

MPG No. 32.3.120 $m'\bar{3}'m$ [Type III, cubic]

Table 1: Wyckoff site: 1o, site symmetry: $m'-3'm$

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: $4'm.m'$

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

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

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

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

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

continued ...

Table 4

No.	position	mapping
10	$[-y, y, 0]$	$[7, 23, 34, 42]$
11	$[y, -y, 0]$	$[6, 22, 35, 43]$
12	$[-y, -y, 0]$	$[8, 24, 33, 41]$

Table 5: Wyckoff site: **24d**, site symmetry: $m'..$

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

Table 6: Wyckoff site: **24e**, site symmetry: $..m$

No.	position	mapping
1	$[x, x, z]$	$[1, 13]$
2	$[-x, -x, z]$	$[4, 16]$
3	$[-x, x, -z]$	$[3, 15]$
4	$[x, -x, -z]$	$[2, 14]$
5	$[z, x, x]$	$[9, 21]$
6	$[z, -x, -x]$	$[10, 22]$
7	$[-z, -x, x]$	$[12, 24]$

continued ...

Table 6

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

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	$[y, x, -z]$	[28]
14	$[-y, -x, -z]$	[25]
15	$[y, -x, z]$	[27]
16	$[-y, x, z]$	[26]
17	$[x, z, -y]$	[32]
18	$[-x, z, y]$	[30]
19	$[-x, -z, -y]$	[29]
20	$[x, -z, y]$	[31]
21	$[z, y, -x]$	[36]
22	$[z, -y, x]$	[35]
23	$[-z, y, x]$	[34]

continued ...

Table 7

No.	position	mapping
24	$[-z, -y, -x]$	[33]
25	$[-x, -y, -z]$	[37]
26	$[x, y, -z]$	[40]
27	$[x, -y, z]$	[39]
28	$[-x, y, z]$	[38]
29	$[-z, -x, -y]$	[45]
30	$[-z, x, y]$	[46]
31	$[z, x, -y]$	[48]
32	$[z, -x, y]$	[47]
33	$[-y, -z, -x]$	[41]
34	$[y, -z, x]$	[43]
35	$[-y, z, x]$	[42]
36	$[y, z, -x]$	[44]
37	$[-y, -x, z]$	[16]
38	$[y, x, z]$	[13]
39	$[-y, x, -z]$	[15]
40	$[y, -x, -z]$	[14]
41	$[-x, -z, y]$	[20]
42	$[x, -z, -y]$	[18]
43	$[x, z, y]$	[17]
44	$[-x, z, -y]$	[19]
45	$[-z, -y, x]$	[24]
46	$[-z, y, -x]$	[23]
47	$[z, -y, -x]$	[22]
48	$[z, y, x]$	[21]