

MSG No. 44.233 I_cmm2 [Type IV, orthorhombic]

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

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

Table 2: Wyckoff site: 4b, site symmetry: $mm2$

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

Table 3: Wyckoff site: 8c, site symmetry: $\dots 2'$

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

Table 4: Wyckoff site: 8d, site symmetry: $\dots m$.

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

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

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

Table 6: Wyckoff site: **16f**, 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	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[6]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[7]
8	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[8]
9	$[x, y, z + \frac{1}{2}]$	[9]
10	$[-x, -y, z + \frac{1}{2}]$	[10]
11	$[-x, y, z + \frac{1}{2}]$	[11]
12	$[x, -y, z + \frac{1}{2}]$	[12]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[13]
14	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[14]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[15]
16	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[16]