

Table 1: Wyckoff site: 3a, site symmetry: 222

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff site: **6f**, site symmetry:  $2..$ 

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

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

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

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

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

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

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

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

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

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

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