

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

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff site: **4f**, site symmetry: $3\bar{m}'$.

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

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

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

Table 8: Wyckoff site: **6h**, site symmetry: $mm'2'$

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

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

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

continued ...

Table 9

No.	position	mapping
12	$[x, x, 0]$	$[21, 24]$

Table 10: Wyckoff site: 12j, site symmetry: $\bar{m}..$

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

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

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

Table 12: Wyckoff site: 24l, site symmetry: $\bar{1}$

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x - y, z]$	$[2]$

continued ...

Table 12

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