

MSG No. 115.290  $P_I\bar{4}m2$  [ Type IV, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry: -4m2

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

Table 2: Wyckoff site: 2b, site symmetry: -4m2

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

Table 3: Wyckoff site: 2c, site symmetry: -4'm2'

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

Table 4: Wyckoff site: 2d, site symmetry: -4'm2'

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

Table 5: Wyckoff site: 4e, site symmetry: 2mm.

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

Table 6: Wyckoff site: 4f, site symmetry: 2mm.

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

Table 7: Wyckoff site: 8g, site symmetry: ..2

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

Table 8: Wyckoff site: 8h, site symmetry: ..2'

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

Table 9: Wyckoff site: 8i, site symmetry: .m.

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

*continued ...*

Table 9

No.	position	mapping
8	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[12,13]

Table 10: Wyckoff site: 16j, site symmetry: 1

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