

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: . . 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: . . 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: . . 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]