

MSG No. 68.513 $Cc'ca$ [Type III, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: $22'2'$

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: $22'2'$

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{4}, 0, z]$	[1, 14]
2	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{2} - z]$	[2, 13]
3	$[\frac{3}{4}, \frac{1}{2}, z + \frac{1}{2}]$	[3, 16]

continued ...

Table 8

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

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

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