

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]