

Table 2 Lattice constants including a and c , formation energy ΔE of calculated Mg_{36} and Mg_{35}R_1 ($\text{R} = \text{Fe}, \text{Mn}, \text{Zn}, \text{Mo}, \text{W}, \text{Li}, \text{Sn}, \text{Sc}, \text{Y}, \text{Gd}, \text{Nd}, \text{Ca}, \text{Sr}, \text{Ba}$) solid solutions.

Solid solution	a (Å)	c (Å)	ΔE (eV/atom)
Mg_{36}	3.180	5.218	0.00000
	3.195 ^[27]	5.178 ^[27]	
$\text{Mg}_{35}\text{Zn}_1$	3.165	5.202	-0.00278
	3.184 ^[27]	5.188 ^[27]	
Mg_{35}Y_1	3.190	5.264	-0.00639
	3.214 ^[27]	5.205 ^[27]	
$\text{Mg}_{35}\text{Ca}_1$	3.214	5.215	-0.00214
	3.221 ^[27]	5.211 ^[27]	
$\text{Mg}_{35}\text{Sr}_1$	3.228	5.235	0.01014
$\text{Mg}_{35}\text{Gd}_1$	3.195	5.256	-0.00578
$\text{Mg}_{35}\text{Mn}_1$	3.155	5.178	0.05383
$\text{Mg}_{35}\text{Nd}_1$	3.206	5.251	-0.00519
$\text{Mg}_{35}\text{Sn}_1$	3.207	5.135	-0.01300
$\text{Mg}_{35}\text{Fe}_1$	3.146	5.190	0.02900
$\text{Mg}_{35}\text{Ba}_1$	3.225	5.295	0.02253
$\text{Mg}_{35}\text{Li}_1$	3.165	5.250	-0.00581
	3.194 ^[28]	5.150 ^[28]	
$\text{Mg}_{35}\text{Mo}_1$	3.164	5.165	0.04150
$\text{Mg}_{35}\text{Sc}_1$	3.177	5.240	-0.00500
Mg_{35}W_1	3.199	5.051	0.06411