

MSG No. 113.273 $P_C\bar{4}2_1m$ [Type IV, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: -4'2'm

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

Table 2: Wyckoff site: 2b, site symmetry: -42'm'

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

Table 3: Wyckoff site: 2c, site symmetry: -42'm'

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

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

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

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

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

Table 6: Wyckoff site: **4f**, site symmetry: **2.m'm'**

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

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

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

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

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

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

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

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

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

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

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