$Cs_3Ga_2F_9$	*hP*84	(185) $P6_3cm$ – $d^3c^6b^2a^2$

$Cs_3Ga_2F_9$ [1]
Structural features: Distorted close-packed CsF_3 layers in h stacking; Ga in octahedral (F_6) voids. Units of two face-linked GaF_6 octahedra. Vacancy derivative of $BaNiO_3$ (perovskite 2H).

De Kozak A. et al. (1994) [1]
$Cs_3F_9Ga_2$
a = 1.0945, c = 1.4756 nm, c/a = 1.348, V = 1.5308 nm^3, Z = 6

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	12*d*	1	0.1819	0.5131	0.3818		single atom Ga
F2	12*d*	1	0.1911	0.522	0.0739		single atom Ga
F3	12*d*	1	0.3368	0.5381	0.2261		non-colinear Ga_2
F4	6*c*	..*m*	0.1255	0	0.4017		non-colinear Ga_2
F5	6*c*	..*m*	0.1405	0	0.7559		single atom Ga
F6	6*c*	..*m*	0.1446	0	0.0547		single atom Ga
Cs7	6*c*	..*m*	0.3205	0	0.225		anticuboctahedron F_{12}
Cs8	6*c*	..*m*	0.3375	0	0.5549		15-vertex Frank-Kasper $F_{12}Ga_3$
Cs9	6*c*	..*m*	0.6558	0	0.4064		anticuboctahedron F_{12}
Ga10	4*b*	3..	$^1/_3$	$^2/_3$	0.1305		octahedron F_6
Ga11	4*b*	3..	$^1/_3$	$^2/_3$	0.3236		octahedron F_6
Ga12	2*a*	3.*m*	0	0	0.0		octahedron F_6
Ga13	2*a*	3.*m*	0	0	0.3071		octahedron F_6

Transformation from published data: -*x*,-*y*,-*z*; origin shift 0 0 0.0936
Experimental: single crystal, diffractometer, X-rays, R = 0.030

Remarks: Space group (193) $P6_3/mcm$ was tested and rejected (R = 0.15).

References: [1] De Kozak A., Mary Y., Gredin P., Renaudin J., Ferey G., Babel D. (1994), Eur. J. Solid State Inorg. Chem. 31, 115-122.