

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: $\dots 2'/\text{m}$

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: $\dots 2'/\text{m}$

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: $\text{m}'2'\text{m}$

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: $\text{m}'2'\text{m}$

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: **8o**, 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: **8p**, 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: **8q**, 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: **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	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[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]