SG No. 164 $D_{3\mathrm{d}}^3$ $P\bar{3}m1$ [trigonal]

Table 1: Wyckoff site: 1a, 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: 1b, 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: 2c, 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: 2d, site symmetry: 3m.

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

Table 5: Wyckoff site: 3e, 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: 3f, 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]

continued ...

Table 6

No.	position	mapping
3	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[3,6,9,12]

Table 7: Wyckoff site: 6g, 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 8: Wyckoff site: 6h, 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 9: Wyckoff site: 6i, 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 10: Wyckoff site: 12j, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x - y, z]$	[2]

continued ...

2

Table 10

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

$[-x + y, -x, z]$

$[y, x, -z]$

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

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