

MSG No. 63.457 *Cmcm* [Type I, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $m2m$

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

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

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

Table 5: Wyckoff site: $8e$, site symmetry: $2..$

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

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

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

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

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

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

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

continued ...

Table 8

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