

MSG No. 123.345  $P4/mm'm'$  [ Type III, tetragonal ]

Table 1: Wyckoff site: **1a**, site symmetry:  $4/\text{mm}'\text{m}'$

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

Table 2: Wyckoff site: **1b**, site symmetry:  $4/\text{mm}'\text{m}'$

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

Table 3: Wyckoff site: **1c**, site symmetry:  $4/\text{mm}'\text{m}'$

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

Table 4: Wyckoff site: **1d**, site symmetry:  $4/\text{mm}'\text{m}'$

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

Table 5: Wyckoff site: **2e**, site symmetry:  $\text{mm}'\text{m}'$ .

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

Table 6: Wyckoff site: **2f**, site symmetry:  $\text{mm}'\text{m}'$ .

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

Table 7: Wyckoff site: 2g, site symmetry:  $4\bar{m}'\bar{m}'$ 

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

Table 8: Wyckoff site: 2h, site symmetry:  $4\bar{m}'\bar{m}'$ 

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

Table 9: Wyckoff site: 4i, site symmetry:  $2\bar{m}'\bar{m}'$ .

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

Table 10: Wyckoff site: 4j, site symmetry:  $\bar{m}.2'\bar{m}'$ 

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

Table 11: Wyckoff site: 4k, site symmetry:  $\bar{m}.2'\bar{m}'$ 

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

Table 12: Wyckoff site: 4l, site symmetry:  $m\bar{2}'m'$ .

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

Table 13: Wyckoff site: 4m, site symmetry:  $m\bar{2}'m'$ .

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

Table 14: Wyckoff site: 4n, site symmetry:  $m\bar{2}'m'$ .

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

Table 15: Wyckoff site: 4o, site symmetry:  $m\bar{2}'m'$ .

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

Table 16: Wyckoff site: 8p, 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]

*continued ...*

Table 16

No.	position	mapping
5	$[x, -y, 0]$	[9,14]
6	$[-x, y, 0]$	[10,13]
7	$[y, x, 0]$	[11,16]
8	$[-y, -x, 0]$	[12,15]

Table 17: Wyckoff site: 8q, site symmetry: m..

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

Table 18: Wyckoff site: 8r, site symmetry: ..m'

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

Table 19: Wyckoff site: 8s, site symmetry: .m'.

No.	position	mapping
1	$[x, 0, z]$	[1,14]
2	$[0, x, z]$	[2,16]
3	$[0, -x, z]$	[3,15]
4	$[-x, 0, z]$	[4,13]
5	$[-x, 0, -z]$	[5,10]
6	$[0, -x, -z]$	[6,12]
7	$[0, x, -z]$	[7,11]

continued ...

Table 19

No.	position	mapping
8	$[x, 0, -z]$	[8,9]

Table 20: Wyckoff site: 8t, site symmetry: .m'.

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

Table 21: Wyckoff site: 16u, 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	$[x, -y, -z]$	[9]
10	$[-x, y, -z]$	[10]
11	$[y, x, -z]$	[11]
12	$[-y, -x, -z]$	[12]
13	$[-x, y, z]$	[13]
14	$[x, -y, z]$	[14]
15	$[-y, -x, z]$	[15]
16	$[y, x, z]$	[16]