

MSG No. 83.48  $P_c4/m$  [ 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:  $m$  . .

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:  $m'$  . .

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]