

MSG No. 83.48  $P_4/m$  [ Type IV, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry:  $4/m..$

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:  $4/m'..$

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

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

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:  $4/m'..$

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

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

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

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

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

Table 7: Wyckoff site: **4g**, site symmetry:  $4$  . .

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

Table 8: Wyckoff site: **4h**, site symmetry:  $4$  . .

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

Table 9: Wyckoff site: **8i**, site symmetry:  $2$  . .

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

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

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

Table 11: Wyckoff site:  $8k$ , site symmetry:  $m' \dots$ 

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

Table 12: Wyckoff site:  $16l$ , site symmetry:  $1$ 

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