

MSG No. 63.468 $C_A mcm$ [Type IV, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: mm'm

No.	position	mapping
1	$[0, \frac{1}{4}, \frac{3}{4}]$	$[1, 3, 6, 8, 18, 20, 21, 23]$
2	$[0, \frac{3}{4}, \frac{1}{4}]$	$[2, 4, 5, 7, 17, 19, 22, 24]$
3	$[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	$[9, 11, 14, 16, 26, 28, 29, 31]$
4	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	$[10, 12, 13, 15, 25, 27, 30, 32]$

Table 2: Wyckoff site: 4b, site symmetry: mm'm

No.	position	mapping
1	$[0, \frac{1}{4}, \frac{1}{4}]$	$[1, 3, 6, 8, 18, 20, 21, 23]$
2	$[0, \frac{3}{4}, \frac{3}{4}]$	$[2, 4, 5, 7, 17, 19, 22, 24]$
3	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	$[9, 11, 14, 16, 26, 28, 29, 31]$
4	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	$[10, 12, 13, 15, 25, 27, 30, 32]$

Table 3: Wyckoff site: 8c, site symmetry: $.2' / \text{m'}$.

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 13, 23, 27]$
2	$[\frac{1}{4}, \frac{3}{4}, 0]$	$[2, 14, 24, 28]$
3	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	$[3, 15, 21, 25]$
4	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	$[4, 16, 22, 26]$
5	$[\frac{3}{4}, \frac{3}{4}, 0]$	$[5, 9, 19, 31]$
6	$[\frac{3}{4}, \frac{1}{4}, 0]$	$[6, 10, 20, 32]$
7	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	$[7, 11, 17, 29]$
8	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$	$[8, 12, 18, 30]$

Table 4: Wyckoff site: 8d, site symmetry: $2/\text{m..}$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 5, 6]$
2	$[0, 0, \frac{1}{2}]$	$[3, 4, 7, 8]$
3	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, 10, 13, 14]$
4	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[11, 12, 15, 16]$
5	$[0, \frac{1}{2}, \frac{1}{2}]$	$[17, 18, 21, 22]$
6	$[0, \frac{1}{2}, 0]$	$[19, 20, 23, 24]$
7	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[25, 26, 29, 30]$
8	$[\frac{1}{2}, 0, 0]$	$[27, 28, 31, 32]$

Table 5: Wyckoff site: 8e, site symmetry: $\dots 2'/\text{m}$

No.	position	mapping
1	$[\frac{1}{4}, 0, \frac{3}{4}]$	[1, 8, 28, 29]
2	$[\frac{1}{4}, 0, \frac{1}{4}]$	[2, 7, 27, 30]
3	$[\frac{3}{4}, 0, \frac{3}{4}]$	[3, 6, 26, 31]
4	$[\frac{3}{4}, 0, \frac{1}{4}]$	[4, 5, 25, 32]
5	$[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}]$	[9, 16, 20, 21]
6	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	[10, 15, 19, 22]
7	$[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$	[11, 14, 18, 23]
8	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	[12, 13, 17, 24]

Table 6: Wyckoff site: 8f, site symmetry: $22'2'$

No.	position	mapping
1	$[\frac{1}{4}, 0, 0]$	[1, 2, 27, 28]
2	$[\frac{3}{4}, 0, \frac{1}{2}]$	[3, 4, 25, 26]
3	$[\frac{3}{4}, 0, 0]$	[5, 6, 31, 32]
4	$[\frac{1}{4}, 0, \frac{1}{2}]$	[7, 8, 29, 30]
5	$[\frac{3}{4}, \frac{1}{2}, 0]$	[9, 10, 19, 20]
6	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}]$	[11, 12, 17, 18]
7	$[\frac{1}{4}, \frac{1}{2}, 0]$	[13, 14, 23, 24]
8	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}]$	[15, 16, 21, 22]

Table 7: Wyckoff site: 8g, site symmetry: $\text{m}2\text{m}$

No.	position	mapping
1	$[0, y, \frac{3}{4}]$	[1, 3, 6, 8]
2	$[0, -y, \frac{1}{4}]$	[2, 4, 5, 7]
3	$[\frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[9, 11, 14, 16]
4	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$	[10, 12, 13, 15]
5	$[0, y + \frac{1}{2}, \frac{1}{4}]$	[17, 19, 22, 24]
6	$[0, \frac{1}{2} - y, \frac{3}{4}]$	[18, 20, 21, 23]
7	$[\frac{1}{2}, y, \frac{1}{4}]$	[25, 27, 30, 32]
8	$[\frac{1}{2}, -y, \frac{3}{4}]$	[26, 28, 29, 31]

Table 8: Wyckoff site: 8h, site symmetry: $2'\text{m}'\text{m}$

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{3}{4}]$	[1, 8, 18, 23]
2	$[x, \frac{3}{4}, \frac{1}{4}]$	[2, 7, 17, 24]
3	$[-x, \frac{1}{4}, \frac{3}{4}]$	[3, 6, 20, 21]

continued ...

