

SG No. 163  $D_{3d}^2$   $P\bar{3}1c$  [ trigonal ]

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

Table 1: Wyckoff site: 2a, site symmetry: 3.2

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

Table 2: Wyckoff site: 2b, site symmetry:  $\bar{3}$ .

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

Table 3: Wyckoff site: 2c, site symmetry: 3.2

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $\bar{3}$ .

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

Table 6: Wyckoff site: 4f, site symmetry:  $3..$ 

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

Table 7: Wyckoff site: 6g, site symmetry:  $-1$ 

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

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

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

Table 9: Wyckoff site: 12i, site symmetry:  $1$ 

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

*continued ...*

Table 9

No.	position	mapping
12	$[-x, -x + y, z + \frac{1}{2}]$	[12]