SG No. 191 D_{6h}^{1} $P6/mmm$ [hexagonal]

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

Table 1: Wyckoff site: `1a`, site symmetry: `6/mmm`

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/mmm`

No.	position	mapping
1	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[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: `-6m2`

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

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

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

Table 5: Wyckoff site: `2e`, site symmetry: `6mm`

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

Table 6: Wyckoff site: `3f`, site symmetry: `mmm`

No.	position	mapping
1	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[1,4,8,11,13,16,20,23]`
2	$\left[0,\ \frac{1}{2},\ 0\right]$	`[2,5,7,10,14,17,19,22]`

3	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[3,6,9,12,15,18,21,24]

Table 7: Wyckoff site: 3g, site symmetry: mmm

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

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

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

Table 9: Wyckoff site: 6i, site symmetry: 2mm

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

Table 10: Wyckoff site: 6j, site symmetry: m2m

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

Table 11: Wyckoff site: `6k`, site symmetry: `m2m`

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

Table 12: Wyckoff site: `6l`, site symmetry: `mm2`

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

Table 13: Wyckoff site: `6m`, site symmetry: `mm2`

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

Table 14: Wyckoff site: `12n`, site symmetry: `..m`

No.	position	mapping
1	$[x,\ 0,\ z]$	`[1,23]`
2	$[0,\ x,\ z]$	`[2,22]`
3	$[-x,\ -x,\ z]$	`[3,24]`
4	$[-x,\ 0,\ z]$	`[4,20]`
5	$[0,\ -x,\ z]$	`[5,19]`
6	$[x,\ x,\ z]$	`[6,21]`
7	$[0,\ x,\ -z]$	`[7,17]`
8	$[x,\ 0,\ -z]$	`[8,16]`
9	$[-x,\ -x,\ -z]$	`[9,18]`

continued ...

Table 14

No.	position	mapping
10	$[0,\ -x,\ -z]$	`[10,14]`
11	$[-x,\ 0,\ -z]$	`[11,13]`
12	$[x,\ x,\ -z]$	`[12,15]`

Table 15: Wyckoff site: `12o`, 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	$[-x,\ -2x,\ z]$	`[4,23]`
5	$[2x,\ x,\ z]$	`[5,22]`
6	$[-x,\ x,\ z]$	`[6,24]`
7	$[2x,\ x,\ -z]$	`[7,14]`
8	$[-x,\ -2x,\ -z]$	`[8,13]`
9	$[-x,\ x,\ -z]$	`[9,15]`
10	$[-2x,\ -x,\ -z]$	`[10,17]`
11	$[x,\ 2x,\ -z]$	`[11,16]`
12	$[x,\ -x,\ -z]$	`[12,18]`

Table 16: Wyckoff site: `12p`, site symmetry: `m..`

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

Table 17: Wyckoff site: 12q, site symmetry: m..

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

Table 18: Wyckoff site: 24r, site symmetry: 1

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