

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]