

MPG No. 32.2.119 $m\bar{3}m1'$ [Type II, cubic]

Table 1: Wyckoff site: 1o, site symmetry: $m\bar{3}m1'$

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, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96]

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

No.	position	mapping
1	[x, 0, 0]	[1, 2, 19, 20, 27, 28, 41, 42, 49, 50, 67, 68, 75, 76, 89, 90]
2	[-x, 0, 0]	[3, 4, 17, 18, 25, 26, 43, 44, 51, 52, 65, 66, 73, 74, 91, 92]
3	[0, x, 0]	[9, 11, 14, 16, 34, 36, 37, 39, 57, 59, 62, 64, 82, 84, 85, 87]
4	[0, -x, 0]	[10, 12, 13, 15, 33, 35, 38, 40, 58, 60, 61, 63, 81, 83, 86, 88]
5	[0, 0, x]	[5, 8, 22, 23, 30, 31, 45, 48, 53, 56, 70, 71, 78, 79, 93, 96]
6	[0, 0, -x]	[6, 7, 21, 24, 29, 32, 46, 47, 54, 55, 69, 72, 77, 80, 94, 95]

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

No.	position	mapping
1	[x, x, x]	[1, 5, 9, 37, 41, 45, 49, 53, 57, 85, 89, 93]
2	[-x, -x, x]	[4, 8, 12, 40, 44, 48, 52, 56, 60, 88, 92, 96]
3	[-x, x, -x]	[3, 7, 11, 39, 43, 47, 51, 55, 59, 87, 91, 95]
4	[x, -x, -x]	[2, 6, 10, 38, 42, 46, 50, 54, 58, 86, 90, 94]
5	[x, x, -x]	[16, 20, 24, 28, 32, 36, 64, 68, 72, 76, 80, 84]
6	[-x, -x, -x]	[13, 17, 21, 25, 29, 33, 61, 65, 69, 73, 77, 81]
7	[x, -x, x]	[15, 19, 23, 27, 31, 35, 63, 67, 71, 75, 79, 83]
8	[-x, x, x]	[14, 18, 22, 26, 30, 34, 62, 66, 70, 74, 78, 82]

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

No.	position	mapping
1	[0, y, y]	[1, 18, 26, 41, 49, 66, 74, 89]
2	[0, -y, y]	[4, 19, 27, 44, 52, 67, 75, 92]
3	[0, y, -y]	[3, 20, 28, 43, 51, 68, 76, 91]
4	[0, -y, -y]	[2, 17, 25, 42, 50, 65, 73, 90]
5	[y, 0, y]	[9, 15, 35, 37, 57, 63, 83, 85]
6	[y, 0, -y]	[10, 16, 36, 38, 58, 64, 84, 86]
7	[-y, 0, y]	[12, 14, 34, 40, 60, 62, 82, 88]

continued ...

Table 4

No.	position	mapping
8	$[-y, 0, -y]$	$[11, 13, 33, 39, 59, 61, 81, 87]$
9	$[y, y, 0]$	$[5, 24, 32, 45, 53, 72, 80, 93]$
10	$[-y, y, 0]$	$[7, 22, 30, 47, 55, 70, 78, 95]$
11	$[y, -y, 0]$	$[6, 23, 31, 46, 54, 71, 79, 94]$
12	$[-y, -y, 0]$	$[8, 21, 29, 48, 56, 69, 77, 96]$

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

No.	position	mapping
1	$[0, y, z]$	$[1, 26, 49, 74]$
2	$[0, -y, z]$	$[4, 27, 52, 75]$
3	$[0, y, -z]$	$[3, 28, 51, 76]$
4	$[0, -y, -z]$	$[2, 25, 50, 73]$
5	$[z, 0, y]$	$[9, 35, 57, 83]$
6	$[z, 0, -y]$	$[10, 36, 58, 84]$
7	$[-z, 0, y]$	$[12, 34, 60, 82]$
8	$[-z, 0, -y]$	$[11, 33, 59, 81]$
9	$[y, z, 0]$	$[5, 32, 53, 80]$
10	$[-y, z, 0]$	$[7, 30, 55, 78]$
11	$[y, -z, 0]$	$[6, 31, 54, 79]$
12	$[-y, -z, 0]$	$[8, 29, 56, 77]$
13	$[y, 0, -z]$	$[16, 38, 64, 86]$
14	$[-y, 0, -z]$	$[13, 39, 61, 87]$
15	$[y, 0, z]$	$[15, 37, 63, 85]$
16	$[-y, 0, z]$	$[14, 40, 62, 88]$
17	$[0, z, -y]$	$[20, 43, 68, 91]$
18	$[0, z, y]$	$[18, 41, 66, 89]$
19	$[0, -z, -y]$	$[17, 42, 65, 90]$
20	$[0, -z, y]$	$[19, 44, 67, 92]$
21	$[z, y, 0]$	$[24, 45, 72, 93]$
22	$[z, -y, 0]$	$[23, 46, 71, 94]$
23	$[-z, y, 0]$	$[22, 47, 70, 95]$
24	$[-z, -y, 0]$	$[21, 48, 69, 96]$

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

No.	position	mapping
1	$[x, x, z]$	$[1, 37, 49, 85]$
2	$[-x, -x, z]$	$[4, 40, 52, 88]$
3	$[-x, x, -z]$	$[3, 39, 51, 87]$
4	$[x, -x, -z]$	$[2, 38, 50, 86]$
5	$[z, x, x]$	$[9, 45, 57, 93]$

continued ...

