

MSG No. 115.289 $P_C\bar{4}m2$ [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	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, 10, 11, 12, 13, 14, 15, 16]$

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: 2.22

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

Table 6: Wyckoff site: 4f, site symmetry: 2.22

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

Table 7: Wyckoff site: 4g, site symmetry: 2mm.

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

Table 8: Wyckoff site: 4h, 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	$[\frac{1}{2}, 0, z]$	[9,10,15,16]
4	$[0, \frac{1}{2}, -z]$	[11,12,13,14]

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

Table 10: Wyckoff site: $8j$, site symmetry: $\cdot\cdot 2'$

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

Table 11: Wyckoff site: $8k$, site symmetry: $\cdot\cdot 2$

No.	position	mapping
1	$[x, x, \frac{1}{2}]$	$[1, 3]$
2	$[-x, -x, \frac{1}{2}]$	$[2, 4]$
3	$[x, -x, \frac{1}{2}]$	$[5, 8]$
4	$[-x, x, \frac{1}{2}]$	$[6, 7]$
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 12: Wyckoff site: $8l$, site symmetry: $\cdot\cdot 2'$

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

Table 13: Wyckoff site: $8m$, site symmetry: $2'\cdot\cdot$

No.	position	mapping
1	$[\frac{3}{4}, \frac{1}{4}, z]$	$[1, 10]$
2	$[\frac{1}{4}, \frac{3}{4}, z]$	$[2, 9]$
3	$[\frac{1}{4}, \frac{3}{4}, -z]$	$[3, 12]$

continued ...

Table 13

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

Table 14: Wyckoff site: 8n, site symmetry: .m.

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

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