Table 8

No.	position	mapping
4	$[-x, \frac{3}{4}, \frac{1}{4}]$	[4,5,19,22]
5	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[9,16,26,31]
6	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[10,15,25,32]
7	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[11,14,28,29]
8	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[12,13,27,30]

Table 9: Wyckoff site: 8i, site symmetry: mm'2'

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	[1,6,20,23]
2	$[0, \frac{3}{4}, -z]$	[2,5,19,24]
3	$[0, \frac{1}{4}, \frac{1}{2} - z]$	[3,8,18,21]
4	$[0, \frac{3}{4}, z + \frac{1}{2}]$	[4,7,17,22]
5	$[\frac{1}{2}, \frac{3}{4}, z]$	[9,14,28,31]
6	$[\frac{1}{2}, \frac{1}{4}, -z]$	[10,13,27,32]
7	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{2} - z]$	[11,16,26,29]
8	$[\frac{1}{2}, \frac{1}{4}, z + \frac{1}{2}]$	[12,15,25,30]

Table 10: Wyckoff site: 16j, site symmetry: $\dots 2'$

No.	position	mapping
1	$[\frac{1}{4}, 0, z]$	[1,28]
2	$[\frac{1}{4}, 0, -z]$	[2,27]
3	$[\frac{3}{4}, 0, \frac{1}{2} - z]$	[3,26]
4	$[\frac{3}{4}, 0, z + \frac{1}{2}]$	[4,25]
5	$[\frac{3}{4}, 0, -z]$	[5,32]
6	$[\frac{3}{4}, 0, z]$	[6,31]
7	$[\frac{1}{4}, 0, z + \frac{1}{2}]$	[7,30]
8	$[\frac{1}{4}, 0, \frac{1}{2} - z]$	[8,29]
9	$[\frac{3}{4}, \frac{1}{2}, z]$	[9,20]
10	$[\frac{3}{4}, \frac{1}{2}, -z]$	[10,19]
11	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{2} - z]$	[11,18]
12	$[\frac{1}{4}, \frac{1}{2}, z + \frac{1}{2}]$	[12,17]
13	$[\frac{1}{4}, \frac{1}{2}, -z]$	[13,24]
14	$[\frac{1}{4}, \frac{1}{2}, z]$	[14,23]
15	$[\frac{3}{4}, \frac{1}{2}, z + \frac{1}{2}]$	[15,22]
16	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{2} - z]$	[16,21]

Table 11: Wyckoff site: 16k, site symmetry: 2..

No.	position	mapping
1	$[x, 0, 0]$	[1,2]
2	$[-x, 0, \frac{1}{2}]$	[3,4]
3	$[-x, 0, 0]$	[5,6]
4	$[x, 0, \frac{1}{2}]$	[7,8]
5	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[9,10]
6	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[11,12]
7	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[13,14]
8	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[15,16]
9	$[x, \frac{1}{2}, \frac{1}{2}]$	[17,18]
10	$[-x, \frac{1}{2}, 0]$	[19,20]
11	$[-x, \frac{1}{2}, \frac{1}{2}]$	[21,22]
12	$[x, \frac{1}{2}, 0]$	[23,24]
13	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[25,26]
14	$[\frac{1}{2} - x, 0, 0]$	[27,28]
15	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[29,30]
16	$[x + \frac{1}{2}, 0, 0]$	[31,32]

Table 12: Wyckoff site: 16l, site symmetry: .2'.

No.	position	mapping
1	$[\frac{1}{4}, y, 0]$	[1,27]
2	$[\frac{1}{4}, -y, 0]$	[2,28]
3	$[\frac{3}{4}, y, \frac{1}{2}]$	[3,25]
4	$[\frac{3}{4}, -y, \frac{1}{2}]$	[4,26]
5	$[\frac{3}{4}, -y, 0]$	[5,31]
6	$[\frac{3}{4}, y, 0]$	[6,32]
7	$[\frac{1}{4}, -y, \frac{1}{2}]$	[7,29]
8	$[\frac{1}{4}, y, \frac{1}{2}]$	[8,30]
9	$[\frac{3}{4}, y + \frac{1}{2}, 0]$	[9,19]
10	$[\frac{3}{4}, \frac{1}{2} - y, 0]$	[10,20]
11	$[\frac{1}{4}, y + \frac{1}{2}, \frac{1}{2}]$	[11,17]
12	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{2}]$	[12,18]
13	$[\frac{1}{4}, \frac{1}{2} - y, 0]$	[13,23]
14	$[\frac{1}{4}, y + \frac{1}{2}, 0]$	[14,24]
15	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{2}]$	[15,21]
16	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2}]$	[16,22]

Table 13: Wyckoff site: 16m, site symmetry: .m'.

