

MSG No. 79.28 I_4 [Type IV, tetragonal]

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x, z]$	[2]
3	$[y, -x, z]$	[3]
4	$[-x, -y, z]$	[4]
5	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[6]
7	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[7]
8	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[8]
9	$[x, y, z + \frac{1}{2}]$	[9]

continued ...

Table 4

No.	position	mapping
10	$[-y, x, z + \frac{1}{2}]$	[10]
11	$[y, -x, z + \frac{1}{2}]$	[11]
12	$[-x, -y, z + \frac{1}{2}]$	[12]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[13]
14	$[\frac{1}{2} - y, x + \frac{1}{2}, z]$	[14]
15	$[y + \frac{1}{2}, \frac{1}{2} - x, z]$	[15]
16	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[16]