

MSG No. 136.501 $P4_2/mn'm'$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: $m.m'm'$

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

Table 2: Wyckoff site: 2b, site symmetry: $m.m'm'$

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

Table 3: Wyckoff site: 4c, site symmetry: $2/m..$

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

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

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

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

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

Table 6: Wyckoff site: **4f**, site symmetry: $m \cdot 2'm'$

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

Table 7: Wyckoff site: **4g**, site symmetry: $m \cdot m'2'$

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

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

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

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

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

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

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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