

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

Table 1: Wyckoff site: 1o, site symmetry: m-3m1'

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:  $\mathbf{m} \cdot \cdot$ 

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:  $\cdot \cdot \mathbf{m}$ 

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]