

MSG No. 134.476 $P4'_2/n'n'm$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: -42m

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: 222.

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

Table 4: Wyckoff site: 4d, site symmetry: 2.2'2'

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

Table 5: Wyckoff site: 4e, site symmetry: ..2'/m

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

Table 6: Wyckoff site: 4f, site symmetry: . . 2¹/m

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

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

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

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

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

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

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

Table 10: Wyckoff site: 8j, site symmetry: .2.

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

Table 11: Wyckoff site: 8k, site symmetry: ..2'

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

Table 12: Wyckoff site: 8l, site symmetry: ..2'

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

Table 13: Wyckoff site: 8m, site symmetry: ...m

No.	position	mapping
1	$[x, -x, z]$	[1,7]
2	$[x, x + \frac{1}{2}, \frac{1}{2} - z]$	[2,6]
3	$[\frac{1}{2} - x, -x, \frac{1}{2} - z]$	[3,5]

continued ...

Table 13

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

Table 14: Wyckoff site: 16n, site symmetry: 1

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