

SG No. 180  $D_6^4$   $P6_222$  [ 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	$[0, 0, \frac{2}{3}]$	$[2, 5, 7, 10]$
3	$[0, 0, \frac{1}{3}]$	$[3, 6, 9, 12]$

Table 2: Wyckoff site: **3b**, site symmetry:  $222$

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

Table 3: Wyckoff site: **3c**, site symmetry:  $222$

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

Table 4: Wyckoff site: **3d**, site symmetry:  $222$

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

Table 5: Wyckoff site: **6e**, site symmetry:  $2. .$

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

*continued ...*

Table 5

No.	position	mapping
6	$[0, 0, \frac{1}{3} - z]$	$[9, 12]$

Table 6: Wyckoff site:  $6\bar{f}$ , site symmetry:  $2..$ 

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

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

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

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

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

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

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

*continued ...*

Table 9

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

Table 10: Wyckoff site: 6j, site symmetry:  $\cdot \cdot 2$ 

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

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

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