

MSG No. 207.43 P_I432 [Type IV, cubic]

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

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: 42.2

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

Table 3: Wyckoff site: 8c, site symmetry: .32'

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

Table 4: Wyckoff site: 12d, site symmetry: 2.2'2'

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

continued ...

Table 4

No.	position	mapping
10	$[\frac{1}{2}, 0, \frac{1}{4}]$	[18,21,28,40]
11	$[\frac{1}{2}, 0, \frac{3}{4}]$	[19,23,29,39]
12	$[0, \frac{3}{4}, \frac{1}{2}]$	[20,22,30,35]

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

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

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

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

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

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

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

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

continued ...

Table 8

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

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

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

Table 10: Wyckoff site: 48j, site symmetry: 1

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

continued ...

Table 10

No.	position	mapping
47	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[47]
48	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - y]$	[48]