

MSG No. 16.5 P_C222 [Type IV, orthorhombic]

Table 1: Wyckoff site: 2a, 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]

Table 2: Wyckoff site: 2b, 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]

Table 3: Wyckoff site: 2c, site symmetry: 222

No.	position	mapping
1	[\frac{1}{2}, 0, \frac{1}{2}]	[1,2,3,4]
2	[0, \frac{1}{2}, \frac{1}{2}]	[5,6,7,8]

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

No.	position	mapping
1	[0, 0, \frac{1}{2}]	[1,2,3,4]
2	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[5,6,7,8]

Table 5: Wyckoff site: 4e, site symmetry: 2..

No.	position	mapping
1	[x, 0, 0]	[1,2]
2	[-x, 0, 0]	[3,4]
3	[x + \frac{1}{2}, \frac{1}{2}, 0]	[5,6]
4	[\frac{1}{2} - x, \frac{1}{2}, 0]	[7,8]

Table 6: Wyckoff site: 4f, site symmetry: 2..

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	[1,2]
2	$[-x, 0, \frac{1}{2}]$	[3,4]
3	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[5,6]
4	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[7,8]

Table 7: Wyckoff site: 4g, 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]

Table 8: Wyckoff site: 4h, site symmetry: .2.

No.	position	mapping
1	$[0, y, \frac{1}{2}]$	[1,3]
2	$[0, -y, \frac{1}{2}]$	[2,4]
3	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[5,7]
4	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[6,8]

Table 9: Wyckoff site: 4i, 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]

Table 10: Wyckoff site: 4j, 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]

Table 11: Wyckoff site: 4k, 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]

Table 12: Wyckoff site: 81, 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]