

Table 1: Wyckoff site: 2a, site symmetry:  $-6m2$ 

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$
2	$[0, 0, \frac{1}{2}]$	$[13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 2: Wyckoff site: 2b, site symmetry:  $-6'm2'$ 

No.	position	mapping
1	$[0, 0, \frac{1}{4}]$	$[1, 2, 3, 10, 11, 12, 16, 17, 18, 19, 20, 21]$
2	$[0, 0, \frac{3}{4}]$	$[4, 5, 6, 7, 8, 9, 13, 14, 15, 22, 23, 24]$

Table 3: Wyckoff site: 2c, site symmetry:  $-6m2$ 

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$
2	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 4: Wyckoff site: 2d, site symmetry:  $-6'm2'$ 

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[1, 2, 3, 10, 11, 12, 16, 17, 18, 19, 20, 21]$
2	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[4, 5, 6, 7, 8, 9, 13, 14, 15, 22, 23, 24]$

Table 5: Wyckoff site: 2e, site symmetry:  $-6m2$ 

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 6: Wyckoff site: 2f, site symmetry:  $-6'm2'$ 

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[1, 2, 3, 10, 11, 12, 16, 17, 18, 19, 20, 21]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[4, 5, 6, 7, 8, 9, 13, 14, 15, 22, 23, 24]$

Table 7: Wyckoff site:  $4g$ , site symmetry:  $3m$ .

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 10, 11, 12]$
2	$[0, 0, -z]$	$[4, 5, 6, 7, 8, 9]$
3	$[0, 0, z + \frac{1}{2}]$	$[13, 14, 15, 22, 23, 24]$
4	$[0, 0, \frac{1}{2} - z]$	$[16, 17, 18, 19, 20, 21]$

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

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 2, 3, 10, 11, 12]$
2	$[\frac{1}{3}, \frac{2}{3}, -z]$	$[4, 5, 6, 7, 8, 9]$
3	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	$[13, 14, 15, 22, 23, 24]$
4	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	$[16, 17, 18, 19, 20, 21]$

Table 9: Wyckoff site:  $4i$ , site symmetry:  $3m$ .

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, z]$	$[1, 2, 3, 10, 11, 12]$
2	$[\frac{2}{3}, \frac{1}{3}, -z]$	$[4, 5, 6, 7, 8, 9]$
3	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	$[13, 14, 15, 22, 23, 24]$
4	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	$[16, 17, 18, 19, 20, 21]$

Table 10: Wyckoff site:  $6j$ , site symmetry:  $mm2$ 

No.	position	mapping
1	$[x, -x, 0]$	$[1, 6, 8, 11]$
2	$[x, 2x, 0]$	$[2, 4, 9, 12]$
3	$[-2x, -x, 0]$	$[3, 5, 7, 10]$
4	$[x, -x, \frac{1}{2}]$	$[13, 18, 20, 23]$
5	$[x, 2x, \frac{1}{2}]$	$[14, 16, 21, 24]$
6	$[-2x, -x, \frac{1}{2}]$	$[15, 17, 19, 22]$

Table 11: Wyckoff site:  $6k$ , site symmetry:  $m'm2'$ 

No.	position	mapping
1	$[x, -x, \frac{1}{4}]$	$[1, 11, 18, 20]$
2	$[x, 2x, \frac{1}{4}]$	$[2, 12, 16, 21]$

*continued ...*

Table 11

No.	position	mapping
3	$[-2x, -x, \frac{1}{4}]$	[3, 10, 17, 19]
4	$[x, 2x, \frac{3}{4}]$	[4, 9, 14, 24]
5	$[-2x, -x, \frac{3}{4}]$	[5, 7, 15, 22]
6	$[x, -x, \frac{3}{4}]$	[6, 8, 13, 23]

