

MPG No. 32.1.118 $m\bar{3}m$ [Type I, cubic]

Table 1: Wyckoff site: **1o**, site symmetry: **m-3m**

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, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]

Table 2: Wyckoff site: **6a**, site symmetry: **4m.m**

No.	position	mapping
1	[x, 0, 0]	[1, 2, 19, 20, 27, 28, 41, 42]
2	[-x, 0, 0]	[3, 4, 17, 18, 25, 26, 43, 44]
3	[0, x, 0]	[9, 11, 14, 16, 34, 36, 37, 39]
4	[0, -x, 0]	[10, 12, 13, 15, 33, 35, 38, 40]
5	[0, 0, x]	[5, 8, 22, 23, 30, 31, 45, 48]
6	[0, 0, -x]	[6, 7, 21, 24, 29, 32, 46, 47]

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

No.	position	mapping
1	[x, x, x]	[1, 5, 9, 37, 41, 45]
2	[-x, -x, x]	[4, 8, 12, 40, 44, 48]
3	[-x, x, -x]	[3, 7, 11, 39, 43, 47]
4	[x, -x, -x]	[2, 6, 10, 38, 42, 46]
5	[x, x, -x]	[16, 20, 24, 28, 32, 36]
6	[-x, -x, -x]	[13, 17, 21, 25, 29, 33]
7	[x, -x, x]	[15, 19, 23, 27, 31, 35]
8	[-x, x, x]	[14, 18, 22, 26, 30, 34]

Table 4: Wyckoff site: **12c**, site symmetry: **m.m2**

No.	position	mapping
1	[0, y, y]	[1, 18, 26, 41]
2	[0, -y, y]	[4, 19, 27, 44]
3	[0, y, -y]	[3, 20, 28, 43]
4	[0, -y, -y]	[2, 17, 25, 42]
5	[y, 0, y]	[9, 15, 35, 37]
6	[y, 0, -y]	[10, 16, 36, 38]
7	[-y, 0, y]	[12, 14, 34, 40]
8	[-y, 0, -y]	[11, 13, 33, 39]
9	[y, y, 0]	[5, 24, 32, 45]

continued ...

Table 4

No.	position	mapping
10	$[-y, y, 0]$	[7,22,30,47]
11	$[y, -y, 0]$	[6,23,31,46]
12	$[-y, -y, 0]$	[8,21,29,48]

Table 5: Wyckoff site: 24d, site symmetry: $\mathbf{m..}$

No.	position	mapping
1	$[0, y, z]$	[1,26]
2	$[0, -y, z]$	[4,27]
3	$[0, y, -z]$	[3,28]
4	$[0, -y, -z]$	[2,25]
5	$[z, 0, y]$	[9,35]
6	$[z, 0, -y]$	[10,36]
7	$[-z, 0, y]$	[12,34]
8	$[-z, 0, -y]$	[11,33]
9	$[y, z, 0]$	[5,32]
10	$[-y, z, 0]$	[7,30]
11	$[y, -z, 0]$	[6,31]
12	$[-y, -z, 0]$	[8,29]
13	$[y, 0, -z]$	[16,38]
14	$[-y, 0, -z]$	[13,39]
15	$[y, 0, z]$	[15,37]
16	$[-y, 0, z]$	[14,40]
17	$[0, z, -y]$	[20,43]
18	$[0, z, y]$	[18,41]
19	$[0, -z, -y]$	[17,42]
20	$[0, -z, y]$	[19,44]
21	$[z, y, 0]$	[24,45]
22	$[z, -y, 0]$	[23,46]
23	$[-z, y, 0]$	[22,47]
24	$[-z, -y, 0]$	[21,48]

Table 6: Wyckoff site: 24e, site symmetry: $\dots\mathbf{m}$

No.	position	mapping
1	$[x, x, z]$	[1,37]
2	$[-x, -x, z]$	[4,40]
3	$[-x, x, -z]$	[3,39]
4	$[x, -x, -z]$	[2,38]
5	$[z, x, x]$	[9,45]
6	$[z, -x, -x]$	[10,46]
7	$[-z, -x, x]$	[12,48]

continued ...

Table 6

No.	position	mapping
8	$[-z, x, -x]$	[11,47]
9	$[x, z, x]$	[5,41]
10	$[-x, z, -x]$	[7,43]
11	$[x, -z, -x]$	[6,42]
12	$[-x, -z, x]$	[8,44]
13	$[x, x, -z]$	[16,28]
14	$[-x, -x, -z]$	[13,25]
15	$[x, -x, z]$	[15,27]
16	$[-x, x, z]$	[14,26]
17	$[x, z, -x]$	[20,32]
18	$[-x, z, x]$	[18,30]
19	$[-x, -z, -x]$	[17,29]
20	$[x, -z, x]$	[19,31]
21	$[z, x, -x]$	[24,36]
22	$[z, -x, x]$	[23,35]
23	$[-z, x, x]$	[22,34]
24	$[-z, -x, -x]$	[21,33]

Table 7: Wyckoff site: 48f, 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	$[y, x, -z]$	[16]
14	$[-y, -x, -z]$	[13]
15	$[y, -x, z]$	[15]
16	$[-y, x, z]$	[14]
17	$[x, z, -y]$	[20]
18	$[-x, z, y]$	[18]
19	$[-x, -z, -y]$	[17]
20	$[x, -z, y]$	[19]
21	$[z, y, -x]$	[24]
22	$[z, -y, x]$	[23]
23	$[-z, y, x]$	[22]

continued ...

Table 7

No.	position	mapping
24	$[-z, -y, -x]$	[21]
25	$[-x, -y, -z]$	[25]
26	$[x, y, -z]$	[28]
27	$[x, -y, z]$	[27]
28	$[-x, y, z]$	[26]
29	$[-z, -x, -y]$	[33]
30	$[-z, x, y]$	[34]
31	$[z, x, -y]$	[36]
32	$[z, -x, y]$	[35]
33	$[-y, -z, -x]$	[29]
34	$[y, -z, x]$	[31]
35	$[-y, z, x]$	[30]
36	$[y, z, -x]$	[32]
37	$[-y, -x, z]$	[40]
38	$[y, x, z]$	[37]
39	$[-y, x, -z]$	[39]
40	$[y, -x, -z]$	[38]
41	$[-x, -z, y]$	[44]
42	$[x, -z, -y]$	[42]
43	$[x, z, y]$	[41]
44	$[-x, z, -y]$	[43]
45	$[-z, -y, x]$	[48]
46	$[-z, y, -x]$	[47]
47	$[z, -y, -x]$	[46]
48	$[z, y, x]$	[45]