

MSG No. 59.416 P_{Immn} [Type IV, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: mmm'

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

Table 2: Wyckoff site: 2b, site symmetry: mmm'

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

Table 3: Wyckoff site: 2c, site symmetry: mmm'

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

Table 4: Wyckoff site: 2d, site symmetry: mmm'

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

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

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

Table 6: Wyckoff site: 4f, site symmetry: mm2

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

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

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

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

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

Table 9: Wyckoff site: 4i, site symmetry: m2'm'

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

Table 10: Wyckoff site: 4j, site symmetry: m2'm'

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

Table 11: Wyckoff site: 8k, site symmetry: -1

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

Table 12: Wyckoff site: 8l, site symmetry: ..m'

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

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

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

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

No.	position	mapping
1	$[x, \frac{1}{4}, z]$	[1,7]
2	$[x + \frac{1}{2}, \frac{3}{4}, -z]$	[2,8]
3	$[-x, \frac{3}{4}, -z]$	[3,5]

continued ...

Table 14

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

Table 15: Wyckoff site: 16o, site symmetry: 1

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