

MSG No. 44.234 $I_a mm2$ [Type IV, orthorhombic]

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

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

Table 2: Wyckoff site: 4b, 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	$[\frac{3}{4}, \frac{1}{2}, z + \frac{1}{2}]$	$[5, 8, 14, 15]$
4	$[\frac{1}{4}, \frac{1}{2}, z + \frac{1}{2}]$	$[6, 7, 13, 16]$

Table 3: Wyckoff site: 8c, site symmetry: $.m.$

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	$[x + \frac{1}{2}, 0, z]$	$[9, 12]$
6	$[\frac{1}{2} - x, 0, z]$	$[10, 11]$
7	$[x, \frac{1}{2}, z + \frac{1}{2}]$	$[13, 16]$
8	$[-x, \frac{1}{2}, z + \frac{1}{2}]$	$[14, 15]$

Table 4: Wyckoff site: 8d, 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	$[\frac{1}{2}, y, z]$	$[9, 11]$
6	$[\frac{1}{2}, -y, z]$	$[10, 12]$
7	$[0, y + \frac{1}{2}, z + \frac{1}{2}]$	$[13, 15]$
8	$[0, \frac{1}{2} - y, z + \frac{1}{2}]$	$[14, 16]$

Table 5: Wyckoff site: $8e$, 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	$[\frac{3}{4}, y + \frac{1}{2}, z + \frac{1}{2}]$	[5,15]
6	$[\frac{1}{4}, \frac{1}{2} - y, z + \frac{1}{2}]$	[6,16]
7	$[\frac{1}{4}, y + \frac{1}{2}, z + \frac{1}{2}]$	[7,13]
8	$[\frac{3}{4}, \frac{1}{2} - y, z + \frac{1}{2}]$	[8,14]

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	$[x + \frac{1}{2}, y, z]$	[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	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[14]
15	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[15]
16	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[16]