

SG No. 99 C_{4v}^1 $P4mm$ [tetragonal]

* plus set: + [0, 0, 0]

Table 1: Wyckoff site: 1a, site symmetry: 4mm

No.	position	mapping
1	[0, 0, z]	[1,2,3,4,5,6,7,8]

Table 2: Wyckoff site: 1b, site symmetry: 4mm

No.	position	mapping
1	[\frac{1}{2}, \frac{1}{2}, z]	[1,2,3,4,5,6,7,8]

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

No.	position	mapping
1	[\frac{1}{2}, 0, z]	[1,2,5,6]
2	[0, \frac{1}{2}, z]	[3,4,7,8]

Table 4: Wyckoff site: 4d, site symmetry: .m

No.	position	mapping
1	[x, x, z]	[1,8]
2	[-x, -x, z]	[2,7]
3	[-x, x, z]	[3,6]
4	[x, -x, z]	[4,5]

Table 5: Wyckoff site: 4e, site symmetry: .m.

No.	position	mapping
1	[x, 0, z]	[1,5]
2	[-x, 0, z]	[2,6]
3	[0, x, z]	[3,8]
4	[0, -x, z]	[4,7]

Table 6: Wyckoff site: 4f, site symmetry: .m.

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

Table 7: Wyckoff site: 8g, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[2]
3	$[-y, x, z]$	[3]
4	$[y, -x, z]$	[4]
5	$[x, -y, z]$	[5]
6	$[-x, y, z]$	[6]
7	$[-y, -x, z]$	[7]
8	$[y, x, z]$	[8]