

MSG No. 74.554 *Imma* [Type I, orthorhombic]

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

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

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

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

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

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

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

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

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

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

continued ...

Table 5

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

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

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

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

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: .m.

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

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

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