$Zn_{58}Gd_{13}$	*hP*142	(186) $P6_3mc$ – $d^4c^{14}b^3a^2$

$Gd_{13}Zn_{58}$ [1]
Structural features: $GdZn_{18}$ and $Gd(Gd,Zn)_n$ polyhedra share atoms to form a dense 3D-framework.

Wang F.E. (1967) [1]
$Gd_{13}Zn_{58}$
a = 1.4352, c = 1.4218 nm, c/a = 0.991, V = 2.5363 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zn1	12*d*	1	0.0244	0.2023	0.0211		bicapped square prism Zn_6Gd_4
Zn2	12*d*	1	0.0856	0.3695	0.2598		icosahedron Zn_8Gd_4
Zn3	12*d*	1	0.3576	0.0304	0.4119		icosahedron Zn_8Gd_4
Zn4	12*d*	1	0.3803	0.0428	0.1128		pseudo Frank-Kasper Zn_7Gd_4
Zn5	6*c*	.*m*.	0.0772	0.9228	0.1655		icosahedron Zn_8Gd_4
Zn6	6*c*	.*m*.	0.1051	0.8949	0.3517		icosahedron Zn_8Gd_4
Gd7	6*c*	.*m*.	0.1993	0.8007	0.0632		pseudo Frank-Kasper Zn_{18}
Gd8	6*c*	.*m*.	0.2102	0.7898	0.4556		pseudo Frank-Kasper Zn_{18}
Zn9	6*c*	.*m*.	0.273	0.727	0.2686		icosahedron $Zn_{10}Gd_2$
Zn10	6*c*	.*m*.	0.4346	0.5654	0.376		pseudo Frank-Kasper $Zn_{10}Gd_3$
Zn11	6*c*	.*m*.	0.438	0.562	0.1736		pseudo Frank-Kasper $Zn_{10}Gd_3$
Zn12	6*c*	.*m*.	0.5064	0.4936	0.0129		square prism (cube) Zn_8
Gd13	6*c*	.*m*.	0.5462	0.4538	0.2515		7-capped pentagonal prism Zn_{17}
Zn14	6*c*	.*m*.	0.6032	0.3968	0.4623		pseudo Frank-Kasper $Zn_{10}Gd_3$
Zn15	6*c*	.*m*.	0.6156	0.3844	0.0726		pseudo Frank-Kasper $Zn_{10}Gd_3$
Zn16	6*c*	.*m*.	0.7556	0.2444	0.1557		bicapped square prism Zn_6Gd_4
Zn17	6*c*	.*m*.	0.7736	0.2264	0.3402		bicapped square prism Zn_6Gd_4
Gd18	6*c*	.*m*.	0.8684	0.1316	0.235		15-vertex Frank-Kasper Zn_{15}
Zn19	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.097		icosahedron Zn_9Gd_3
Zn20	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.413		icosahedron Zn_9Gd_3
Zn21	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.7402		15-vertex Frank-Kasper $Zn_{12}Gd_3$
Gd22	2*a*	3*m*.	0	0	0.0		14-vertex polyhedron Zn_{14}
Zn23	2*a*	3*m*.	0	0	0.2491		pseudo Frank-Kasper Zn_6Gd_5

Transformation from published data: origin shift 0 0 0.265
Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.130

Remarks: Phase referred to as η-(GdZn). In table 1 of [1] the z-coordinate of former Zn(13) is misprinted as 0.3148 instead of 0.362 (see [2]). In table 2 of [1] the number of Gd atoms at 0.437 nm from former Gd2 is misprinted as 1 instead of 2 and the coordination polyhedron is consequently stated to contain one instead of two Gd atoms. The structure was redetermined in space group (194) $P6_3/mmc$ in [3].

References: [1] Wang F.E. (1967), Acta Crystallogr. 22, 579-584. [2] Bruzzone G., Fornasini M.L., Merlo F. (1970), J. Less-Common Met. 21, 225-253. [3] Cromer D.T., Larson A.C. (1972), Acta Crystallogr. B 28, 1016-1022.