

SG No. 194  $D_{6h}^4$   $P6_3/mmc$  [ hexagonal ]

\* plus set:  $+ [0, 0, 0]$

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

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

Table 2: Wyckoff site: 2b, site symmetry:  $-6m2$

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

Table 3: Wyckoff site: 2c, site symmetry:  $-6m2$

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

Table 4: Wyckoff site: 2d, site symmetry:  $-6m2$

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

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

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

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

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

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

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

Table 8: Wyckoff site: **6h**, site symmetry: **mm2**

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

Table 9: Wyckoff site: **12i**, site symmetry: **.2**.

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

*continued ...*

Table 9

No.	position	mapping
12	$[-x, -x, \frac{1}{2}]$	[18,24]

Table 10: Wyckoff site: 12j, site symmetry:  $m..$ 

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

Table 11: Wyckoff site: 12k, site symmetry:  $.m.$ 

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

Table 12: Wyckoff site: 241, 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	$[-x, -y, z + \frac{1}{2}]$	[4]
5	$[y, -x + y, z + \frac{1}{2}]$	[5]
6	$[x - y, x, z + \frac{1}{2}]$	[6]
7	$[y, x, -z]$	[7]
8	$[x - y, -y, -z]$	[8]
9	$[-x, -x + y, -z]$	[9]
10	$[-y, -x, \frac{1}{2} - z]$	[10]
11	$[-x + y, y, \frac{1}{2} - z]$	[11]
12	$[x, x - y, \frac{1}{2} - z]$	[12]
13	$[-x, -y, -z]$	[13]
14	$[y, -x + y, -z]$	[14]
15	$[x - y, x, -z]$	[15]
16	$[x, y, \frac{1}{2} - z]$	[16]
17	$[-y, x - y, \frac{1}{2} - z]$	[17]
18	$[-x + y, -x, \frac{1}{2} - z]$	[18]
19	$[-y, -x, z]$	[19]
20	$[-x + y, y, z]$	[20]
21	$[x, x - y, z]$	[21]
22	$[y, x, z + \frac{1}{2}]$	[22]
23	$[x - y, -y, z + \frac{1}{2}]$	[23]
24	$[-x, -x + y, z + \frac{1}{2}]$	[24]