

MSG No. 64.478 $C_c mca$ [Type IV, orthorhombic]

Table 1: Wyckoff site: 8a, site symmetry: 2'22'

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

Table 2: Wyckoff site: 8b, site symmetry: 22'2'

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

Table 3: Wyckoff site: 8c, site symmetry: .2/m'.

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

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

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

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

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

Table 6: Wyckoff site: 8f, site symmetry: $2/\text{m}..$

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

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

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	[1, 6, 28, 31]
2	$[0, \frac{3}{4}, -z]$	[2, 5, 27, 32]
3	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - z]$	[3, 8, 26, 29]

continued ...

Table 7

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

Table 8: Wyckoff site: 16h, site symmetry: .2.

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

Table 9: Wyckoff site: 16i, site symmetry: .2'.

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

continued ...

Table 9

No.	position	mapping
14	$[\frac{3}{4}, y + \frac{1}{2}, 0]$	[14,32]
15	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{2}]$	[15,29]
16	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2}]$	[16,30]

Table 10: Wyckoff site: 16j, site symmetry: $2^3\ldots$

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

Table 11: Wyckoff site: 16k, site symmetry: $2\ldots$

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

continued ...

Table 11

No.	position	mapping
16	$[x, \frac{1}{2}, 0]$	[31,32]

Table 12: Wyckoff site: 16l, site symmetry: $\dots 2'$

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

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

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

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

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

Table 15: Wyckoff site: 32o, site symmetry: 1

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

continued ...

Table 15

No.	position	mapping
24	$[x + \frac{1}{2}, y, -z]$	[24]
25	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[25]
26	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[26]
27	$[-x, y + \frac{1}{2}, -z]$	[27]
28	$[-x, \frac{1}{2} - y, z]$	[28]
29	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[29]
30	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[30]
31	$[x, \frac{1}{2} - y, z]$	[31]
32	$[x, y + \frac{1}{2}, -z]$	[32]