

MSG No. 222.102 $Pn'\bar{3}'n'$ [Type III, cubic]

Table 1: Wyckoff site: 2a, site symmetry: 432

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[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	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[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: 42.2

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

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

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

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

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

continued ...

Table 4

No.	position	mapping
10	$[\frac{3}{4}, \frac{1}{4}, 0]$	[18,21,29,39]
11	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[19,23,28,40]
12	$[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$	[20,22,31,36]

Table 5: Wyckoff site: 12e, site symmetry: 4..

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

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

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

Table 7: Wyckoff site: 24g, site symmetry: 2..

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

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

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

continued ...

Table 8

No.	position	mapping
16	$[-y, -y, \frac{3}{4}]$	[28,42]
17	$[y + \frac{1}{2}, -y, \frac{3}{4}]$	[29,43]
18	$[y + \frac{1}{2}, \frac{3}{4}, -y]$	[30,44]
19	$[-y, \frac{3}{4}, -y]$	[31,41]
20	$[\frac{3}{4}, y + \frac{1}{2}, y + \frac{1}{2}]$	[32,38]
21	$[-y, \frac{3}{4}, y + \frac{1}{2}]$	[35,46]
22	$[y + \frac{1}{2}, \frac{3}{4}, y + \frac{1}{2}]$	[36,48]
23	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	[39,47]
24	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[40,45]

Table 9: Wyckoff site: 48i, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, \frac{1}{2} - z, y]$	[2]
3	$[x, z, \frac{1}{2} - y]$	[3]
4	$[z, y, \frac{1}{2} - x]$	[4]
5	$[\frac{1}{2} - z, y, x]$	[5]
6	$[\frac{1}{2} - y, x, z]$	[6]
7	$[y, \frac{1}{2} - x, z]$	[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	$[y, x, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[12]
13	$[\frac{1}{2} - x, z, y]$	[13]
14	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[14]
15	$[z, \frac{1}{2} - y, x]$	[15]
16	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$	[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	$[-x, z + \frac{1}{2}, -y]$	[26]
27	$[-x, -z, y + \frac{1}{2}]$	[27]
28	$[-z, -y, x + \frac{1}{2}]$	[28]
29	$[z + \frac{1}{2}, -y, -x]$	[29]
30	$[y + \frac{1}{2}, -x, -z]$	[30]
31	$[-y, x + \frac{1}{2}, -z]$	[31]

continued ...

Table 9

No.	position	mapping
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	$[-y, -x, z + \frac{1}{2}]$	[35]
36	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[36]
37	$[x + \frac{1}{2}, -z, -y]$	[37]
38	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[38]
39	$[-z, y + \frac{1}{2}, -x]$	[39]
40	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[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]