

MSG No. 223.108  $Pm'\bar{3}'n'$  [ Type III, cubic ]

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

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

Table 2: Wyckoff site: 6b, site symmetry:  $m'm'm'..$

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

Table 3: Wyckoff site: 6c, site symmetry:  $-4'm'.2$

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

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

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

Table 5: Wyckoff site:  $8e$ , site symmetry:  $.32$ 

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

Table 6: Wyckoff site:  $12f$ , site symmetry:  $2m'm'..$ 

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

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

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

Table 8: Wyckoff site: 12h, site symmetry:  $2\mathfrak{m}'\mathfrak{m}'\dots$ 

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

Table 9: Wyckoff site: 16i, site symmetry:  $\dots 3$ .

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

Table 10: Wyckoff site: 24j, site symmetry:  $\dots 2$ 

No.	position	mapping
1	$[\frac{1}{4}, y, y + \frac{1}{2}]$	$[1, 13]$
2	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	$[2, 10]$
3	$[\frac{3}{4}, y, \frac{1}{2} - y]$	$[3, 9]$
4	$[y, y + \frac{1}{2}, \frac{1}{4}]$	$[4, 18]$
5	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	$[5, 19]$

*continued ...*

Table 10

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

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

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

*continued ...*

Table 11

No.	position	mapping
22	$[z, 0, -y]$	[22,44]
23	$[y, -z, 0]$	[23,43]
24	$[-z, 0, -y]$	[24,41]

Table 12: Wyckoff site: 481, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[2]
3	$[x + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[3]
4	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - x]$	[4]
5	$[\frac{1}{2} - z, y + \frac{1}{2}, x + \frac{1}{2}]$	[5]
6	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[6]
7	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[7]
8	$[x, -y, -z]$	[8]
9	$[-x, y, -z]$	[9]
10	$[-x, -y, z]$	[10]
11	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[12]
13	$[\frac{1}{2} - x, z + \frac{1}{2}, y + \frac{1}{2}]$	[13]
14	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[14]
15	$[z + \frac{1}{2}, \frac{1}{2} - y, x + \frac{1}{2}]$	[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	$[-y, z, -x]$	[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	$[-x, -y, -z]$	[25]
26	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y]$	[26]
27	$[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}]$	[27]
28	$[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}]$	[28]
29	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x]$	[29]
30	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[30]
31	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[31]
32	$[-x, y, z]$	[32]
33	$[x, -y, z]$	[33]
34	$[x, y, -z]$	[34]
35	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[35]
36	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[36]
37	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[37]

continued ...

Table 12

No.	position	mapping
38	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[38]
39	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x]$	[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	$[y, -z, x]$	[43]
44	$[z, x, -y]$	[44]
45	$[y, z, -x]$	[45]
46	$[-z, x, y]$	[46]
47	$[-y, z, x]$	[47]
48	$[z, -x, y]$	[48]