

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: $\mathbf{m}..$

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: $.\mathbf{m}.$

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: 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	$[-x, -y, z + \frac{1}{2}]$	[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]