

MSG No. 63.459 $Cm'cm$ [Type III, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry: $m'2'm$

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	[1,4]
2	$[x, -y, \frac{3}{4}]$	[2,3]
3	$[-x, y, \frac{1}{4}]$	[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	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{3}{4}]$	[10,11]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{4}]$	[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	$[x, -y, -z]$	[2]
3	$[x, -y, z + \frac{1}{2}]$	[3]

continued ...

Table 8

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