

MSG No. 136.502 $P4'_2/m'nm'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site: 4g, site symmetry: $m' . m' 2$

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

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	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[5, 6]
4	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[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	$[0, \frac{1}{2}, -z]$	[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, 14]
2	$[-x, -y, 0]$	[2, 13]
3	$[y, x, 0]$	[3, 16]
4	$[-y, -x, 0]$	[4, 15]
5	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[5, 10]
6	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2}]$	[6, 9]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	[7, 12]
8	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[8, 11]

Table 10: Wyckoff site: 8j, site symmetry: $\dots m'$

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

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	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[5]
6	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[6]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[7]
8	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[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	$[-x, -y, -z]$	[13]
14	$[x, y, -z]$	[14]
15	$[-y, -x, z]$	[15]
16	$[y, x, z]$	[16]