

MSG No. 22.46 $F\bar{2}221'$ [Type II, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: 2221'

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,17,18,19,20]
2	[0, $\frac{1}{2}$, $\frac{1}{2}$]	[5,6,7,8,21,22,23,24]
3	[$\frac{1}{2}$, 0, $\frac{1}{2}$]	[9,10,11,12,25,26,27,28]
4	[$\frac{1}{2}$, $\frac{1}{2}$, 0]	[13,14,15,16,29,30,31,32]

Table 2: Wyckoff site: 4b, site symmetry: 2221'

No.	position	mapping
1	[0, 0, $\frac{1}{2}$]	[1,2,3,4,17,18,19,20]
2	[0, $\frac{1}{2}$, 0]	[5,6,7,8,21,22,23,24]
3	[$\frac{1}{2}$, 0, 0]	[9,10,11,12,25,26,27,28]
4	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[13,14,15,16,29,30,31,32]

Table 3: Wyckoff site: 4c, site symmetry: 2221'

No.	position	mapping
1	[$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$]	[1,6,11,16,17,22,27,32]
2	[$\frac{1}{4}$, $\frac{3}{4}$, $\frac{3}{4}$]	[2,5,12,15,18,21,28,31]
3	[$\frac{3}{4}$, $\frac{1}{4}$, $\frac{3}{4}$]	[3,8,9,14,19,24,25,30]
4	[$\frac{3}{4}$, $\frac{3}{4}$, $\frac{1}{4}$]	[4,7,10,13,20,23,26,29]

Table 4: Wyckoff site: 4d, site symmetry: 2221'

No.	position	mapping
1	[$\frac{1}{4}$, $\frac{1}{4}$, $\frac{3}{4}$]	[1,6,11,16,17,22,27,32]
2	[$\frac{1}{4}$, $\frac{3}{4}$, $\frac{1}{4}$]	[2,5,12,15,18,21,28,31]
3	[$\frac{3}{4}$, $\frac{1}{4}$, $\frac{1}{4}$]	[3,8,9,14,19,24,25,30]
4	[$\frac{3}{4}$, $\frac{3}{4}$, $\frac{3}{4}$]	[4,7,10,13,20,23,26,29]

Table 5: Wyckoff site: 8e, site symmetry: 2..1'

No.	position	mapping
1	[x, 0, 0]	[1,2,17,18]
2	[-x, 0, 0]	[3,4,19,20]

continued ...

Table 5

No.	position	mapping
3	$[x, \frac{1}{2}, \frac{1}{2}]$	[5,6,21,22]
4	$[-x, \frac{1}{2}, \frac{1}{2}]$	[7,8,23,24]
5	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[9,10,25,26]
6	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[11,12,27,28]
7	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[13,14,29,30]
8	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[15,16,31,32]

Table 6: Wyckoff site: 8f, site symmetry: .2.1'

No.	position	mapping
1	$[0, y, 0]$	[1,3,17,19]
2	$[0, -y, 0]$	[2,4,18,20]
3	$[0, y + \frac{1}{2}, \frac{1}{2}]$	[5,7,21,23]
4	$[0, \frac{1}{2} - y, \frac{1}{2}]$	[6,8,22,24]
5	$[\frac{1}{2}, y, \frac{1}{2}]$	[9,11,25,27]
6	$[\frac{1}{2}, -y, \frac{1}{2}]$	[10,12,26,28]
7	$[\frac{1}{2}, y + \frac{1}{2}, 0]$	[13,15,29,31]
8	$[\frac{1}{2}, \frac{1}{2} - y, 0]$	[14,16,30,32]

Table 7: Wyckoff site: 8g, site symmetry: ..21'

No.	position	mapping
1	$[0, 0, z]$	[1,4,17,20]
2	$[0, 0, -z]$	[2,3,18,19]
3	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[5,8,21,24]
4	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[6,7,22,23]
5	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[9,12,25,28]
6	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[10,11,26,27]
7	$[\frac{1}{2}, \frac{1}{2}, z]$	[13,16,29,32]
8	$[\frac{1}{2}, \frac{1}{2}, -z]$	[14,15,30,31]

Table 8: Wyckoff site: 8h, site symmetry: ..21'

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, z]$	[1,16,17,32]
2	$[\frac{1}{4}, \frac{3}{4}, -z]$	[2,15,18,31]
3	$[\frac{3}{4}, \frac{1}{4}, -z]$	[3,14,19,30]
4	$[\frac{3}{4}, \frac{3}{4}, z]$	[4,13,20,29]
5	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[5,12,21,28]

continued ...

Table 8

No.	position	mapping
6	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[6,11,22,27]
7	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[7,10,23,26]
8	$[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[8,9,24,25]

Table 9: Wyckoff site: 8i, site symmetry: .2.1'

No.	position	mapping
1	$[\frac{1}{4}, y, \frac{1}{4}]$	[1,11,17,27]
2	$[\frac{1}{4}, -y, \frac{3}{4}]$	[2,12,18,28]
3	$[\frac{3}{4}, y, \frac{3}{4}]$	[3,9,19,25]
4	$[\frac{3}{4}, -y, \frac{1}{4}]$	[4,10,20,26]
5	$[\frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}]$	[5,15,21,31]
6	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{4}]$	[6,16,22,32]
7	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{4}]$	[7,13,23,29]
8	$[\frac{3}{4}, \frac{1}{2} - y, \frac{3}{4}]$	[8,14,24,30]

Table 10: Wyckoff site: 8j, site symmetry: 2..1'

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	[1,6,17,22]
2	$[x, \frac{3}{4}, \frac{3}{4}]$	[2,5,18,21]
3	$[-x, \frac{1}{4}, \frac{3}{4}]$	[3,8,19,24]
4	$[-x, \frac{3}{4}, \frac{1}{4}]$	[4,7,20,23]
5	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[9,14,25,30]
6	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[10,13,26,29]
7	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[11,16,27,32]
8	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[12,15,28,31]

Table 11: Wyckoff site: 16k, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1,17]
2	$[x, -y, -z]$	[2,18]
3	$[-x, y, -z]$	[3,19]
4	$[-x, -y, z]$	[4,20]
5	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[5,21]
6	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[6,22]
7	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[7,23]
8	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[8,24]

continued ...

Table 11

No.	position	mapping
9	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[9,25]
10	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[10,26]
11	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[11,27]
12	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[12,28]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[13,29]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[14,30]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[15,31]
16	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[16,32]