

MSG No. 74.555  $Imma1'$  [ Type II, orthorhombic ]

Table 1: Wyckoff site: 4a, site symmetry:  $2/m..1'$

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

Table 2: Wyckoff site: 4b, site symmetry:  $2/m..1'$

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

Table 3: Wyckoff site: 4c, site symmetry:  $.2/m.1'$

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

Table 4: Wyckoff site: 4d, site symmetry:  $.2/m.1'$

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

Table 5: Wyckoff site: 4e, site symmetry:  $mm21'$

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	$[1, 4, 6, 7, 17, 20, 22, 23]$
2	$[0, \frac{3}{4}, -z]$	$[2, 3, 5, 8, 18, 19, 21, 24]$

*continued ...*

Table 5

No.	position	mapping
3	$[\frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$	[9, 12, 14, 15, 25, 28, 30, 31]
4	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - z]$	[10, 11, 13, 16, 26, 27, 29, 32]

Table 6: Wyckoff site: 8f, site symmetry:  $2..1'$ 

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

Table 7: Wyckoff site: 8g, 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	$[\frac{3}{4}, y + \frac{1}{2}, \frac{3}{4}]$	[3, 9, 19, 25]
4	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{4}]$	[4, 10, 20, 26]
5	$[\frac{3}{4}, -y, \frac{3}{4}]$	[5, 15, 21, 31]
6	$[\frac{3}{4}, y, \frac{1}{4}]$	[6, 16, 22, 32]
7	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{4}]$	[7, 13, 23, 29]
8	$[\frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}]$	[8, 14, 24, 30]

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

No.	position	mapping
1	$[0, y, z]$	[1, 6, 17, 22]
2	$[0, -y, -z]$	[2, 5, 18, 21]
3	$[0, y + \frac{1}{2}, -z]$	[3, 8, 19, 24]
4	$[0, \frac{1}{2} - y, z]$	[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	$[\frac{1}{2}, y, \frac{1}{2} - z]$	[11, 16, 27, 32]
8	$[\frac{1}{2}, -y, z + \frac{1}{2}]$	[12, 15, 28, 31]

Table 9: Wyckoff site:  $8i$ , site symmetry:  $.m.1'$ 

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

Table 10: Wyckoff site:  $16j$ , site symmetry:  $11'$ 

No.	position	mapping
1	$[x, y, z]$	[1, 17]
2	$[x, -y, -z]$	[2, 18]
3	$[-x, y + \frac{1}{2}, -z]$	[3, 19]
4	$[-x, \frac{1}{2} - y, z]$	[4, 20]
5	$[-x, -y, -z]$	[5, 21]
6	$[-x, y, z]$	[6, 22]
7	$[x, \frac{1}{2} - y, z]$	[7, 23]
8	$[x, y + \frac{1}{2}, -z]$	[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	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[11, 27]
12	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[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	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[15, 31]
16	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[16, 32]