub>3</sub>Ni), trigonal bipyramidal (U<sub>5</sub> and U<sub>4</sub>Ni) and trigonal (U<sub>3</sub>) voids.

Yamamoto T. et al. (1998) [1]

AlD<sub>2.20</sub>NiU $a = 0.71713$ ,  $c = 0.39757$  nm,  $c/a = 0.554$ ,  $V = 0.1771$  nm<sup>3</sup>,  $Z = 3$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
D1	6 <i>j</i>	<i>m</i> ..	0.207	0.233	0	0.09	
D2	4 <i>h</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.432	0.4	
D3	3 <i>g</i>	<i>m2m</i>	0.331	0	<sup>1</sup> / <sub>2</sub>		non-colinear Al <sub>2</sub>
U4	3 <i>g</i>	<i>m2m</i>	0.659	0	<sup>1</sup> / <sub>2</sub>		
Al5	3 <i>f</i>	<i>m2m</i>	0.347	0	0		trigonal bipyramid D <sub>5</sub>
D6	3 <i>f</i>	<i>m2m</i>	0.577	0	0	0.15	
D7	2 <i>e</i>	3. <i>m</i>	0	0	0.43	0.5	
Ni8	2 <i>c</i>	-6..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0		colinear D <sub>2</sub>
Ni9	1 <i>a</i>	-62 <i>m</i>	0	0	0		

Experimental: powder, diffractometer, neutrons

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

References: [1] Yamamoto T., Ishii Y., Kayano H. (1998), J. Alloys Compd. 269, 162-165.