

MSG No. 73.548 *Ibca* [Type I, orthorhombic]

Table 1: Wyckoff site: 8a, site symmetry: -1

No.	position	mapping
1	[0, 0, 0]	[1,5]
2	[0, 0, $\frac{1}{2}$]	[2,6]
3	[$\frac{1}{2}$, 0, 0]	[3,7]
4	[0, $\frac{1}{2}$, 0]	[4,8]
5	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[9,13]
6	[$\frac{1}{2}$, $\frac{1}{2}$, 0]	[10,14]
7	[0, $\frac{1}{2}$, $\frac{1}{2}$]	[11,15]
8	[$\frac{1}{2}$, 0, $\frac{1}{2}$]	[12,16]

Table 2: Wyckoff site: 8b, site symmetry: -1

No.	position	mapping
1	[$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$]	[1,13]
2	[$\frac{1}{4}$, $\frac{3}{4}$, $\frac{1}{4}$]	[2,14]
3	[$\frac{1}{4}$, $\frac{1}{4}$, $\frac{3}{4}$]	[3,15]
4	[$\frac{3}{4}$, $\frac{1}{4}$, $\frac{1}{4}$]	[4,16]
5	[$\frac{3}{4}$, $\frac{3}{4}$, $\frac{3}{4}$]	[5,9]
6	[$\frac{3}{4}$, $\frac{1}{4}$, $\frac{3}{4}$]	[6,10]
7	[$\frac{3}{4}$, $\frac{3}{4}$, $\frac{1}{4}$]	[7,11]
8	[$\frac{1}{4}$, $\frac{3}{4}$, $\frac{3}{4}$]	[8,12]

Table 3: Wyckoff site: 8c, site symmetry: 2..

No.	position	mapping
1	[x , 0, $\frac{1}{4}$]	[1,2]
2	[$\frac{1}{2} - x$, 0, $\frac{3}{4}$]	[3,12]
3	[$-x$, $\frac{1}{2}$, $\frac{1}{4}$]	[4,11]
4	[$-x$, 0, $\frac{3}{4}$]	[5,6]
5	[$x + \frac{1}{2}$, 0, $\frac{1}{4}$]	[7,16]
6	[x , $\frac{1}{2}$, $\frac{3}{4}$]	[8,15]
7	[$x + \frac{1}{2}$, $\frac{1}{2}$, $\frac{3}{4}$]	[9,10]
8	[$\frac{1}{2} - x$, $\frac{1}{2}$, $\frac{1}{4}$]	[13,14]

Table 4: Wyckoff site: 8d, site symmetry: .2.

No.	position	mapping
1	$[\frac{1}{4}, y, 0]$	[1,3]
2	$[\frac{1}{4}, -y, \frac{1}{2}]$	[2,12]
3	$[\frac{3}{4}, \frac{1}{2} - y, 0]$	[4,10]
4	$[\frac{3}{4}, -y, 0]$	[5,7]
5	$[\frac{3}{4}, y, \frac{1}{2}]$	[6,16]
6	$[\frac{1}{4}, y + \frac{1}{2}, 0]$	[8,14]
7	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2}]$	[9,11]
8	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{2}]$	[13,15]

Table 5: Wyckoff site: 8e, site symmetry: ..2

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	[1,4]
2	$[0, \frac{3}{4}, \frac{1}{2} - z]$	[2,11]
3	$[\frac{1}{2}, \frac{1}{4}, -z]$	[3,10]
4	$[0, \frac{3}{4}, -z]$	[5,8]
5	$[0, \frac{1}{4}, z + \frac{1}{2}]$	[6,15]
6	$[\frac{1}{2}, \frac{3}{4}, z]$	[7,14]
7	$[\frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$	[9,12]
8	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - z]$	[13,16]

Table 6: Wyckoff site: 16f, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, -y, \frac{1}{2} - z]$	[2]
3	$[\frac{1}{2} - x, y, -z]$	[3]
4	$[-x, \frac{1}{2} - y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[-x, y, z + \frac{1}{2}]$	[6]
7	$[x + \frac{1}{2}, -y, z]$	[7]
8	$[x, y + \frac{1}{2}, -z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[10]
11	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[12]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[13]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[14]
15	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[15]
16	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[16]