

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]