SG No. 181 D_6^5 $P6_422$ [hexagonal]

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

Table 1: Wyckoff site: `3a`, site symmetry: `222`

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

Table 2: Wyckoff site: `3b`, site symmetry: `222`

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

Table 3: Wyckoff site: `3c`, site symmetry: `222`

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

Table 4: Wyckoff site: `3d`, site symmetry: `222`

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

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

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

continued ...

Table 5

No.	position	mapping
6	$\left[0,\ 0,\ \frac{2}{3}-z\right]$	[9,12]

Table 6: Wyckoff site: 6f, site symmetry: 2..

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

Table 7: Wyckoff site: 6g, site symmetry: .2.

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

Table 8: Wyckoff site: 6h, site symmetry: .2.

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

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

No.	position	mapping
1	$[x,\ 2x,\ 0]$	[1,11]
2	$\left[-2x,\ -x,\ \frac{1}{3}\right]$	[2,10]

continued ...

Table 9

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

Table 10: Wyckoff site: 6j, site symmetry: ..2

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

Table 11: Wyckoff site: 12k, site symmetry: 1

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