

MSG No. 22.46 $F2221'$ [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]