

MSG No. 80.32 I_c4_1 [Type IV, tetragonal]

Table 1: Wyckoff site: 8a, site symmetry: $2'..$

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

Table 2: Wyckoff site: 8b, site symmetry: $2'..$

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

Table 3: Wyckoff site: 8c, site symmetry: $2..$

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

Table 4: Wyckoff site: 16d, site symmetry: 1

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