

MSG No. 177.152  $P6'22'$  [ Type III, hexagonal ]

Table 1: Wyckoff site: 1a, site symmetry: 6'22'

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

Table 2: Wyckoff site: 1b, site symmetry: 6'22'

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

Table 3: Wyckoff site: 2c, site symmetry: 3.2'

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

Table 4: Wyckoff site: 2d, site symmetry: 3.2'

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

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

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

Table 6: Wyckoff site: 3f, site symmetry: 2'22'

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

Table 7: Wyckoff site: 3g, site symmetry: 2'22'

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

Table 8: Wyckoff site: 4h, site symmetry: 3..

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

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

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

Table 10: Wyckoff site: 6j, site symmetry: .2.

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

Table 11: Wyckoff site: 6k, site symmetry: .2.

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	[1,4]

*continued ...*

Table 11

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

Table 12: Wyckoff site: 61, site symmetry:  $\dots 2'$ 

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

Table 13: Wyckoff site: 6m, site symmetry:  $\dots 2'$ 

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

Table 14: Wyckoff site: 12n, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x - y, z]$	[2]
3	$[-x + y, -x, z]$	[3]
4	$[x - y, -y, -z]$	[4]
5	$[y, x, -z]$	[5]
6	$[-x, -x + y, -z]$	[6]
7	$[x - y, x, z]$	[7]
8	$[-x, -y, z]$	[8]
9	$[y, -x + y, z]$	[9]
10	$[x, x - y, -z]$	[10]

continued ...

Table 14

No.	position	mapping
11	$[-x + y, y, -z]$	[11]
12	$[-y, -x, -z]$	[12]