Table 12: Wyckoff site: 12l, site symmetry:  $m..$ 

No.	position	mapping
1	$[x, y, 0]$	[1, 8]
2	$[-y, x - y, 0]$	[2, 9]
3	$[-x + y, -x, 0]$	[3, 7]
4	$[x, x - y, 0]$	[4, 12]
5	$[-x + y, y, 0]$	[5, 10]
6	$[-y, -x, 0]$	[6, 11]
7	$[x, y, \frac{1}{2}]$	[13, 20]
8	$[-y, x - y, \frac{1}{2}]$	[14, 21]
9	$[-x + y, -x, \frac{1}{2}]$	[15, 19]
10	$[x, x - y, \frac{1}{2}]$	[16, 24]
11	$[-x + y, y, \frac{1}{2}]$	[17, 22]
12	$[-y, -x, \frac{1}{2}]$	[18, 23]

Table 13: Wyckoff site: 12m, site symmetry:  $m'..$ 

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	[1, 20]
2	$[-y, x - y, \frac{1}{4}]$	[2, 21]
3	$[-x + y, -x, \frac{1}{4}]$	[3, 19]
4	$[x, x - y, \frac{3}{4}]$	[4, 24]
5	$[-x + y, y, \frac{3}{4}]$	[5, 22]
6	$[-y, -x, \frac{3}{4}]$	[6, 23]
7	$[-x + y, -x, \frac{3}{4}]$	[7, 15]
8	$[x, y, \frac{3}{4}]$	[8, 13]
9	$[-y, x - y, \frac{3}{4}]$	[9, 14]
10	$[-x + y, y, \frac{1}{4}]$	[10, 17]
11	$[-y, -x, \frac{1}{4}]$	[11, 18]
12	$[x, x - y, \frac{1}{4}]$	[12, 16]

Table 14: Wyckoff site: **12n**, site symmetry: **.m**.

No.	position	mapping
1	$[x, -x, z]$	$[1, 11]$
2	$[x, 2x, z]$	$[2, 12]$
3	$[-2x, -x, z]$	$[3, 10]$
4	$[x, 2x, -z]$	$[4, 9]$
5	$[-2x, -x, -z]$	$[5, 7]$
6	$[x, -x, -z]$	$[6, 8]$
7	$[x, -x, z + \frac{1}{2}]$	$[13, 23]$
8	$[x, 2x, z + \frac{1}{2}]$	$[14, 24]$
9	$[-2x, -x, z + \frac{1}{2}]$	$[15, 22]$
10	$[x, 2x, \frac{1}{2} - z]$	$[16, 21]$
11	$[-2x, -x, \frac{1}{2} - z]$	$[17, 19]$
12	$[x, -x, \frac{1}{2} - z]$	$[18, 20]$

Table 15: Wyckoff site: **24o**, site symmetry: **1**

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x - y, z]$	$[2]$
3	$[-x + y, -x, z]$	$[3]$
4	$[x, x - y, -z]$	$[4]$
5	$[-x + y, y, -z]$	$[5]$
6	$[-y, -x, -z]$	$[6]$
7	$[-x + y, -x, -z]$	$[7]$
8	$[x, y, -z]$	$[8]$
9	$[-y, x - y, -z]$	$[9]$
10	$[-x + y, y, z]$	$[10]$
11	$[-y, -x, z]$	$[11]$
12	$[x, x - y, z]$	$[12]$
13	$[x, y, z + \frac{1}{2}]$	$[13]$
14	$[-y, x - y, z + \frac{1}{2}]$	$[14]$
15	$[-x + y, -x, z + \frac{1}{2}]$	$[15]$
16	$[x, x - y, \frac{1}{2} - z]$	$[16]$
17	$[-x + y, y, \frac{1}{2} - z]$	$[17]$
18	$[-y, -x, \frac{1}{2} - z]$	$[18]$
19	$[-x + y, -x, \frac{1}{2} - z]$	$[19]$
20	$[x, y, \frac{1}{2} - z]$	$[20]$
21	$[-y, x - y, \frac{1}{2} - z]$	$[21]$
22	$[-x + y, y, z + \frac{1}{2}]$	$[22]$
23	$[-y, -x, z + \frac{1}{2}]$	$[23]$
24	$[x, x - y, z + \frac{1}{2}]$	$[24]$