

MSG No. 64.470 *Cmca1'* [Type II, orthorhombic]

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

No.	position	mapping
1	[0, 0, 0]	[1, 2, 5, 6, 17, 18, 21, 22]
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	[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	$[0, \frac{1}{2}, \frac{1}{2}]$	[11, 12, 15, 16, 27, 28, 31, 32]

Table 2: Wyckoff site: **4b**, site symmetry: $2/m \dots 1'$

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

Table 3: Wyckoff site: **8c**, site symmetry: $-11'$

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

Table 4: Wyckoff site: **8d**, site symmetry: $2 \dots 1'$

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

Table 5: Wyckoff site: 8e, site symmetry: .2.1'

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

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

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

Table 7: Wyckoff site: 16g, site symmetry: 11'

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