

MSG No. 88.84 $I4_1/a'$ [Type III, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: -4' . .

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

Table 2: Wyckoff site: 4b, site symmetry: -4' . .

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

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

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

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

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

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

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

Table 6: Wyckoff site: 16f, site symmetry: 1

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