

MSG No. 71.534 *Immm1'* [ Type II, orthorhombic ]

Table 1: Wyckoff site: 2a, site symmetry:  $\text{mmm}1'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $\text{mmm}1'$

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

Table 3: Wyckoff site: 2c, site symmetry:  $\text{mmm}1'$

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

Table 4: Wyckoff site: 2d, site symmetry:  $\text{mmm}1'$

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	$[0, \frac{1}{2}, 0]$	[9, 10, 11, 12, 13, 14, 15, 16, 25, 26, 27, 28, 29, 30, 31, 32]

Table 5: Wyckoff site: 4e, site symmetry:  $2\text{mm}1'$

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	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[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 6: Wyckoff site: 4f, site symmetry: 2mm1'

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

Table 7: Wyckoff site: 4g, 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	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[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 8: Wyckoff site: 4h, 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	$[\frac{1}{2}, y + \frac{1}{2}, 0]$	[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 9: Wyckoff site: 4i, 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	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[9, 12, 14, 15, 25, 28, 30, 31]
4	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[10, 11, 13, 16, 26, 27, 29, 32]

Table 10: Wyckoff site: 4j, site symmetry: mm21'

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

Table 11: Wyckoff site: 8k, site symmetry: -11'

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

Table 12: Wyckoff site: 8l, 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	$[\frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9,14,25,30]
6	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[10,13,26,29]
7	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[11,16,27,32]
8	$[\frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[12,15,28,31]

Table 13: Wyckoff site: 8m, 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	$[x + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[9,15,25,31]
6	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[10,16,26,32]
7	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2} - z]$	[11,13,27,29]
8	$[\frac{1}{2} - x, \frac{1}{2}, z + \frac{1}{2}]$	[12,14,28,30]

Table 14: Wyckoff site: 8n, 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]

*continued ...*

Table 14

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

Table 15: Wyckoff site: 16o, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1,17]
2	$[x, -y, -z]$	[2,18]
3	$[-x, y, -z]$	[3,19]
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	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9,25]
10	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[10,26]
11	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[11,27]
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[12,28]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[13,29]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[14,30]
15	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[15,31]
16	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[16,32]