

MSG No. 99.170  $P_I4mm$  [ Type IV, tetragonal ]

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

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

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]	[2,3,7,8]
3	[\frac{1}{2}, 0, z + \frac{1}{2}]	[9,12,13,14]
4	[0, \frac{1}{2}, z + \frac{1}{2}]	[10,11,15,16]

Table 3: Wyckoff site: 8c, site symmetry: ...m

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

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

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

Table 5: Wyckoff site: **16e**, 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	$[-x, y, z]$	[5]
6	$[x, -y, z]$	[6]
7	$[-y, -x, z]$	[7]
8	$[y, x, z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[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	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[12]
13	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[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]