

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

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: $-6'm'2$

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: $-6'm'2$

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: $-6'm'2$

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: $3\bar{m}'$.

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: $m'm'2$

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: $\mathbf{m}'..$

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: $\mathbf{1}$

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]