

Table 1: Wyckoff site: 1a, site symmetry: $62'2'$

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: $62'2'$

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	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1, 3, 5, 10, 11, 12]$
2	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[2, 4, 6, 7, 8, 9]$

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	$[1, 7]$

continued ...

Table 11

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

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

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

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

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

Table 14: Wyckoff site: 12n, site symmetry: 1

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

continued ...

Table 14

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