

MSG No. 65.482 *Cmmm1'* [Type II, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: **mmm1'**

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

Table 2: Wyckoff site: 2b, site symmetry: **mmm1'**

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

Table 3: Wyckoff site: 2c, site symmetry: **mmm1'**

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

Table 4: Wyckoff site: 2d, site symmetry: **mmm1'**

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

Table 5: Wyckoff site: 4e, site symmetry: **..2/m1'**

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

Table 6: Wyckoff site: 4f, site symmetry: $\dots 2/m1'$

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

Table 7: Wyckoff site: 4g, site symmetry: $2mm1'$

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

Table 8: Wyckoff site: 4h, site symmetry: $2mm1'$

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

Table 9: Wyckoff site: 4i, site symmetry: $m2m1'$

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

Table 10: Wyckoff site: 4j, site symmetry: $m2m1'$

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

Table 11: Wyckoff site: 4k, site symmetry: mm21'

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

Table 12: Wyckoff site: 4l, site symmetry: mm21'

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

Table 13: Wyckoff site: 8m, site symmetry: .21'

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

Table 14: Wyckoff site: 8n, site symmetry: m..1'

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

Table 15: Wyckoff site: 8o, site symmetry: .m.1'

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

Table 16: Wyckoff site: 8p, site symmetry: ..m1'

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

Table 17: Wyckoff site: 8q, site symmetry: ..m1'

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

Table 18: Wyckoff site: 16r, site symmetry: 11'

No.	position	mapping
1	[x, y, z]	[1, 17]
2	[x, -y, -z]	[2, 18]
3	[-x, y, -z]	[3, 19]

continued ...

Table 18

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