

MSG No. 63.460  $Cmc'm$  [ Type III, orthorhombic ]

Table 1: Wyckoff site: **4a**, site symmetry:  $2'/m..$

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

Table 2: Wyckoff site: **4b**, site symmetry:  $2'/m..$

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

Table 3: Wyckoff site: **4c**, site symmetry:  $m\bar{2}m$

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

Table 4: Wyckoff site: **8d**, site symmetry:  $-1'$

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

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

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

Table 6: Wyckoff site: 8f, site symmetry: m..

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

Table 7: Wyckoff site: 8g, site symmetry: ...m

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

Table 8: Wyckoff site: 16h, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, y, \frac{1}{2} - z]$	[2]
3	$[-x, y, z]$	[3]

continued ...

Table 8

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