

MSG No. 134.474 $P4'_2/nm'm$ [Type III, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: 22'2'.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, -x, z]$	[1,7]
2	$[\frac{1}{2} - x, x + \frac{1}{2}, z]$	[2,8]
3	$[-x, x, -z]$	[3,5]

continued ...

Table 13

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

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

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