

MSG No. 132.447  $P4_2/mcm$  [ Type I, tetragonal ]

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

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

Table 2: Wyckoff site: 2b, site symmetry:  $-42m$

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

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

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

Table 4: Wyckoff site: 2d, site symmetry:  $-42m$

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

Table 5: Wyckoff site: 4e, site symmetry:  $222.$

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

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

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

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

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

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

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

Table 9: Wyckoff site: **4i**, site symmetry:  $m.2m$ 

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

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

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

Table 11: Wyckoff site:  $8\mathbf{k}$ , site symmetry:  $2..$ 

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

Table 12: Wyckoff site:  $8\mathbf{l}$ , site symmetry:  $.2.$ 

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

Table 13: Wyckoff site:  $8\mathbf{m}$ , site symmetry:  $.2.$ 

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

Table 14: Wyckoff site:  $8\mathbf{n}$ , site symmetry:  $\mathbf{m}..$ 

No.	position	mapping
1	$[x, y, 0]$	$[1, 14]$
2	$[-y, x, \frac{1}{2}]$	$[2, 11]$
3	$[y, -x, \frac{1}{2}]$	$[3, 10]$

*continued ...*

Table 14

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

Table 15: Wyckoff site: 8o, site symmetry:  $\bar{3}m$ 

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

Table 16: Wyckoff site: 16p, site symmetry: 1

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