

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: 12l, 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]