

MSG No. 84.54 $P4_2/m'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x, z + \frac{1}{2}]$	[2]
3	$[y, -x, z + \frac{1}{2}]$	[3]
4	$[-x, -y, z]$	[4]

continued ...

Table 11

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