

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]