

MSG No. 134.471 $P4_2/nm$ [Type I, tetragonal]

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: 2.22

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, -x, z]$	[1,15]
2	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	[2,13]
3	$[-x, \frac{1}{2} - x, z + \frac{1}{2}]$	[3,12]

continued ...

Table 13

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

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

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