

MSG No. 16.4 P_a222 [Type IV, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: 222

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

Table 2: Wyckoff site: 2b, site symmetry: 22'2'

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

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

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

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

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

Table 5: Wyckoff site: 2e, site symmetry: 22'2'

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

Table 6: Wyckoff site: 2f, site symmetry: 22'2'

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

Table 7: Wyckoff site: $2g$, site symmetry: 222

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

Table 8: Wyckoff site: $2h$, site symmetry: $22'2'$

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

Table 9: Wyckoff site: $4i$, site symmetry: $2..$

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

Table 10: Wyckoff site: $4j$, site symmetry: $2..$

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

Table 11: Wyckoff site: $4k$, site symmetry: $2..$

No.	position	mapping
1	$[x, \frac{1}{2}, 0]$	[1,2]
2	$[-x, \frac{1}{2}, 0]$	[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 12: Wyckoff site: $4l$, site symmetry: $2..$

No.	position	mapping
1	$[x, \frac{1}{2}, \frac{1}{2}]$	[1,2]
2	$[-x, \frac{1}{2}, \frac{1}{2}]$	[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 13: Wyckoff site: $4m$, site symmetry: $.2.$

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

Table 14: Wyckoff site: $4n$, site symmetry: $.2.$

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

Table 15: Wyckoff site: $4o$, site symmetry: $.2'$.

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

Table 16: Wyckoff site: $4p$, site symmetry: $.2'$.

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

Table 17: Wyckoff site: $4q$, site symmetry: $\dots 2$

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

Table 18: Wyckoff site: $4r$, site symmetry: $\dots 2'$

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

Table 19: Wyckoff site: $4s$, site symmetry: $\dots 2$

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

Table 20: Wyckoff site: $4t$, site symmetry: $\dots 2'$

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

Table 21: Wyckoff site: $8u$, site symmetry: 1

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

continued ...

Table 21

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