

MSG No. 21.42 C_c222 [Type IV, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: 222

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

Table 2: Wyckoff site: 4b, site symmetry: 222

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

Table 3: Wyckoff site: 4c, site symmetry: 2'2'2

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

Table 4: Wyckoff site: 4d, site symmetry: 2'2'2

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

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

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2]$
2	$[-x, 0, 0]$	$[3, 4]$

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: $2'$. .

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

Table 7: Wyckoff site: 8g, site symmetry: $.2$.

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

Table 8: Wyckoff site: 8h, site symmetry: $.2'$.

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

continued ...

Table 8

No.	position	mapping
6	$[\frac{1}{2}, \frac{1}{2} - y, \frac{3}{4}]$	[6,16]
7	$[\frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[7,13]
8	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$	[8,14]

Table 9: Wyckoff site: 8i, site symmetry: $\dots 2$

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

Table 10: Wyckoff site: 8j, site symmetry: $\dots 2$

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

Table 11: Wyckoff site: 8k, site symmetry: $\dots 2$

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

Table 12: Wyckoff site: 161, 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	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[6]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[7]
8	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[8]
9	$[x, y, z + \frac{1}{2}]$	[9]
10	$[x, -y, \frac{1}{2} - z]$	[10]
11	$[-x, y, \frac{1}{2} - z]$	[11]
12	$[-x, -y, z + \frac{1}{2}]$	[12]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[14]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[15]
16	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[16]