

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]