SG No. 165　$D_{3\mathrm{d}}^4$　$P\bar{3}c1$　[trigonal]

Table 1: Wyckoff site: `2a`, site symmetry: `32.`

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

Table 2: Wyckoff site: `2b`, site symmetry: `-3..`

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

Table 3: Wyckoff site: `4c`, site symmetry: `3..`

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

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

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

Table 5: Wyckoff site: `6e`, site symmetry: `-1`

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

continued ...

Table 5

No.	position	mapping
6	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[6,12]

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

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

Table 7: Wyckoff site: `12g`, site symmetry: `1`

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