

MSG No. 65.484 $Cmmm'$ [Type III, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: mmm'

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8]$
2	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, 10, 11, 12, 13, 14, 15, 16]$

Table 2: Wyckoff site: 2b, site symmetry: mmm'

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8]$
2	$[0, \frac{1}{2}, 0]$	$[9, 10, 11, 12, 13, 14, 15, 16]$

Table 3: Wyckoff site: 2c, site symmetry: mmm'

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8]$
2	$[0, \frac{1}{2}, \frac{1}{2}]$	$[9, 10, 11, 12, 13, 14, 15, 16]$

Table 4: Wyckoff site: 2d, site symmetry: mmm'

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[9, 10, 11, 12, 13, 14, 15, 16]$

Table 5: Wyckoff site: 4e, site symmetry: $. . 2/m'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 8, 10, 15]$
2	$[\frac{3}{4}, \frac{3}{4}, 0]$	$[2, 7, 9, 16]$
3	$[\frac{3}{4}, \frac{1}{4}, 0]$	$[3, 6, 12, 13]$
4	$[\frac{1}{4}, \frac{3}{4}, 0]$	$[4, 5, 11, 14]$

Table 6: Wyckoff site: 4f, site symmetry: $\dots/2/m'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$	[1, 8, 10, 15]
2	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	[2, 7, 9, 16]
3	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[3, 6, 12, 13]
4	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	[4, 5, 11, 14]

Table 7: Wyckoff site: 4g, site symmetry: $2'mm'$

No.	position	mapping
1	$[x, 0, 0]$	[1, 4, 5, 8]
2	$[-x, 0, 0]$	[2, 3, 6, 7]
3	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[9, 12, 13, 16]
4	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[10, 11, 14, 15]

Table 8: Wyckoff site: 4h, site symmetry: $2'mm'$

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	[1, 4, 5, 8]
2	$[-x, 0, \frac{1}{2}]$	[2, 3, 6, 7]
3	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9, 12, 13, 16]
4	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[10, 11, 14, 15]

Table 9: Wyckoff site: 4i, site symmetry: $m2'm'$

No.	position	mapping
1	$[0, y, 0]$	[1, 3, 6, 8]
2	$[0, -y, 0]$	[2, 4, 5, 7]
3	$[\frac{1}{2}, y + \frac{1}{2}, 0]$	[9, 11, 14, 16]
4	$[\frac{1}{2}, \frac{1}{2} - y, 0]$	[10, 12, 13, 15]

Table 10: Wyckoff site: 4j, site symmetry: $m2'm'$

No.	position	mapping
1	$[0, y, \frac{1}{2}]$	[1, 3, 6, 8]
2	$[0, -y, \frac{1}{2}]$	[2, 4, 5, 7]
3	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[9, 11, 14, 16]
4	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[10, 12, 13, 15]

Table 11: Wyckoff site: 4k, site symmetry: mm2

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4]$
2	$[0, 0, -z]$	$[5, 6, 7, 8]$
3	$[\frac{1}{2}, \frac{1}{2}, z]$	$[9, 10, 11, 12]$
4	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[13, 14, 15, 16]$

Table 12: Wyckoff site: 4l, site symmetry: mm2

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 2, 3, 4]$
2	$[0, \frac{1}{2}, -z]$	$[5, 6, 7, 8]$
3	$[\frac{1}{2}, 0, z]$	$[9, 10, 11, 12]$
4	$[\frac{1}{2}, 0, -z]$	$[13, 14, 15, 16]$

Table 13: Wyckoff site: 8m, site symmetry: . . 2

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, z]$	$[1, 10]$
2	$[\frac{3}{4}, \frac{3}{4}, z]$	$[2, 9]$
3	$[\frac{3}{4}, \frac{1}{4}, z]$	$[3, 12]$
4	$[\frac{1}{4}, \frac{3}{4}, z]$	$[4, 11]$
5	$[\frac{1}{4}, \frac{3}{4}, -z]$	$[5, 14]$
6	$[\frac{3}{4}, \frac{1}{4}, -z]$	$[6, 13]$
7	$[\frac{3}{4}, \frac{3}{4}, -z]$	$[7, 16]$
8	$[\frac{1}{4}, \frac{1}{4}, -z]$	$[8, 15]$

Table 14: Wyckoff site: 8n, site symmetry: m . .

No.	position	mapping
1	$[0, y, z]$	$[1, 3]$
2	$[0, -y, z]$	$[2, 4]$
3	$[0, -y, -z]$	$[5, 7]$
4	$[0, y, -z]$	$[6, 8]$
5	$[\frac{1}{2}, y + \frac{1}{2}, z]$	$[9, 11]$
6	$[\frac{1}{2}, \frac{1}{2} - y, z]$	$[10, 12]$
7	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	$[13, 15]$
8	$[\frac{1}{2}, y + \frac{1}{2}, -z]$	$[14, 16]$

Table 15: Wyckoff site: $8o$, site symmetry: $.m$.

No.	position	mapping
1	$[x, 0, z]$	[1,4]
2	$[-x, 0, z]$	[2,3]
3	$[x, 0, -z]$	[5,8]
4	$[-x, 0, -z]$	[6,7]
5	$[x + \frac{1}{2}, \frac{1}{2}, z]$	[9,12]
6	$[\frac{1}{2} - x, \frac{1}{2}, z]$	[10,11]
7	$[x + \frac{1}{2}, \frac{1}{2}, -z]$	[13,16]
8	$[\frac{1}{2} - x, \frac{1}{2}, -z]$	[14,15]

Table 16: Wyckoff site: $8p$, site symmetry: $.m'$

No.	position	mapping
1	$[x, y, 0]$	[1,8]
2	$[-x, -y, 0]$	[2,7]
3	$[-x, y, 0]$	[3,6]
4	$[x, -y, 0]$	[4,5]
5	$[x + \frac{1}{2}, y + \frac{1}{2}, 0]$	[9,16]
6	$[\frac{1}{2} - x, \frac{1}{2} - y, 0]$	[10,15]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	[11,14]
8	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	[12,13]

Table 17: Wyckoff site: $8q$, site symmetry: $.m'$

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	[1,8]
2	$[-x, -y, \frac{1}{2}]$	[2,7]
3	$[-x, y, \frac{1}{2}]$	[3,6]
4	$[x, -y, \frac{1}{2}]$	[4,5]
5	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[9,16]
6	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2}]$	[10,15]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	[11,14]
8	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[12,13]

Table 18: Wyckoff site: $16r$, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[2]
3	$[-x, y, z]$	[3]

continued ...

Table 18

No.	position	mapping
4	$[x, -y, z]$	[4]
5	$[x, -y, -z]$	[5]
6	$[-x, y, -z]$	[6]
7	$[-x, -y, -z]$	[7]
8	$[x, y, -z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[9]
10	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[10]
11	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[11]
12	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[12]
13	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[13]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[14]
15	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[15]
16	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[16]