

Table 1: Wyckoff site: 2a, site symmetry:  $32'$  .

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

Table 2: Wyckoff site: 2b, site symmetry:  $-6'$  . .

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:  $-6'$  . .

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

Table 4: Wyckoff site: 2d, site symmetry:  $-6'$  . .

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

Table 5: Wyckoff site: 4e, site symmetry:  $3$  . .

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

Table 6: Wyckoff site: **4f**, site symmetry: **3** .

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

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

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

Table 8: Wyckoff site: **6h**, site symmetry: **m'** .

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

Table 9: Wyckoff site: **12i**, site symmetry: **1**

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

*continued ...*

Table 9

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