

MSG No. 105.217  $P_{C42}mc$  [ Type IV, tetragonal ]

Table 1: Wyckoff site: 4a, site symmetry: 2mm.

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

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

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

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

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

Table 4: Wyckoff site: 8d, site symmetry: .m.

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

Table 5: Wyckoff site: **16e**, site symmetry: 1

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