No.	position	mapping
1	$[x, \frac{1}{4}, z]$	[1,23]

continued ...

Table 13

No.	position	mapping
2	$[x, \frac{3}{4}, -z]$	[2,24]
3	$[-x, \frac{1}{4}, \frac{1}{2} - z]$	[3,21]
4	$[-x, \frac{3}{4}, z + \frac{1}{2}]$	[4,22]
5	$[-x, \frac{3}{4}, -z]$	[5,19]
6	$[-x, \frac{1}{4}, z]$	[6,20]
7	$[x, \frac{3}{4}, z + \frac{1}{2}]$	[7,17]
8	$[x, \frac{1}{4}, \frac{1}{2} - z]$	[8,18]
9	$[x + \frac{1}{2}, \frac{3}{4}, z]$	[9,31]
10	$[x + \frac{1}{2}, \frac{1}{4}, -z]$	[10,32]
11	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{2} - z]$	[11,29]
12	$[\frac{1}{2} - x, \frac{1}{4}, z + \frac{1}{2}]$	[12,30]
13	$[\frac{1}{2} - x, \frac{1}{4}, -z]$	[13,27]
14	$[\frac{1}{2} - x, \frac{3}{4}, z]$	[14,28]
15	$[x + \frac{1}{2}, \frac{1}{4}, z + \frac{1}{2}]$	[15,25]
16	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - z]$	[16,26]

Table 14: Wyckoff site: 16n, site symmetry: m..

No.	position	mapping
1	$[0, y, z]$	[1,6]
2	$[0, -y, -z]$	[2,5]
3	$[0, y, \frac{1}{2} - z]$	[3,8]
4	$[0, -y, z + \frac{1}{2}]$	[4,7]
5	$[\frac{1}{2}, y + \frac{1}{2}, z]$	[9,14]
6	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	[10,13]
7	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[11,16]
8	$[\frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[12,15]
9	$[0, y + \frac{1}{2}, z + \frac{1}{2}]$	[17,22]
10	$[0, \frac{1}{2} - y, \frac{1}{2} - z]$	[18,21]
11	$[0, y + \frac{1}{2}, -z]$	[19,24]
12	$[0, \frac{1}{2} - y, z]$	[20,23]
13	$[\frac{1}{2}, y, z + \frac{1}{2}]$	[25,30]
14	$[\frac{1}{2}, -y, \frac{1}{2} - z]$	[26,29]
15	$[\frac{1}{2}, y, -z]$	[27,32]
16	$[\frac{1}{2}, -y, z]$	[28,31]

Table 15: Wyckoff site: 16o, site symmetry: ..m

No.	position	mapping
1	$[x, y, \frac{3}{4}]$	[1,8]
2	$[x, -y, \frac{1}{4}]$	[2,7]
3	$[-x, y, \frac{3}{4}]$	[3,6]

continued ...

Table 15

No.	position	mapping
4	$[-x, -y, \frac{1}{4}]$	[4,5]
5	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[9,16]
6	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$	[10,15]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{3}{4}]$	[11,14]
8	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{4}]$	[12,13]
9	$[x, y + \frac{1}{2}, \frac{1}{4}]$	[17,24]
10	$[x, \frac{1}{2} - y, \frac{3}{4}]$	[18,23]
11	$[-x, y + \frac{1}{2}, \frac{1}{4}]$	[19,22]
12	$[-x, \frac{1}{2} - y, \frac{3}{4}]$	[20,21]
13	$[x + \frac{1}{2}, y, \frac{1}{4}]$	[25,32]
14	$[x + \frac{1}{2}, -y, \frac{3}{4}]$	[26,31]
15	$[\frac{1}{2} - x, y, \frac{1}{4}]$	[27,30]
16	$[\frac{1}{2} - x, -y, \frac{3}{4}]$	[28,29]

Table 16: Wyckoff site: 32p, site symmetry: 1

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

continued ...

Table 16

No.	position	mapping
28	$[\frac{1}{2} - x, -y, z]$	[28]
29	$[\frac{1}{2} - x, -y, \frac{1}{2} - z]$	[29]
30	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[30]
31	$[x + \frac{1}{2}, -y, z]$	[31]
32	$[x + \frac{1}{2}, y, -z]$	[32]