

MSG No. 71.534  $Immm1'$  [ Type II, orthorhombic ]

Table 1: Wyckoff site: 2a, site symmetry:  $mmm1'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $mmm1'$

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

Table 3: Wyckoff site: 2c, site symmetry:  $mmm1'$

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

Table 4: Wyckoff site: 2d, site symmetry:  $mmm1'$

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

Table 5: Wyckoff site: 4e, site symmetry:  $2mm1'$

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

Table 6: Wyckoff site: 4f, site symmetry:  $2mm1'$ 

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

Table 7: Wyckoff site: 4g, site symmetry:  $m2m1'$ 

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

Table 8: Wyckoff site: 4h, site symmetry:  $m2m1'$ 

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

Table 9: Wyckoff site: 4i, site symmetry:  $mm21'$ 

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

Table 10: Wyckoff site: 4j, site symmetry:  $mm21'$ 

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

Table 11: Wyckoff site:  $8k$ , site symmetry:  $-11'$ 

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

Table 12: Wyckoff site:  $8l$ , site symmetry:  $m..1'$ 

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

Table 13: Wyckoff site:  $8m$ , site symmetry:  $.m.1'$ 

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

Table 14: Wyckoff site:  $8n$ , site symmetry:  $..m1'$ 

No.	position	mapping
1	$[x, y, 0]$	[1, 8, 17, 24]
2	$[x, -y, 0]$	[2, 7, 18, 23]
3	$[-x, y, 0]$	[3, 6, 19, 22]

*continued ...*

Table 14

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

Table 15: Wyckoff site: 16o, 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	$[-x, -y, -z]$	[5, 21]
6	$[-x, y, z]$	[6, 22]
7	$[x, -y, z]$	[7, 23]
8	$[x, y, -z]$	[8, 24]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9, 25]
10	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[10, 26]
11	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[11, 27]
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[12, 28]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[13, 29]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[14, 30]
15	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[15, 31]
16	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[16, 32]