

MSG No. 194.266  $P6'_3/mm'c$  [ Type III, hexagonal ]

Table 1: Wyckoff site: 2a, site symmetry:  $-3'm'$ .

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

Table 2: Wyckoff site: 2b, site symmetry:  $-6m'2'$

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $3m'$ .

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

Table 6: Wyckoff site: 4f, site symmetry: 3m'.

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

Table 7: Wyckoff site: 6g, site symmetry: .2/m'.

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

Table 8: Wyckoff site: 6h, site symmetry: mm'2'

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

Table 9: Wyckoff site: 12i, 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	$[-x, -x, \frac{1}{2}]$	[7,10]
5	$[x, 0, \frac{1}{2}]$	[8,11]
6	$[0, x, \frac{1}{2}]$	[9,12]
7	$[x, x, \frac{1}{2}]$	[13,16]
8	$[-x, 0, \frac{1}{2}]$	[14,17]
9	$[0, -x, \frac{1}{2}]$	[15,18]
10	$[-x, 0, 0]$	[19,22]
11	$[0, -x, 0]$	[20,23]

continued ...

Table 9

No.	position	mapping
12	[ $x, x, 0$ ]	[21,24]

Table 10: Wyckoff site: 12j, site symmetry:  $\mathbf{m}..$ 

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

Table 11: Wyckoff site: 12k, site symmetry:  $.\mathbf{m}'.$ 

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

Table 12: Wyckoff site: 24l, site symmetry: 1

No.	position	mapping
1	[ $x, y, z$ ]	[1]
2	[ $-y, x - y, z$ ]	[2]

*continued ...*

Table 12

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