

MSG No. 175.138 $P6/m1'$ [Type II, hexagonal]

Table 1: Wyckoff site: 1a, site symmetry: $6/m..1'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 2: Wyckoff site: 1b, site symmetry: $6/m..1'$

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 3: Wyckoff site: 2c, site symmetry: $-6..1'$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1, 3, 5, 8, 10, 12, 13, 15, 17, 20, 22, 24]$
2	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[2, 4, 6, 7, 9, 11, 14, 16, 18, 19, 21, 23]$

Table 4: Wyckoff site: 2d, site symmetry: $-6..1'$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[1, 3, 5, 8, 10, 12, 13, 15, 17, 20, 22, 24]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[2, 4, 6, 7, 9, 11, 14, 16, 18, 19, 21, 23]$

Table 5: Wyckoff site: 2e, site symmetry: $6..1'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 5, 6, 13, 14, 15, 16, 17, 18]$
2	$[0, 0, -z]$	$[7, 8, 9, 10, 11, 12, 19, 20, 21, 22, 23, 24]$

Table 6: Wyckoff site: 3f, site symmetry: $2/m..1'$

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	$[1, 4, 7, 10, 13, 16, 19, 22]$
2	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[2, 5, 8, 11, 14, 17, 20, 23]$
3	$[0, \frac{1}{2}, 0]$	$[3, 6, 9, 12, 15, 18, 21, 24]$

Table 7: Wyckoff site: $3g$, site symmetry: $2/m..1'$

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, 4, 7, 10, 13, 16, 19, 22]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, 5, 8, 11, 14, 17, 20, 23]$
3	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, 6, 9, 12, 15, 18, 21, 24]$

Table 8: Wyckoff site: $4h$, site symmetry: $3..1'$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 3, 5, 13, 15, 17]$
2	$[\frac{2}{3}, \frac{1}{3}, z]$	$[2, 4, 6, 14, 16, 18]$
3	$[\frac{2}{3}, \frac{1}{3}, -z]$	$[7, 9, 11, 19, 21, 23]$
4	$[\frac{1}{3}, \frac{2}{3}, -z]$	$[8, 10, 12, 20, 22, 24]$

Table 9: Wyckoff site: $6i$, site symmetry: $2..1'$

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	$[1, 4, 13, 16]$
2	$[\frac{1}{2}, \frac{1}{2}, z]$	$[2, 5, 14, 17]$
3	$[0, \frac{1}{2}, z]$	$[3, 6, 15, 18]$
4	$[\frac{1}{2}, 0, -z]$	$[7, 10, 19, 22]$
5	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[8, 11, 20, 23]$
6	$[0, \frac{1}{2}, -z]$	$[9, 12, 21, 24]$

Table 10: Wyckoff site: $6j$, site symmetry: $m..1'$

No.	position	mapping
1	$[x, y, 0]$	$[1, 10, 13, 22]$
2	$[x - y, x, 0]$	$[2, 11, 14, 23]$
3	$[-y, x - y, 0]$	$[3, 12, 15, 24]$
4	$[-x, -y, 0]$	$[4, 7, 16, 19]$
5	$[-x + y, -x, 0]$	$[5, 8, 17, 20]$
6	$[y, -x + y, 0]$	$[6, 9, 18, 21]$

Table 11: Wyckoff site: $6k$, site symmetry: $m..1'$

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	$[1, 10, 13, 22]$

continued ...

Table 11

No.	position	mapping
2	$[x - y, x, \frac{1}{2}]$	[2, 11, 14, 23]
3	$[-y, x - y, \frac{1}{2}]$	[3, 12, 15, 24]
4	$[-x, -y, \frac{1}{2}]$	[4, 7, 16, 19]
5	$[-x + y, -x, \frac{1}{2}]$	[5, 8, 17, 20]
6	$[y, -x + y, \frac{1}{2}]$	[6, 9, 18, 21]

Table 12: Wyckoff site: 121, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	[1, 13]
2	$[x - y, x, z]$	[2, 14]
3	$[-y, x - y, z]$	[3, 15]
4	$[-x, -y, z]$	[4, 16]
5	$[-x + y, -x, z]$	[5, 17]
6	$[y, -x + y, z]$	[6, 18]
7	$[-x, -y, -z]$	[7, 19]
8	$[-x + y, -x, -z]$	[8, 20]
9	$[y, -x + y, -z]$	[9, 21]
10	$[x, y, -z]$	[10, 22]
11	$[x - y, x, -z]$	[11, 23]
12	$[-y, x - y, -z]$	[12, 24]