

MPG No. 29.3.111 $m'\bar{3}'$ [Type III, cubic]

Table 1: Wyckoff site: **1o**, site symmetry: $\mathbf{m}'\mathbf{-3}'$

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: **6a**, site symmetry: $\mathbf{2mm}$.

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

Table 3: Wyckoff site: **8b**, site symmetry: $.3.$

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

Table 4: Wyckoff site: **12c**, site symmetry: $\mathbf{m}'\mathbf{\cdot\cdot\cdot}$

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

continued ...

Table 4

No.	position	mapping
11	[$y, -z, 0$]	[6,19]
12	[$-y, -z, 0$]	[8,17]

Table 5: Wyckoff site: 24d, site symmetry: 1

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