

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

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

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: $\text{m}'.\text{m}2'$

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: $m' \dots$

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: $\dots m$

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]