

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

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

Table 2: Wyckoff site: 2b, site symmetry:  $3.2'$

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

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

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

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

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

Table 5: Wyckoff site: 2e, site symmetry:  $3.2$

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

Table 6: Wyckoff site: 2f, site symmetry:  $3.2'$

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

Table 7: Wyckoff site:  $4\mathbf{g}$ , site symmetry:  $3..$ 

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

Table 8: Wyckoff site:  $4\mathbf{h}$ , site symmetry:  $3..$ 

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

Table 9: Wyckoff site:  $4\mathbf{i}$ , site symmetry:  $3..$ 

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

Table 10: Wyckoff site:  $6\mathbf{j}$ , site symmetry:  $..2$ 

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

Table 11: Wyckoff site:  $6\mathbf{k}$ , site symmetry:  $..2'$ 

No.	position	mapping
1	$[x, -x, \frac{1}{4}]$	$[1, 12]$
2	$[x, 2x, \frac{1}{4}]$	$[2, 10]$

*continued ...*

Table 11

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

Table 12: Wyckoff site: 121, site symmetry: 1

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