

MSG No. 62.453 P_{Anma} [Type IV, orthorhombic]

Table 1: Wyckoff site: **4a**, site symmetry: $.2'/\text{m}$.

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

Table 2: Wyckoff site: **4b**, site symmetry: $.2'/\text{m}$.

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

Table 3: Wyckoff site: **4c**, site symmetry: $\text{m}'\text{m}2'$

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: .2¹.

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

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

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

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

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

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

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

continued ...

Table 8

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