

MSG No. 84.53 $P4'_2/m$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 2/m..

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

Table 2: Wyckoff site: 2b, site symmetry: 2/m..

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

Table 3: Wyckoff site: 2c, site symmetry: 2/m..

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

Table 4: Wyckoff site: 2d, site symmetry: 2/m..

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

Table 5: Wyckoff site: 2e, site symmetry: -4'..

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

Table 6: Wyckoff site: 2f, site symmetry: -4'..

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

Table 7: Wyckoff site: 4g, site symmetry: 2..

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

Table 8: Wyckoff site: 4h, site symmetry: 2..

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

Table 9: Wyckoff site: 4i, site symmetry: 2..

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

Table 10: Wyckoff site: 4j, site symmetry: m..

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

Table 11: Wyckoff site: 8k, site symmetry: 1

No.	position	mapping
1	[x, y, z]	[1]
2	[-x, -y, z]	[2]
3	[-x, -y, -z]	[3]
4	[x, y, -z]	[4]

continued ...

Table 11

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