

PG No. 11 C_{4h} $4/m$ [tetragonal]

Table 1: Wyckoff site: 1o, site symmetry: 4/m..

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

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

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

Table 3: Wyckoff site: 4b, site symmetry: m..

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

Table 4: Wyckoff site: 8c, 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]