

MSG No. 204.30 $Im\bar{3}$ [Type I, cubic]

Table 1: Wyckoff site: 2a, site symmetry: $m-3$.

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

Table 2: Wyckoff site: 6b, site symmetry: $mmm..$

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

Table 3: Wyckoff site: 8c, site symmetry: $..-3$.

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

Table 4: Wyckoff site: 12d, site symmetry: $2mm..$

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

continued ...

Table 4

No.	position	mapping
10	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[30, 33, 43, 47]
11	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[31, 35, 42, 45]
12	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[32, 34, 41, 48]

Table 5: Wyckoff site: 12e, site symmetry: $2mm..$

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

Table 6: Wyckoff site: 16f, site symmetry: $..3.$

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

Table 7: Wyckoff site: **24g**, site symmetry: **m** . .

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

Table 8: Wyckoff site: **48h**, site symmetry: **1**

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[x, -y, -z]$	$[2]$
3	$[-x, y, -z]$	$[3]$
4	$[-x, -y, z]$	$[4]$
5	$[z, x, y]$	$[5]$
6	$[y, z, x]$	$[6]$
7	$[-y, z, -x]$	$[7]$
8	$[-z, -x, y]$	$[8]$
9	$[-y, -z, x]$	$[9]$
10	$[z, -x, -y]$	$[10]$
11	$[y, -z, -x]$	$[11]$
12	$[-z, x, -y]$	$[12]$
13	$[-x, -y, -z]$	$[13]$
14	$[-x, y, z]$	$[14]$
15	$[x, -y, z]$	$[15]$

continued ...

Table 8

No.	position	mapping
16	$[x, y, -z]$	[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	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[25]
26	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[26]
27	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[27]
28	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[28]
29	$[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$	[29]
30	$[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[30]
31	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{2} - x]$	[31]
32	$[\frac{1}{2} - z, \frac{1}{2} - x, y + \frac{1}{2}]$	[32]
33	$[\frac{1}{2} - y, \frac{1}{2} - z, x + \frac{1}{2}]$	[33]
34	$[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - y]$	[34]
35	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[35]
36	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - y]$	[36]
37	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[37]
38	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[38]
39	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[39]
40	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[40]
41	$[\frac{1}{2} - z, \frac{1}{2} - x, \frac{1}{2} - y]$	[41]
42	$[\frac{1}{2} - y, \frac{1}{2} - z, \frac{1}{2} - x]$	[42]
43	$[y + \frac{1}{2}, \frac{1}{2} - z, x + \frac{1}{2}]$	[43]
44	$[z + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - y]$	[44]
45	$[y + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - x]$	[45]
46	$[\frac{1}{2} - z, x + \frac{1}{2}, y + \frac{1}{2}]$	[46]
47	$[\frac{1}{2} - y, z + \frac{1}{2}, x + \frac{1}{2}]$	[47]
48	$[z + \frac{1}{2}, \frac{1}{2} - x, y + \frac{1}{2}]$	[48]