

MSG No. 131.440 $P4'_2/m'm'c$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site: 4g, site symmetry: $2\bar{m}'\bar{m}'$.

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

Table 8: Wyckoff site: 4h, site symmetry: $2\bar{m}'\bar{m}'$.

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

Table 9: Wyckoff site: 4i, site symmetry: $2\bar{m}'\bar{m}'$.

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

Table 10: Wyckoff site: 4j, site symmetry: $\bar{m}'2\bar{m}'$.

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

Table 11: Wyckoff site: 4k, site symmetry: $\bar{m}'2\bar{m}'$.

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

Table 12: Wyckoff site: 41, site symmetry: $m'2m'$.

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

Table 13: Wyckoff site: 4m, site symmetry: $m'2m'$.

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

Table 14: Wyckoff site: 8n, site symmetry: $\dots 2'$

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

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

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

Table 16: Wyckoff site: 8p, site symmetry: .m'.

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

Table 17: Wyckoff site: 8q, site symmetry: m'..

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

Table 18: Wyckoff site: 16r, 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]
5	$[y, -x, \frac{1}{2} - z]$	[5]
6	$[-y, x, \frac{1}{2} - z]$	[6]
7	$[-y, -x, z + \frac{1}{2}]$	[7]
8	$[y, x, z + \frac{1}{2}]$	[8]
9	$[-y, x, z + \frac{1}{2}]$	[9]
10	$[y, -x, z + \frac{1}{2}]$	[10]
11	$[y, x, \frac{1}{2} - z]$	[11]
12	$[-y, -x, \frac{1}{2} - z]$	[12]
13	$[-x, -y, -z]$	[13]
14	$[-x, y, z]$	[14]
15	$[x, -y, z]$	[15]
16	$[x, y, -z]$	[16]