

MSG No. 44.233 I_cmm2 [Type IV, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: $\text{mm}2$

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: $\text{mm}2$

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: $.m.$

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]