

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: . . 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: 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]