

Table 1: Wyckoff site: 2a, site symmetry:  $-3m$ .

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 8: Wyckoff site: **6h**, site symmetry: **mm2**

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

Table 9: Wyckoff site: **12i**, site symmetry: **.2**.

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

*continued ...*

Table 9

No.	position	mapping
12	$[0, x, \frac{1}{2}]$	$[18, 24]$

Table 10: Wyckoff site: 12j, site symmetry:  $m..$ 

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

Table 11: Wyckoff site: 12k, site symmetry:  $.m.$ 

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

Table 12: Wyckoff site: 24l, site symmetry:  $1$ 

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

*continued ...*

Table 12

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