

MSG No. 115.288 $P_c\bar{4}m2$ [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	$[0, 0, \frac{1}{2}]$	$[9, 10, 11, 12, 13, 14, 15, 16]$

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, z]$	[1,2,7,8]
2	$[\frac{1}{2}, \frac{1}{2}, -z]$	[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 7: Wyckoff site: **4g**, 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	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[9,10,15,16]
4	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[11,12,13,14]

Table 8: Wyckoff site: **8h**, 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	$[x, x, \frac{1}{2}]$	[9,11]
6	$[-x, -x, \frac{1}{2}]$	[10,12]
7	$[x, -x, \frac{1}{2}]$	[13,16]
8	$[-x, x, \frac{1}{2}]$	[14,15]

Table 9: Wyckoff site: **8i**, site symmetry: $. . 2'$

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

Table 10: Wyckoff site: 8j, 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	$[x, 0, z + \frac{1}{2}]$	[9,16]
6	$[-x, 0, z + \frac{1}{2}]$	[10,15]
7	$[0, x, \frac{1}{2} - z]$	[11,14]
8	$[0, -x, \frac{1}{2} - z]$	[12,13]

Table 11: Wyckoff site: 8k, site symmetry: .m.

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

Table 12: Wyckoff site: 16l, 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	$[x, y, z + \frac{1}{2}]$	[9]
10	$[-x, -y, z + \frac{1}{2}]$	[10]
11	$[y, x, \frac{1}{2} - z]$	[11]
12	$[-y, -x, \frac{1}{2} - z]$	[12]
13	$[y, -x, \frac{1}{2} - z]$	[13]
14	$[-y, x, \frac{1}{2} - z]$	[14]
15	$[-x, y, z + \frac{1}{2}]$	[15]
16	$[x, -y, z + \frac{1}{2}]$	[16]