

Table 1: Wyckoff site: 1a, site symmetry:  $6'22'$

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:  $6'22'$

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

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

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

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

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

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

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

Table 6: Wyckoff site: 3f, site symmetry:  $2'22'$

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

Table 7: Wyckoff site:  $3g$ , site symmetry:  $2'22'$ 

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

Table 8: Wyckoff site:  $4h$ , site symmetry:  $3..$ 

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

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

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

Table 10: Wyckoff site:  $6j$ , site symmetry:  $.2.$ 

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

Table 11: Wyckoff site:  $6k$ , site symmetry:  $.2.$ 

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	$[1, 4]$

*continued ...*

Table 11

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

Table 12: Wyckoff site:  $6\bar{1}$ , site symmetry:  $\bar{3}2'$ 

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

Table 13: Wyckoff site:  $6\bar{m}$ , site symmetry:  $\bar{3}2'$ 

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

Table 14: Wyckoff site:  $12\bar{n}$ , site symmetry:  $\bar{6}$ 

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

*continued ...*

Table 14

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