

MSG No. 224.114 $Pn'\bar{3}'m'$ [Type III, cubic]

Table 1: Wyckoff site: 2a, site symmetry: $-4'3m'$

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

Table 2: Wyckoff site: 4b, site symmetry: $.-3'm'$

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

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: $.3m'$

No.	position	mapping
1	$[x, x, x]$	[1, 17, 18, 36, 38, 40]
2	$[x + \frac{1}{2}, -x, x + \frac{1}{2}]$	[2, 7, 15, 33, 43, 48]

continued ...

Table 5

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

Table 6: Wyckoff site: 12f, site symmetry: 2.22

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

Table 7: Wyckoff site: 12g, site symmetry: 2.m'm'

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

Table 8: Wyckoff site: 24h, site symmetry: 2..

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

Table 9: Wyckoff site: 24i, site symmetry: ..2

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

continued ...

Table 9

No.	position	mapping
16	$[-y, \frac{1}{2} - y, \frac{1}{2}]$	[28,42]
17	$[y + \frac{1}{2}, \frac{1}{2} - y, 0]$	[29,43]
18	$[y, 0, -y]$	[30,44]
19	$[\frac{1}{2} - y, \frac{1}{2}, -y]$	[31,41]
20	$[\frac{1}{2}, y + \frac{1}{2}, y]$	[32,38]
21	$[\frac{1}{2} - y, 0, y + \frac{1}{2}]$	[35,46]
22	$[y, \frac{1}{2}, y + \frac{1}{2}]$	[36,48]
23	$[-y, y, 0]$	[39,47]
24	$[y + \frac{1}{2}, y, \frac{1}{2}]$	[40,45]

Table 10: Wyckoff site: 24j, site symmetry: ..2

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

Table 11: Wyckoff site: 24k, site symmetry: . . m'

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

Table 12: Wyckoff site: 48l, site symmetry: 1

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

continued ...

Table 12

No.	position	mapping
16	$[-z, -y, -x]$	[16]
17	$[z, x, y]$	[17]
18	$[y, z, x]$	[18]
19	$[\frac{1}{2} - y, z, \frac{1}{2} - x]$	[19]
20	$[\frac{1}{2} - z, \frac{1}{2} - x, y]$	[20]
21	$[\frac{1}{2} - y, \frac{1}{2} - z, x]$	[21]
22	$[z, \frac{1}{2} - x, \frac{1}{2} - y]$	[22]
23	$[y, \frac{1}{2} - z, \frac{1}{2} - x]$	[23]
24	$[\frac{1}{2} - z, x, \frac{1}{2} - y]$	[24]
25	$[-x, -y, -z]$	[25]
26	$[\frac{1}{2} - x, z, \frac{1}{2} - y]$	[26]
27	$[\frac{1}{2} - x, \frac{1}{2} - z, y]$	[27]
28	$[\frac{1}{2} - z, \frac{1}{2} - y, x]$	[28]
29	$[z, \frac{1}{2} - y, \frac{1}{2} - x]$	[29]
30	$[y, \frac{1}{2} - x, \frac{1}{2} - z]$	[30]
31	$[\frac{1}{2} - y, x, \frac{1}{2} - z]$	[31]
32	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[32]
33	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[33]
34	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[34]
35	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[35]
36	$[y, x, z]$	[36]
37	$[x, \frac{1}{2} - z, \frac{1}{2} - y]$	[37]
38	$[x, z, y]$	[38]
39	$[\frac{1}{2} - z, y, \frac{1}{2} - x]$	[39]
40	$[z, y, x]$	[40]
41	$[-z, -x, -y]$	[41]
42	$[-y, -z, -x]$	[42]
43	$[y + \frac{1}{2}, -z, x + \frac{1}{2}]$	[43]
44	$[z + \frac{1}{2}, x + \frac{1}{2}, -y]$	[44]
45	$[y + \frac{1}{2}, z + \frac{1}{2}, -x]$	[45]
46	$[-z, x + \frac{1}{2}, y + \frac{1}{2}]$	[46]
47	$[-y, z + \frac{1}{2}, x + \frac{1}{2}]$	[47]
48	$[z + \frac{1}{2}, -x, y + \frac{1}{2}]$	[48]