

GdSI	<i>hP12</i>	(174) <i>P</i> -6 – $kj^2fca$
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**GdSI** [1]

Beck H.P., Strobel C. (1986) [1]

GdIS

$a = 1.0737$ ,  $c = 0.4179$  nm,  $c/a = 0.389$ ,  $V = 0.4172$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
I1	$3k$	$m..$	0.14967	0.31433	$\frac{1}{2}$		bicapped hexagonal prism Gd <sub>6</sub> S <sub>6</sub> I <sub>2</sub>
S2	$3j$	$m..$	0.03467	0.51733	0		single atom Gd
Gd3	$3j$	$m..$	0.30167	0.15433	0		single atom S
I4	$1f$	$-6..$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{2}$		bicapped hexagonal prism Gd <sub>6</sub> S <sub>6</sub> I <sub>2</sub>
Gd5	$1c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	0		coplanar triangle S <sub>3</sub>
S6	$1a$	$-6..$	0	0	0		coplanar triangle Gd <sub>3</sub>

Transformation from published data:  $y,x,z$ ; origin shift  $\frac{1}{3} \frac{2}{3} \frac{1}{2}$

Experimental: powder, film, X-rays

References: [1] Beck H.P., Strobel C. (1986), Z. Anorg. Allg. Chem. 535, 229-239.