

MSG No. 48.264 P_{Innn} [Type IV, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: $m'm'm'$

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

Table 2: Wyckoff site: 2b, site symmetry: $m'm'm'$

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

Table 3: Wyckoff site: 2c, site symmetry: $m'm'm'$

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

Table 4: Wyckoff site: 2d, site symmetry: $m'm'm'$

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

Table 5: Wyckoff site: 4e, site symmetry: $2m'm'$

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

Table 6: Wyckoff site: 4f, site symmetry: 2m'm'

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

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

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

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

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

Table 9: Wyckoff site: 4i, site symmetry: m'm'2

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

Table 10: Wyckoff site: 4j, site symmetry: m'm'2

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	[1,16]
2	$[x, \frac{1}{2} - y, \frac{1}{4}]$	[2,15]
3	$[\frac{1}{2} - x, y, \frac{1}{4}]$	[3,14]

continued ...

Table 14

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

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

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