

MSG No. 223.108 $Pm\bar{3}n'$ [Type III, cubic]

Table 1: Wyckoff site: **2a**, site symmetry: $m' \bar{3}'$.

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

Table 2: Wyckoff site: **6b**, site symmetry: $m'm'm'..$

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

Table 3: Wyckoff site: **6c**, site symmetry: $-4'm'.2$

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

Table 4: Wyckoff site: **6d**, site symmetry: $-4'm'.2$

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

Table 5: Wyckoff site: 8e, site symmetry: .32

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

Table 6: Wyckoff site: 12f, site symmetry: $2\bar{m}'\bar{m}'\dots$

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

Table 7: Wyckoff site: 12g, site symmetry: $2\bar{m}'\bar{m}'\dots$

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

Table 8: Wyckoff site: 12h, site symmetry: $2\bar{m}'\bar{m}'\dots$

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

Table 9: Wyckoff site: 16i, site symmetry: $.3.$

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

Table 10: Wyckoff site: 24j, site symmetry: $\dots 2$

No.	position	mapping
1	$[\frac{1}{4}, y, y + \frac{1}{2}]$	[1, 13]
2	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	[2, 10]
3	$[\frac{3}{4}, y, \frac{1}{2} - y]$	[3, 9]
4	$[y, y + \frac{1}{2}, \frac{1}{4}]$	[4, 18]
5	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	[5, 19]

continued ...

Table 10

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

Table 11: Wyckoff site: 24k, site symmetry: $m' \dots$

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

continued ...

Table 11

No.	position	mapping
22	$[z, 0, -y]$	[22,44]
23	$[y, -z, 0]$	[23,43]
24	$[-z, 0, -y]$	[24,41]

Table 12: Wyckoff site: 481, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[2]
3	$[x + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[3]
4	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - x]$	[4]
5	$[\frac{1}{2} - z, y + \frac{1}{2}, x + \frac{1}{2}]$	[5]
6	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[6]
7	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[7]
8	$[x, -y, -z]$	[8]
9	$[-x, y, -z]$	[9]
10	$[-x, -y, z]$	[10]
11	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[12]
13	$[\frac{1}{2} - x, z + \frac{1}{2}, y + \frac{1}{2}]$	[13]
14	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[14]
15	$[z + \frac{1}{2}, \frac{1}{2} - y, x + \frac{1}{2}]$	[15]
16	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$	[16]
17	$[z, x, y]$	[17]
18	$[y, z, x]$	[18]
19	$[-y, z, -x]$	[19]
20	$[-z, -x, y]$	[20]
21	$[-y, -z, x]$	[21]
22	$[z, -x, -y]$	[22]
23	$[y, -z, -x]$	[23]
24	$[-z, x, -y]$	[24]
25	$[-x, -y, -z]$	[25]
26	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y]$	[26]
27	$[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}]$	[27]
28	$[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}]$	[28]
29	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x]$	[29]
30	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[30]
31	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[31]
32	$[-x, y, z]$	[32]
33	$[x, -y, z]$	[33]
34	$[x, y, -z]$	[34]
35	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[35]
36	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[36]
37	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[37]

continued ...

Table 12

No.	position	mapping
38	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[38]
39	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x]$	[39]
40	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[40]
41	$[-z, -x, -y]$	[41]
42	$[-y, -z, -x]$	[42]
43	$[y, -z, x]$	[43]
44	$[z, x, -y]$	[44]
45	$[y, z, -x]$	[45]
46	$[-z, x, y]$	[46]
47	$[-y, z, x]$	[47]
48	$[z, -x, y]$	[48]