

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

Table 1: Wyckoff site: **4a**, site symmetry:  $2/m\ldots 1'$

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:  $2/m\ldots 1'$

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:  $mm\bar{2}1'$

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]