

MSG No. 59.412 P_bmmn [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

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

continued ...

Table 5

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

Table 6: Wyckoff site: $4f$, site symmetry: $mm'2'$

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

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

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

Table 8: Wyckoff site: $8h$, site symmetry: $.2'$

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

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

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

Table 10: Wyckoff site: $8j$, site symmetry: $.m'$.

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

Table 11: Wyckoff site: $8k$, site symmetry: m .

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

Table 12: Wyckoff site: $16l$, site symmetry: 1

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

continued ...

Table 12

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