

MSG No. 63.461  $Cmcm'$  [ 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:  $m2'm'$

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

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

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

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	$[0, -y, z + \frac{1}{2}]$	$[2, 4]$
3	$[0, -y, -z]$	$[5, 7]$
4	$[0, y, \frac{1}{2} - z]$	$[6, 8]$
5	$[\frac{1}{2}, y + \frac{1}{2}, z]$	$[9, 11]$
6	$[\frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	$[10, 12]$
7	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	$[13, 15]$
8	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	$[14, 16]$

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

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

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

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

*continued ...*

Table 8

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