

MSG No. 65.481 *Cmmm* [Type I, 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]	[1,8,12,13]
2	[\frac{1}{4}, \frac{3}{4}, 0]	[2,7,11,14]
3	[\frac{3}{4}, \frac{1}{4}, 0]	[3,6,10,15]
4	[\frac{3}{4}, \frac{3}{4}, 0]	[4,5,9,16]

Table 6: Wyckoff site: 4f, site symmetry: . . 2/m

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

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

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

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

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

Table 9: Wyckoff site: 4i, site symmetry: m2m

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: m2m

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

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

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

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

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

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

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

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

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

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	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	[10,15]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	[11,14]
8	$[\frac{1}{2} - x, \frac{1}{2} - y, 0]$	[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	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[10,15]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	[11,14]
8	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2}]$	[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	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[10]
11	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[11]
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[12]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[13]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[14]
15	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[15]
16	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[16]