SG No. 177 D_6^1 $P622$ [hexagonal]

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

Table 1: Wyckoff site: `1a`, site symmetry: `622`

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: `622`

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

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

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

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

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

Table 6: Wyckoff site: `3f`, site symmetry: `222`

No.	position	mapping
1	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[1,4,8,11]`
2	$\left[0,\ \frac{1}{2},\ 0\right]$	`[2,5,7,10]`

3	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[3,6,9,12]`

Table 7: Wyckoff site: `3g`, site symmetry: `222`

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

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

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

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

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

Table 10: Wyckoff site: `6j`, 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	$[-x, 0, 0]$	`[4,11]`
5	$[0, -x, 0]$	`[5,10]`
6	$[x, x, 0]$	`[6,12]`

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

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

Table 12: Wyckoff site: `6l`, site symmetry: `..2`

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

Table 13: Wyckoff site: `6m`, site symmetry: `..2`

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

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	$[-x,\ -y,\ z]$	`[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]`

continued ...

Table 14

No.	position	mapping
10	$[-y, -x, -z]$	`[10]`
11	$[-x+y, y, -z]$	`[11]`
12	$[x, x-y, -z]$	`[12]`