

MSG No. 73.550 *Ib'ca* [Type III, orthorhombic]

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

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

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

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

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

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

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

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

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

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

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	$[x + \frac{1}{2}, -y, z]$	[3]
4	$[x, y + \frac{1}{2}, -z]$	[4]
5	$[\frac{1}{2} - x, y, -z]$	[5]
6	$[-x, \frac{1}{2} - y, z]$	[6]
7	$[-x, -y, -z]$	[7]
8	$[-x, y, z + \frac{1}{2}]$	[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	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[11]
12	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[12]
13	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[13]
14	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[14]
15	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[15]
16	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[16]