

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]