

Table 1: Wyckoff site: 3a, site symmetry: $2'2'2$

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

Table 2: Wyckoff site: 3b, site symmetry: $2'2'2$

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

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

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

Table 4: Wyckoff site: 3d, site symmetry: $2'2'2$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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