

MSG No. 51.304 *P_Imma* [Type IV, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: .2/m.

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

Table 2: Wyckoff site: 4b, site symmetry: .2/m.

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

Table 3: Wyckoff site: 4c, site symmetry: 2'/m..

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

Table 4: Wyckoff site: 4d, site symmetry: 2'/m..

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

Table 5: Wyckoff site: 4e, site symmetry: mm2

No.	position	mapping
1	[\frac{1}{4}, 0, z]	[1,4,6,7]
2	[\frac{3}{4}, 0, -z]	[2,3,5,8]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: .2.

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

Table 7: Wyckoff site: 8g, site symmetry: 2'..

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: $\mathbf{m..}$

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

Table 10: Wyckoff site: 16j, site symmetry: 1

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