

MSG No. 136.498 $P4'_2/mn'm$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: m.m̄m̄

No.	position	mapping
1	[0, 0, 0]	[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 2: Wyckoff site: 2b, site symmetry: m.m̄m̄

No.	position	mapping
1	[0, 0, \frac{1}{2}]	[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 3: Wyckoff site: 4c, site symmetry: 2/m..

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

Table 4: Wyckoff site: 4d, site symmetry: -4'..

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

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

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 + \frac{1}{2}]	[9,10,15,16]
4	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]	[11,12,13,14]

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

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

Table 7: Wyckoff site: 4g, site symmetry: m.m2

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

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

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

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

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

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

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

Table 11: Wyckoff site: 16k, 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	[-x, -y, -z]	[5]
6	[x, y, -z]	[6]
7	[-y, -x, z]	[7]
8	[y, x, z]	[8]
9	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[10]
11	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[12]
13	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[13]
14	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[14]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[15]
16	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[16]