

MSG No. 83.48 P_c4/m [Type IV, tetragonal]

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

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,5,6,7,8]
2	[0, 0, $\frac{1}{2}$]	[9,10,11,12,13,14,15,16]

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

No.	position	mapping
1	[0, 0, $\frac{1}{4}$]	[1,2,3,4,13,14,15,16]
2	[0, 0, $\frac{3}{4}$]	[5,6,7,8,9,10,11,12]

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

No.	position	mapping
1	[$\frac{1}{2}$, $\frac{1}{2}$, 0]	[1,2,3,4,5,6,7,8]
2	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[9,10,11,12,13,14,15,16]

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

No.	position	mapping
1	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{4}$]	[1,2,3,4,13,14,15,16]
2	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{3}{4}$]	[5,6,7,8,9,10,11,12]

Table 5: Wyckoff site: 4e, site symmetry: 2/m..

No.	position	mapping
1	[0, $\frac{1}{2}$, 0]	[1,4,5,8]
2	[$\frac{1}{2}$, 0, 0]	[2,3,6,7]
3	[0, $\frac{1}{2}$, $\frac{1}{2}$]	[9,12,13,16]
4	[$\frac{1}{2}$, 0, $\frac{1}{2}$]	[10,11,14,15]

Table 6: Wyckoff site: **4f**, site symmetry: $2/m \cdot \cdot \cdot$

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{4}]$	[1, 4, 13, 16]
2	$[\frac{1}{2}, 0, \frac{1}{4}]$	[2, 3, 14, 15]
3	$[0, \frac{1}{2}, \frac{3}{4}]$	[5, 8, 9, 12]
4	$[\frac{1}{2}, 0, \frac{3}{4}]$	[6, 7, 10, 11]

Table 7: Wyckoff site: **4g**, site symmetry: $4 \cdot \cdot \cdot$

No.	position	mapping
1	$[0, 0, z]$	[1, 2, 3, 4]
2	$[0, 0, -z]$	[5, 6, 7, 8]
3	$[0, 0, z + \frac{1}{2}]$	[9, 10, 11, 12]
4	$[0, 0, \frac{1}{2} - z]$	[13, 14, 15, 16]

Table 8: Wyckoff site: **4h**, site symmetry: $4 \cdot \cdot \cdot$

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, z]$	[1, 2, 3, 4]
2	$[\frac{1}{2}, \frac{1}{2}, -z]$	[5, 6, 7, 8]
3	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[9, 10, 11, 12]
4	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[13, 14, 15, 16]

Table 9: Wyckoff site: **8i**, site symmetry: $2 \cdot \cdot \cdot$

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	[1, 4]
2	$[\frac{1}{2}, 0, z]$	[2, 3]
3	$[0, \frac{1}{2}, -z]$	[5, 8]
4	$[\frac{1}{2}, 0, -z]$	[6, 7]
5	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[9, 12]
6	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[10, 11]
7	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[13, 16]
8	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[14, 15]

Table 10: Wyckoff site: 8j, site symmetry: $\mathbf{m} \cdot \cdot$

No.	position	mapping
1	$[x, y, 0]$	[1,8]
2	$[-y, x, 0]$	[2,7]
3	$[y, -x, 0]$	[3,6]
4	$[-x, -y, 0]$	[4,5]
5	$[x, y, \frac{1}{2}]$	[9,16]
6	$[-y, x, \frac{1}{2}]$	[10,15]
7	$[y, -x, \frac{1}{2}]$	[11,14]
8	$[-x, -y, \frac{1}{2}]$	[12,13]

Table 11: Wyckoff site: 8k, site symmetry: $\mathbf{m}' \cdot \cdot \cdot$

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	[1,16]
2	$[-y, x, \frac{1}{4}]$	[2,15]
3	$[y, -x, \frac{1}{4}]$	[3,14]
4	$[-x, -y, \frac{1}{4}]$	[4,13]
5	$[-x, -y, \frac{3}{4}]$	[5,12]
6	$[y, -x, \frac{3}{4}]$	[6,11]
7	$[-y, x, \frac{3}{4}]$	[7,10]
8	$[x, y, \frac{3}{4}]$	[8,9]

Table 12: Wyckoff site: 16l, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x, z]$	[2]
3	$[y, -x, z]$	[3]
4	$[-x, -y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[y, -x, -z]$	[6]
7	$[-y, x, -z]$	[7]
8	$[x, y, -z]$	[8]
9	$[x, y, z + \frac{1}{2}]$	[9]
10	$[-y, x, z + \frac{1}{2}]$	[10]
11	$[y, -x, z + \frac{1}{2}]$	[11]
12	$[-x, -y, z + \frac{1}{2}]$	[12]
13	$[-x, -y, \frac{1}{2} - z]$	[13]
14	$[y, -x, \frac{1}{2} - z]$	[14]
15	$[-y, x, \frac{1}{2} - z]$	[15]
16	$[x, y, \frac{1}{2} - z]$	[16]