

MSG No. 68.515 $Cc'c'a$ [Type III, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: **8c**, site symmetry: -1

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

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

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

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

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

Table 6: Wyckoff site: 8f, site symmetry: $.2'$

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

Table 7: Wyckoff site: 8g, site symmetry: $..2$

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

Table 8: Wyckoff site: 8h, site symmetry: $..2$

No.	position	mapping
1	$[\frac{1}{4}, 0, z]$	[1,10]
2	$[\frac{3}{4}, \frac{1}{2}, z]$	[2,9]
3	$[\frac{1}{4}, \frac{1}{2}, -z]$	[3,12]

continued ...

Table 8

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

Table 9: Wyckoff site: 16i, site symmetry: 1

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