

MSG No. 73.549 *Ibca1'* [Type II, orthorhombic]

Table 1: Wyckoff site: 8a, site symmetry: $-11'$

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

Table 2: Wyckoff site: 8b, site symmetry: $-11'$

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

Table 3: Wyckoff site: 8c, site symmetry: $2..1'$

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

Table 4: Wyckoff site: **8d**, site symmetry: $\cdot 2.1'$

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

Table 5: Wyckoff site: **8e**, site symmetry: $\cdot \cdot 21'$

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

Table 6: Wyckoff site: **16f**, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 17]$
2	$[x, -y, \frac{1}{2} - z]$	$[2, 18]$
3	$[\frac{1}{2} - x, y, -z]$	$[3, 19]$
4	$[-x, \frac{1}{2} - y, z]$	$[4, 20]$
5	$[-x, -y, -z]$	$[5, 21]$
6	$[-x, y, z + \frac{1}{2}]$	$[6, 22]$
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	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	$[10, 26]$
11	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	$[11, 27]$
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	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	$[14, 30]$
15	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	$[15, 31]$
16	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	$[16, 32]$