SG No. 91 D_4^3 $P4_122$ [tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: .2.

No.	position	mapping
1	$[0, y, 0]$	[1,5]
2	$\left[0, -y, \frac{1}{2}\right]$	[2,6]
3	$\left[-y, 0, \frac{1}{4}\right]$	[3,8]
4	$\left[y, 0, \frac{3}{4}\right]$	[4,7]

Table 2: Wyckoff site: 4b, site symmetry: .2.

No.	position	mapping
1	$\left[\frac{1}{2}, y, 0\right]$	[1,5]
2	$\left[\frac{1}{2}, -y, \frac{1}{2}\right]$	[2,6]
3	$\left[-y, \frac{1}{2}, \frac{1}{4}\right]$	[3,8]
4	$\left[y, \frac{1}{2}, \frac{3}{4}\right]$	[4,7]

Table 3: Wyckoff site: 4c, site symmetry: ..2

No.	position	mapping
1	$\left[x, x, \frac{3}{8}\right]$	[1,7]
2	$\left[-x, -x, \frac{7}{8}\right]$	[2,8]
3	$\left[-x, x, \frac{5}{8}\right]$	[3,5]
4	$\left[x, -x, \frac{1}{8}\right]$	[4,6]

Table 4: Wyckoff site: 8d, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$\left[-x, -y, z + \frac{1}{2}\right]$	[2]
3	$\left[-y, x, z + \frac{1}{4}\right]$	[3]
4	$\left[y, -x, z + \frac{3}{4}\right]$	[4]
5	$[-x, y, -z]$	[5]
6	$\left[x, -y, \frac{1}{2} - z\right]$	[6]
7	$\left[y, x, \frac{3}{4} - z\right]$	[7]
8	$\left[-y, -x, \frac{1}{4} - z\right]$	[8]