

MSG No. 65.483 $Cm'mm$ [Type III, orthorhombic]

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

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: $m'mm$

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: $m'mm$

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: $m'mm$

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	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 4, 14, 15]$
2	$[\frac{1}{4}, \frac{3}{4}, 0]$	$[2, 3, 13, 16]$
3	$[\frac{3}{4}, \frac{1}{4}, 0]$	$[5, 8, 10, 11]$
4	$[\frac{3}{4}, \frac{3}{4}, 0]$	$[6, 7, 9, 12]$

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

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

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

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

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

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

Table 9: Wyckoff site: 4i, site symmetry: $m'2'm$

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

Table 10: Wyckoff site: 4j, site symmetry: $m'2'm$

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

Table 11: Wyckoff site: 4k, site symmetry: $m'm2'$

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

Table 12: Wyckoff site: 4l, site symmetry: $m'm2'$

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

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

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

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

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

Table 15: Wyckoff site: $8\mathfrak{o}$, site symmetry: $.m$.

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

Table 16: Wyckoff site: $8\mathfrak{p}$, site symmetry: $.m$

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

Table 17: Wyckoff site: $8\mathfrak{q}$, site symmetry: $.m$

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

Table 18: Wyckoff site: $16\mathfrak{r}$, 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	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[10]
11	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[11]
12	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[12]
13	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[13]
14	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[14]
15	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[15]
16	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[16]