

MSG No. 102.194  $P_I4_2nm$  [ Type IV, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry:  $4'm'm$

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

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

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

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

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

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

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