

MSG No. 35.170 $C_a mm2$ [Type IV, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: $mm2$

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

Table 2: Wyckoff site: 4b, site symmetry: $mm'2'$

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

Table 3: Wyckoff site: 4c, site symmetry: $m'm2'$

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: $.m.$

No.	position	mapping
1	$[x, 0, z]$	$[1, 4]$
2	$[-x, 0, z]$	$[2, 3]$

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

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

Table 9: Wyckoff site: 16i, site symmetry: 1

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