

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

Table 1: Wyckoff site: 1a, site symmetry: $4/mm'm'$

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: $4/mm'm'$

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: $4/mm'm'$

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: $4/mm'm'$

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: $mm'm'$.

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: $mm'm'$.

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: $4m'm'$

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: $4m'm'$

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: $2m'm'$.

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: $m.2'm'$

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: $m.2'm'$

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: $m2'm'$.

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: $m2'm'$.

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: $m2'm'$.

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: $m2'm'$.

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]