

MSG No. 132.450  $P4'_2/mc'm$  [ Type III, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry:  $\text{m.m}\bar{\text{m}}$

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

Table 2: Wyckoff site: 2b, site symmetry:  $-4'2'\text{m}$

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

Table 3: Wyckoff site: 2c, site symmetry:  $\text{m.m}\bar{\text{m}}$

No.	position	mapping
1	[ $\frac{1}{2}$ , $\frac{1}{2}$ , 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 4: Wyckoff site: 2d, site symmetry:  $-4'2'\text{m}$

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

Table 5: Wyckoff site: 4e, site symmetry:  $22'2'$ .

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

Table 6: Wyckoff site: 4f, 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	[ $\frac{1}{2}$ , 0, $\frac{1}{2}$ ]	[9,10,13,14]
4	[0, $\frac{1}{2}$ , $\frac{1}{2}$ ]	[11,12,15,16]

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

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

Table 8: Wyckoff site: 4h, site symmetry: 2.mm

No.	position	mapping
1	[ $\frac{1}{2}$ , $\frac{1}{2}$ , z]	[1,2,7,8]
2	[ $\frac{1}{2}$ , $\frac{1}{2}$ , -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 9: Wyckoff site: 4i, site symmetry: m.2m

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

Table 10: Wyckoff site: 4j, site symmetry: m.2m

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

Table 11: Wyckoff site: 8k, 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	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[9,10]
6	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[11,12]
7	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[13,14]
8	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[15,16]

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

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

Table 13: Wyckoff site: 8m, site symmetry: .2'.

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

Table 14: Wyckoff site: 8n, site symmetry: m..

No.	position	mapping
1	$[x, y, 0]$	[1,6]
2	$[-x, -y, 0]$	[2,5]
3	$[y, x, 0]$	[3,8]

*continued ...*

Table 14

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

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

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