

MSG No. 193.262 P_63/mcm [Type IV, hexagonal]

Table 1: Wyckoff site: 2a, site symmetry: $6'/mm'm$

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $6'm'm$

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

Table 6: Wyckoff site: 6f, site symmetry: $mm'm$

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

Table 7: Wyckoff site: 6g, site symmetry: $m'm'm$

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

Table 8: Wyckoff site: 8h, site symmetry: $3m'$

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

Table 9: Wyckoff site: 12i, site symmetry: $2'm'm$

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	[1, 23, 28, 43]
2	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[2, 21, 29, 46]
3	$[0, \frac{1}{2}, z]$	[3, 24, 30, 44]
4	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[4, 19, 25, 47]
5	$[\frac{1}{2}, \frac{1}{2}, z]$	[5, 22, 26, 45]
6	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[6, 20, 27, 48]
7	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[7, 16, 35, 37]

continued ...

Table 9

No.	position	mapping
8	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[8, 18, 36, 39]
9	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[9, 14, 34, 41]
10	$[\frac{1}{2}, \frac{1}{2}, -z]$	[10, 17, 33, 38]
11	$[\frac{1}{2}, 0, -z]$	[11, 13, 31, 40]
12	$[0, \frac{1}{2}, -z]$	[12, 15, 32, 42]

Table 10: Wyckoff site: 12j, site symmetry: m2m

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

Table 11: Wyckoff site: 12k, site symmetry: m'2'm

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

Table 12: Wyckoff site: 121, site symmetry: $mm'2'$

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

Table 13: Wyckoff site: 12m, site symmetry: $m'm'2$

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

Table 14: Wyckoff site: 24n, site symmetry: $..m$

No.	position	mapping
1	$[x, 0, z]$	[1, 23]
2	$[x, x, z + \frac{1}{2}]$	[2, 21]
3	$[0, x, z]$	[3, 24]
4	$[-x, 0, z + \frac{1}{2}]$	[4, 19]
5	$[-x, -x, z]$	[5, 22]
6	$[0, -x, z + \frac{1}{2}]$	[6, 20]
7	$[x, 0, \frac{1}{2} - z]$	[7, 16]
8	$[0, x, \frac{1}{2} - z]$	[8, 18]
9	$[-x, -x, \frac{1}{2} - z]$	[9, 14]

continued ...

Table 14

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

Table 15: Wyckoff site: 24o, site symmetry: $.m'$.

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

Table 16: Wyckoff site: 24p, site symmetry: $m \dots$

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

Table 17: Wyckoff site: 24q, site symmetry: $m' \dots$

No.	position	mapping
1	$[x, y, 0]$	[1,40]
2	$[x - y, x, \frac{1}{2}]$	[2,41]
3	$[-y, x - y, 0]$	[3,42]
4	$[-x, -y, \frac{1}{2}]$	[4,37]
5	$[-x + y, -x, 0]$	[5,38]
6	$[y, -x + y, \frac{1}{2}]$	[6,39]
7	$[x - y, -y, \frac{1}{2}]$	[7,47]
8	$[y, x, \frac{1}{2}]$	[8,48]
9	$[-x, -x + y, \frac{1}{2}]$	[9,46]
10	$[x, x - y, 0]$	[10,45]
11	$[-x + y, y, 0]$	[11,43]
12	$[-y, -x, 0]$	[12,44]
13	$[-x, -y, 0]$	[13,28]
14	$[-x + y, -x, \frac{1}{2}]$	[14,29]
15	$[y, -x + y, 0]$	[15,30]

continued ...

Table 17

No.	position	mapping
16	$[x, y, \frac{1}{2}]$	[16,25]
17	$[x - y, x, 0]$	[17,26]
18	$[-y, x - y, \frac{1}{2}]$	[18,27]
19	$[-x + y, y, \frac{1}{2}]$	[19,35]
20	$[-y, -x, \frac{1}{2}]$	[20,36]
21	$[x, x - y, \frac{1}{2}]$	[21,34]
22	$[-x, -x + y, 0]$	[22,33]
23	$[x - y, -y, 0]$	[23,31]
24	$[y, x, 0]$	[24,32]

Table 18: Wyckoff site: 48r, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x - y, x, z + \frac{1}{2}]$	[2]
3	$[-y, x - y, z]$	[3]
4	$[-x, -y, z + \frac{1}{2}]$	[4]
5	$[-x + y, -x, z]$	[5]
6	$[y, -x + y, z + \frac{1}{2}]$	[6]
7	$[x - y, -y, \frac{1}{2} - z]$	[7]
8	$[y, x, \frac{1}{2} - z]$	[8]
9	$[-x, -x + y, \frac{1}{2} - z]$	[9]
10	$[x, x - y, -z]$	[10]
11	$[-x + y, y, -z]$	[11]
12	$[-y, -x, -z]$	[12]
13	$[-x, -y, -z]$	[13]
14	$[-x + y, -x, \frac{1}{2} - z]$	[14]
15	$[y, -x + y, -z]$	[15]
16	$[x, y, \frac{1}{2} - z]$	[16]
17	$[x - y, x, -z]$	[17]
18	$[-y, x - y, \frac{1}{2} - z]$	[18]
19	$[-x + y, y, z + \frac{1}{2}]$	[19]
20	$[-y, -x, z + \frac{1}{2}]$	[20]
21	$[x, x - y, z + \frac{1}{2}]$	[21]
22	$[-x, -x + y, z]$	[22]
23	$[x - y, -y, z]$	[23]
24	$[y, x, z]$	[24]
25	$[x, y, z + \frac{1}{2}]$	[25]
26	$[x - y, x, z]$	[26]
27	$[-y, x - y, z + \frac{1}{2}]$	[27]
28	$[-x, -y, z]$	[28]
29	$[-x + y, -x, z + \frac{1}{2}]$	[29]
30	$[y, -x + y, z]$	[30]
31	$[x - y, -y, -z]$	[31]

continued ...

Table 18

No.	position	mapping
32	$[y, x, -z]$	[32]
33	$[-x, -x + y, -z]$	[33]
34	$[x, x - y, \frac{1}{2} - z]$	[34]
35	$[-x + y, y, \frac{1}{2} - z]$	[35]
36	$[-y, -x, \frac{1}{2} - z]$	[36]
37	$[-x, -y, \frac{1}{2} - z]$	[37]
38	$[-x + y, -x, -z]$	[38]
39	$[y, -x + y, \frac{1}{2} - z]$	[39]
40	$[x, y, -z]$	[40]
41	$[x - y, x, \frac{1}{2} - z]$	[41]
42	$[-y, x - y, -z]$	[42]
43	$[-x + y, y, z]$	[43]
44	$[-y, -x, z]$	[44]
45	$[x, x - y, z]$	[45]
46	$[-x, -x + y, z + \frac{1}{2}]$	[46]
47	$[x - y, -y, z + \frac{1}{2}]$	[47]
48	$[y, x, z + \frac{1}{2}]$	[48]