

MSG No. 51.301 *P_Amma* [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	[0, \frac{1}{2}, \frac{1}{2}]	[9,11,13,15]
4	[\frac{1}{2}, \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	[0, \frac{1}{2}, 0]	[9,11,13,15]
4	[\frac{1}{2}, \frac{1}{2}, 0]	[10,12,14,16]

Table 3: Wyckoff site: 4c, 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]
3	[\frac{1}{4}, \frac{1}{2}, z + \frac{1}{2}]	[9,12,14,15]
4	[\frac{3}{4}, \frac{1}{2}, \frac{1}{2} - z]	[10,11,13,16]

Table 4: Wyckoff site: 8d, site symmetry: -1'

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

Table 5: Wyckoff site: 8e, 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	[0, y + \frac{1}{2}, \frac{1}{2}]	[9,11]
6	[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]	[10,12]
7	[0, \frac{1}{2} - y, \frac{1}{2}]	[13,15]
8	[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]	[14,16]

Table 6: Wyckoff site: 8f, 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}, z + \frac{1}{2}]	[9,15]
6	[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]	[10,16]
7	[-x, \frac{1}{2}, \frac{1}{2} - z]	[11,13]
8	[\frac{1}{2} - x, \frac{1}{2}, z + \frac{1}{2}]	[12,14]

Table 7: Wyckoff site: 8g, 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, -z]	[3,8]
4	[\frac{1}{4}, -y, z]	[4,7]
5	[\frac{1}{4}, y + \frac{1}{2}, z + \frac{1}{2}]	[9,14]
6	[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{2} - z]	[10,13]
7	[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2} - z]	[11,16]
8	[\frac{1}{4}, \frac{1}{2} - y, z + \frac{1}{2}]	[12,15]

Table 8: Wyckoff site: 16h, site symmetry: 1

No.	position	mapping
1	[x, y, z]	[1]
2	[x + \frac{1}{2}, -y, -z]	[2]
3	[-x, y, -z]	[3]

continued ...

Table 8

No.	position	mapping
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	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[10]
11	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[12]
13	$[-x, \frac{1}{2} - y, \frac{1}{2} - z]$	[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	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[16]