

MSG No. 215.70 $P\bar{4}3m$ [Type I, cubic]

Table 1: Wyckoff site: **1a**, site symmetry: **-43m**

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 2: Wyckoff site: **1b**, site symmetry: **-43m**

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 3: Wyckoff site: **3c**, site symmetry: **-42.m**

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, 3, 4, 13, 14, 21, 22]$
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, 8, 10, 12, 17, 18, 19, 20]$
3	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[6, 7, 9, 11, 15, 16, 23, 24]$

Table 4: Wyckoff site: **3d**, site symmetry: **-42.m**

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	$[1, 2, 3, 4, 13, 14, 21, 22]$
2	$[0, \frac{1}{2}, 0]$	$[5, 8, 10, 12, 17, 18, 19, 20]$
3	$[0, 0, \frac{1}{2}]$	$[6, 7, 9, 11, 15, 16, 23, 24]$

Table 5: Wyckoff site: **4e**, site symmetry: **.3m**

No.	position	mapping
1	$[x, x, x]$	$[1, 5, 6, 20, 22, 24]$
2	$[x, -x, -x]$	$[2, 10, 11, 16, 17, 21]$
3	$[-x, x, -x]$	$[3, 7, 12, 13, 18, 23]$
4	$[-x, -x, x]$	$[4, 8, 9, 14, 15, 19]$

Table 6: Wyckoff site: 6f, site symmetry: 2..mm

No.	position	mapping
1	[$x, 0, 0$]	[1, 2, 21, 22]
2	[$-x, 0, 0$]	[3, 4, 13, 14]
3	[$0, x, 0$]	[5, 12, 18, 20]
4	[$0, 0, x$]	[6, 9, 15, 24]
5	[$0, 0, -x$]	[7, 11, 16, 23]
6	[$0, -x, 0$]	[8, 10, 17, 19]

Table 7: Wyckoff site: 6g, site symmetry: 2..mm

No.	position	mapping
1	[$x, \frac{1}{2}, \frac{1}{2}$]	[1, 2, 21, 22]
2	[$-x, \frac{1}{2}, \frac{1}{2}$]	[3, 4, 13, 14]
3	[$\frac{1}{2}, x, \frac{1}{2}$]	[5, 12, 18, 20]
4	[$\frac{1}{2}, \frac{1}{2}, x$]	[6, 9, 15, 24]
5	[$\frac{1}{2}, \frac{1}{2}, -x$]	[7, 11, 16, 23]
6	[$\frac{1}{2}, -x, \frac{1}{2}$]	[8, 10, 17, 19]

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

No.	position	mapping
1	[$x, \frac{1}{2}, 0$]	[1, 2]
2	[$-x, \frac{1}{2}, 0$]	[3, 4]
3	[$0, x, \frac{1}{2}$]	[5, 12]
4	[$\frac{1}{2}, 0, x$]	[6, 9]
5	[$\frac{1}{2}, 0, -x$]	[7, 11]
6	[$0, -x, \frac{1}{2}$]	[8, 10]
7	[$-x, 0, \frac{1}{2}$]	[13, 14]
8	[$0, \frac{1}{2}, x$]	[15, 24]
9	[$0, \frac{1}{2}, -x$]	[16, 23]
10	[$\frac{1}{2}, -x, 0$]	[17, 19]
11	[$\frac{1}{2}, x, 0$]	[18, 20]
12	[$x, 0, \frac{1}{2}$]	[21, 22]

Table 9: Wyckoff site: 12i, site symmetry: ...m

No.	position	mapping
1	[x, x, z]	[1, 20]
2	[$x, -x, -z$]	[2, 17]
3	[$-x, x, -z$]	[3, 18]

continued ...

Table 9

No.	position	mapping
4	$[-x, -x, z]$	[4,19]
5	$[z, x, x]$	[5,24]
6	$[x, z, x]$	[6,22]
7	$[-x, z, -x]$	[7,13]
8	$[-z, -x, x]$	[8,15]
9	$[-x, -z, x]$	[9,14]
10	$[z, -x, -x]$	[10,16]
11	$[x, -z, -x]$	[11,21]
12	$[-z, x, -x]$	[12,23]

Table 10: Wyckoff site: 24j, 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	$[z, x, y]$	[5]
6	$[y, z, x]$	[6]
7	$[-y, z, -x]$	[7]
8	$[-z, -x, y]$	[8]
9	$[-y, -z, x]$	[9]
10	$[z, -x, -y]$	[10]
11	$[y, -z, -x]$	[11]
12	$[-z, x, -y]$	[12]
13	$[-x, z, -y]$	[13]
14	$[-x, -z, y]$	[14]
15	$[-z, -y, x]$	[15]
16	$[z, -y, -x]$	[16]
17	$[y, -x, -z]$	[17]
18	$[-y, x, -z]$	[18]
19	$[-y, -x, z]$	[19]
20	$[y, x, z]$	[20]
21	$[x, -z, -y]$	[21]
22	$[x, z, y]$	[22]
23	$[-z, y, -x]$	[23]
24	$[z, y, x]$	[24]