

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: $\dots 2'$

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: $\dots 2$

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: $\dots 2'$

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: $2' \dots$

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]