

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:  $.2.1'$ 

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:  $.21'$ 

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]