

MSG No. 113.272 $P_c\bar{4}2_1m$ [Type IV, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $2.mm$

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

Table 4: Wyckoff site: 8d, site symmetry: $2..$

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

Table 5: Wyckoff site: **8e**, site symmetry: $\bar{3}m$

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

Table 6: Wyckoff site: **16f**, site symmetry: $\bar{1}$

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