

MSG No. 217.78 $I\bar{4}3m$ [Type I, cubic]

Table 1: Wyckoff site: 2a, site symmetry: -43m

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: -42.m

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

Table 3: Wyckoff site: 8c, site symmetry: .3m

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

Table 4: Wyckoff site: 12d, site symmetry: -4..

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

continued ...

Table 4

No.	position	mapping
10	$[\frac{1}{2}, \frac{3}{4}, 0]$	[17, 19, 29, 36]
11	$[\frac{1}{2}, \frac{1}{4}, 0]$	[18, 20, 32, 34]
12	$[\frac{1}{4}, 0, \frac{1}{2}]$	[21, 22, 27, 28]

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

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

Table 6: Wyckoff site: 24f, site symmetry: 2..

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

continued ...

Table 6

No.	position	mapping
20	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[39,48]
21	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[40,47]
22	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[41,43]
23	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[42,44]
24	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[45,46]

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

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

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]

continued ...

Table 8

No.	position	mapping
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	$[-x, z, -y]$	[13]
14	$[-x, -z, y]$	[14]
15	$[-z, -y, x]$	[15]
16	$[z, -y, -x]$	[16]
17	$[y, -x, -z]$	[17]
18	$[-y, x, -z]$	[18]
19	$[-y, -x, z]$	[19]
20	$[y, x, z]$	[20]
21	$[x, -z, -y]$	[21]
22	$[x, z, y]$	[22]
23	$[-z, y, -x]$	[23]
24	$[z, y, x]$	[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	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y]$	[37]
38	$[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}]$	[38]
39	$[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}]$	[39]
40	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x]$	[40]
41	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[41]
42	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[42]
43	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[43]
44	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[44]
45	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[45]
46	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[46]
47	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x]$	[47]
48	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[48]