

MSG No. 35.169 C_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	$[\frac{1}{2}, \frac{1}{2}, z]$	[5,6,7,8]
3	$[0, 0, z + \frac{1}{2}]$	[9,10,11,12]
4	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[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	$[\frac{1}{2}, 0, z]$	[5,6,7,8]
3	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[9,10,11,12]
4	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[13,14,15,16]

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

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

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

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