

MSG No. 132.451 $P4'_2/mcm'$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: $m \cdot m' \cdot m'$

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

Table 2: Wyckoff site: 2b, site symmetry: $-4'2m'$

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: $m \cdot m' \cdot m'$

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

Table 4: Wyckoff site: 2d, site symmetry: $-4'2m'$

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: 222.

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

Table 6: Wyckoff site: 4f, site symmetry: 2/m..

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

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

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

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

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

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

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

Table 10: Wyckoff site: 4j, site symmetry: m.2'm'

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

Table 11: Wyckoff site: 8k, site symmetry: 2..

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

Table 12: Wyckoff site: 8l, site symmetry: .2.

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

Table 13: Wyckoff site: 8m, site symmetry: .2.

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

Table 14: Wyckoff site: 8n, site symmetry: m..

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

continued ...

Table 14

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

Table 15: Wyckoff site: 8o, site symmetry: . .m'

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

Table 16: Wyckoff site: 16p, site symmetry: 1

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