

Table 1: Wyckoff site: **3a**, site symmetry:  $22'2'$

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:  $22'2'$

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:  $22'2'$

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:  $22'2'$

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, 4, 7, 11]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{5}{6}]$	$[2, 5, 9, 10]$
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:  $\cdot \cdot 2'$ 

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	$[-y, -x, \frac{2}{3} - z]$	$[12]$