Table 6

No.	position	mapping
6	$[z, -x, -x]$	$[10, 46, 58, 94]$
7	$[-z, -x, x]$	$[12, 48, 60, 96]$
8	$[-z, x, -x]$	$[11, 47, 59, 95]$
9	$[x, z, x]$	$[5, 41, 53, 89]$
10	$[-x, z, -x]$	$[7, 43, 55, 91]$
11	$[x, -z, -x]$	$[6, 42, 54, 90]$
12	$[-x, -z, x]$	$[8, 44, 56, 92]$
13	$[x, x, -z]$	$[16, 28, 64, 76]$
14	$[-x, -x, -z]$	$[13, 25, 61, 73]$
15	$[x, -x, z]$	$[15, 27, 63, 75]$
16	$[-x, x, z]$	$[14, 26, 62, 74]$
17	$[x, z, -x]$	$[20, 32, 68, 80]$
18	$[-x, z, x]$	$[18, 30, 66, 78]$
19	$[-x, -z, -x]$	$[17, 29, 65, 77]$
20	$[x, -z, x]$	$[19, 31, 67, 79]$
21	$[z, x, -x]$	$[24, 36, 72, 84]$
22	$[z, -x, x]$	$[23, 35, 71, 83]$
23	$[-z, x, x]$	$[22, 34, 70, 82]$
24	$[-z, -x, -x]$	$[21, 33, 69, 81]$

Table 7: Wyckoff site: **48f**, site symmetry: **1**

No.	position	mapping
1	$[x, y, z]$	$[1, 49]$
2	$[-x, -y, z]$	$[4, 52]$
3	$[-x, y, -z]$	$[3, 51]$
4	$[x, -y, -z]$	$[2, 50]$
5	$[z, x, y]$	$[9, 57]$
6	$[z, -x, -y]$	$[10, 58]$
7	$[-z, -x, y]$	$[12, 60]$
8	$[-z, x, -y]$	$[11, 59]$
9	$[y, z, x]$	$[5, 53]$
10	$[-y, z, -x]$	$[7, 55]$
11	$[y, -z, -x]$	$[6, 54]$
12	$[-y, -z, x]$	$[8, 56]$
13	$[y, x, -z]$	$[16, 64]$
14	$[-y, -x, -z]$	$[13, 61]$
15	$[y, -x, z]$	$[15, 63]$
16	$[-y, x, z]$	$[14, 62]$
17	$[x, z, -y]$	$[20, 68]$
18	$[-x, z, y]$	$[18, 66]$
19	$[-x, -z, -y]$	$[17, 65]$
20	$[x, -z, y]$	$[19, 67]$
21	$[z, y, -x]$	$[24, 72]$

continued ...

Table 7

No.	position	mapping
22	$[z, -y, x]$	$[23, 71]$
23	$[-z, y, x]$	$[22, 70]$
24	$[-z, -y, -x]$	$[21, 69]$
25	$[-x, -y, -z]$	$[25, 73]$
26	$[x, y, -z]$	$[28, 76]$
27	$[x, -y, z]$	$[27, 75]$
28	$[-x, y, z]$	$[26, 74]$
29	$[-z, -x, -y]$	$[33, 81]$
30	$[-z, x, y]$	$[34, 82]$
31	$[z, x, -y]$	$[36, 84]$
32	$[z, -x, y]$	$[35, 83]$
33	$[-y, -z, -x]$	$[29, 77]$
34	$[y, -z, x]$	$[31, 79]$
35	$[-y, z, x]$	$[30, 78]$
36	$[y, z, -x]$	$[32, 80]$
37	$[-y, -x, z]$	$[40, 88]$
38	$[y, x, z]$	$[37, 85]$
39	$[-y, x, -z]$	$[39, 87]$
40	$[y, -x, -z]$	$[38, 86]$
41	$[-x, -z, y]$	$[44, 92]$
42	$[x, -z, -y]$	$[42, 90]$
43	$[x, z, y]$	$[41, 89]$
44	$[-x, z, -y]$	$[43, 91]$
45	$[-z, -y, x]$	$[48, 96]$
46	$[-z, y, -x]$	$[47, 95]$
47	$[z, -y, -x]$	$[46, 94]$
48	$[z, y, x]$	$[45, 93]$