

MSG No. 220.89 $I\bar{4}3d$ [Type I, cubic]

Table 1: Wyckoff site: 12a, site symmetry: -4..

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

Table 2: Wyckoff site: 12b, site symmetry: -4..

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

Table 3: Wyckoff site: 16c, site symmetry: .3.

No.	position	mapping
1	$[x, x, x]$	[1, 5, 6]
2	$[x, -x, \frac{1}{2} - x]$	[2, 10, 11]
3	$[\frac{1}{2} - x, x, -x]$	[3, 7, 12]
4	$[-x, \frac{1}{2} - x, x]$	[4, 8, 9]
5	$[\frac{1}{4} - x, x + \frac{1}{4}, \frac{3}{4} - x]$	[13, 18, 23]
6	$[\frac{3}{4} - x, \frac{1}{4} - x, x + \frac{1}{4}]$	[14, 15, 19]
7	$[x + \frac{1}{4}, \frac{3}{4} - x, \frac{1}{4} - x]$	[16, 17, 21]

continued ...

Table 3

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

Table 4: Wyckoff site: 24d, site symmetry: 2..

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

Table 5: Wyckoff site: 48e, site symmetry: 1

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

continued ...

Table 5

No.	position	mapping
47	$\left[\frac{3}{4} - z, y + \frac{3}{4}, \frac{1}{4} - x\right]$	[47]
48	$\left[z + \frac{3}{4}, y + \frac{3}{4}, x + \frac{3}{4}\right]$	[48]