

MSG No. 88.82 $I4_1/a1'$ [Type II, tetragonal]

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

No.	position	mapping
1	$[0, \frac{1}{4}, \frac{1}{8}]$	[1,4,14,15,17,20,30,31]
2	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{8}]$	[2,3,13,16,18,19,29,32]
3	$[0, \frac{3}{4}, \frac{7}{8}]$	[5,8,10,11,21,24,26,27]
4	$[\frac{1}{2}, \frac{3}{4}, \frac{5}{8}]$	[6,7,9,12,22,23,25,28]

Table 2: Wyckoff site: 4b, site symmetry: -4..1'

No.	position	mapping
1	$[0, \frac{1}{4}, \frac{5}{8}]$	[1,4,14,15,17,20,30,31]
2	$[\frac{1}{2}, \frac{1}{4}, \frac{7}{8}]$	[2,3,13,16,18,19,29,32]
3	$[0, \frac{3}{4}, \frac{3}{8}]$	[5,8,10,11,21,24,26,27]
4	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{8}]$	[6,7,9,12,22,23,25,28]

Table 3: Wyckoff site: 8c, site symmetry: -11'

No.	position	mapping
1	$[0, 0, 0]$	[1,5,17,21]
2	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[2,14,18,30]
3	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[3,15,19,31]
4	$[0, \frac{1}{2}, 0]$	[4,8,20,24]
5	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[6,10,22,26]
6	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[7,11,23,27]
7	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9,13,25,29]
8	$[\frac{1}{2}, 0, \frac{1}{2}]$	[12,16,28,32]

Table 4: Wyckoff site: 8d, site symmetry: -11'

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	[1,5,17,21]
2	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[2,14,18,30]
3	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[3,15,19,31]
4	$[0, \frac{1}{2}, \frac{1}{2}]$	[4,8,20,24]
5	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[6,10,22,26]
6	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[7,11,23,27]
7	$[\frac{1}{2}, \frac{1}{2}, 0]$	[9,13,25,29]
8	$[\frac{1}{2}, 0, 0]$	[12,16,28,32]

Table 5: Wyckoff site: 8e, site symmetry: 2..1'

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	[1,4,17,20]
2	$[\frac{1}{2}, \frac{1}{4}, z + \frac{1}{4}]$	[2,3,18,19]
3	$[0, \frac{3}{4}, -z]$	[5,8,21,24]
4	$[\frac{1}{2}, \frac{3}{4}, \frac{3}{4} - z]$	[6,7,22,23]
5	$[\frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$	[9,12,25,28]
6	$[0, \frac{3}{4}, z + \frac{3}{4}]$	[10,11,26,27]
7	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - z]$	[13,16,29,32]
8	$[0, \frac{1}{4}, \frac{1}{4} - z]$	[14,15,30,31]

Table 6: Wyckoff site: 16f, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1,17]
2	$[\frac{3}{4} - y, x + \frac{1}{4}, z + \frac{1}{4}]$	[2,18]
3	$[y + \frac{1}{4}, \frac{1}{4} - x, z + \frac{1}{4}]$	[3,19]
4	$[-x, \frac{1}{2} - y, z]$	[4,20]
5	$[-x, -y, -z]$	[5,21]
6	$[y + \frac{1}{4}, \frac{3}{4} - x, \frac{3}{4} - z]$	[6,22]
7	$[\frac{3}{4} - y, x + \frac{3}{4}, \frac{3}{4} - z]$	[7,23]
8	$[x, y + \frac{1}{2}, -z]$	[8,24]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9,25]
10	$[\frac{1}{4} - y, x + \frac{3}{4}, z + \frac{3}{4}]$	[10,26]
11	$[y + \frac{3}{4}, \frac{3}{4} - x, z + \frac{3}{4}]$	[11,27]
12	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[12,28]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[13,29]
14	$[y + \frac{3}{4}, \frac{1}{4} - x, \frac{1}{4} - z]$	[14,30]
15	$[\frac{1}{4} - y, x + \frac{1}{4}, \frac{1}{4} - z]$	[15,31]
16	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[16,32]