SG No. 166 D_{3d}^{5} $R\bar{3}m$ [trigonal]

* plus set: $+[0,\ 0,\ 0]$, $+\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{3}\right]$, $+\left[\frac{1}{3},\ \frac{2}{3},\ \frac{2}{3}\right]$

Table 1: Wyckoff site: `3a`, site symmetry: `-3m`

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

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

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: `6c`, site symmetry: `3m`

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

Table 4: Wyckoff site: `9d`, site symmetry: `.2/m`

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

Table 5: Wyckoff site: `9e`, site symmetry: `.2/m`

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

Table 6: Wyckoff site: `18f`, site symmetry: `.2`

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

Table 7: Wyckoff site: `18g`, site symmetry: `.2`

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

Table 8: Wyckoff site: `18h`, site symmetry: `.m`

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

Table 9: Wyckoff site: `36i`, site symmetry: `1`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1]`
2	$[-y,\ x-y,\ z]$	`[2]`
3	$[-x+y,\ -x,\ z]$	`[3]`
4	$[y,\ x,\ -z]$	`[4]`
5	$[x-y,\ -y,\ -z]$	`[5]`
6	$[-x,\ -x+y,\ -z]$	`[6]`
7	$[-x,\ -y,\ -z]$	`[7]`
8	$[y,\ -x+y,\ -z]$	`[8]`
9	$[x-y,\ x,\ -z]$	`[9]`

continued ...

Table 9

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