

GdAg_{3.6} [1]; Hf₁₄Cu₅₁ [3]; PuAg₃ (see remark)

Structural features: Gd₂Ag₂₄ units (two Gd inside a double hexagonal antiprism capped by two triangles) and GdAg₁₄ polyhedra share atoms to form a dense 3D-framework. See Fig. IV.87.

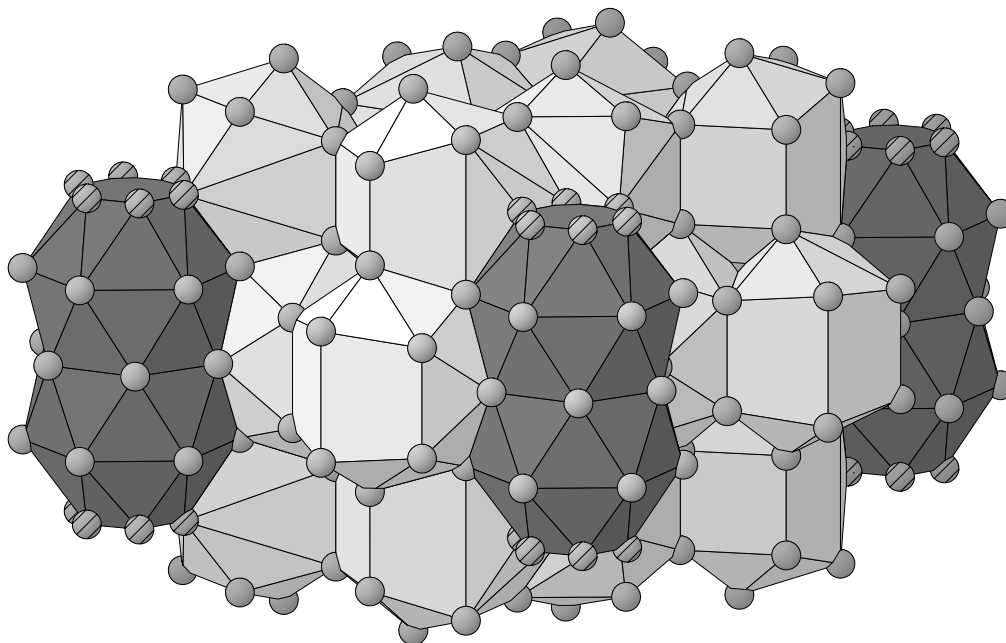


Fig. IV.87. **GdAg_{3.6}**

Arrangement of GdAg₁₂ polyhedra (light) and Gd₂Ag₂₄ units (dark): two Gd atoms inside a double hexagonal antiprism capped by two triangles (the Ag atoms from the partly occupied site forming the latter are hatched).

Bailey D.M., Kline G.R. (1971) [1]

Ag_{50.85}Gd₁₄

$a = 1.2670$, $c = 0.9332$ nm, $c/a = 0.737$, $V = 1.2974$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	12l	1	0.1049	0.439	0.3305		pseudo Frank-Kasper Ag ₉ Gd ₄
Ag2	12l	1	0.2662	0.0744	0.2370		pseudo Frank-Kasper Ag ₉ Gd ₄
Ag3	12l	1	0.4944	0.1155	0.1526		icosahedron Ag ₈ Gd ₄
Ag4	6k	$m..$	0.0589	0.2383	$\frac{1}{2}$		icosahedron Ag ₈ Gd ₄
Gd5	6k	$m..$	0.4680	0.1394	$\frac{1}{2}$		14-vertex polyhedron Ag ₁₄
Ag6	6j	$m..$	0.0193	0.1324	0	0.4742	
Gd7	6j	$m..$	0.1138	0.3898	0		15-vertex Frank-Kasper Ag ₁₅
Ag8	4h	3.. $\bar{3}$	$\frac{1}{3}$	$\frac{2}{3}$	0.2987		bicapped square prism Ag ₇ Gd ₃
Gd9	2e	6.. $\bar{6}$	0	0	0.3060		
Ag10	2c	-6.. $\bar{6}$	$\frac{1}{3}$	$\frac{2}{3}$	0		pseudo Frank-Kasper Ag ₈ Gd ₃

Transformation from published data: $y, x, -z$

Experimental: single crystal, diffractometer, X-rays, R = 0.045

Remarks: Identical to the phase called Gd_2Ag_7 in [4], same sample studied. The authors suggest splitting of site Gd7 to avoid short interatomic distances $d(\text{Gd7}-\text{Ag6})$. Non-centrosymmetric space groups were tested and rejected. The atom coordinates have not been determined for PuAg_3 (cell parameters in [2], isotypism stated in [1]). Short interatomic distances for partly occupied site(s).

References: [1] Bailey D.M., Kline G.R. (1971), *Acta Crystallogr. B* 27, 650-653. [2] Runnalls O.J.C. (1956), *Can. J. Chem.* 34, 133-145. [3] Gabathuler J.P., White P., Parthé E. (1975), *Acta Crystallogr. B* 31, 608-610. [4] McMasters O.D., Gschneidner K.A. Jr., Venteicher R.F. (1970), *Acta Crystallogr. B* 26, 1224-1229.