

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

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: $-6'm2'$

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	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[4, 5, 6, 7, 8, 9, 13, 14, 15, 22, 23, 24]$

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

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

Table 5: Wyckoff site: 4e, 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 6: Wyckoff site: **4f**, site symmetry: **3m**.

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 2, 3, 10, 11, 12]$
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	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	$[16, 17, 18, 19, 20, 21]$

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

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

Table 8: Wyckoff site: **6h**, site symmetry: **m'm2'**

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

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	$[-x, 0, 0]$	$[7, 10]$
5	$[0, -x, 0]$	$[8, 11]$
6	$[x, x, 0]$	$[9, 12]$
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	$[-x, -x, \frac{1}{2}]$	$[19, 22]$
11	$[x, 0, \frac{1}{2}]$	$[20, 23]$

continued ...

Table 9

No.	position	mapping
12	$[0, x, \frac{1}{2}]$	[21, 24]

Table 10: Wyckoff site: 12j, site symmetry: $m'\bar{1}$.

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	$[x - y, -y, \frac{3}{4}]$	[4, 23]
5	$[y, x, \frac{3}{4}]$	[5, 24]
6	$[-x, -x + y, \frac{3}{4}]$	[6, 22]
7	$[-x, -y, \frac{3}{4}]$	[7, 14]
8	$[y, -x + y, \frac{3}{4}]$	[8, 15]
9	$[x - y, x, \frac{3}{4}]$	[9, 13]
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 11: Wyckoff site: 12k, site symmetry: $\bar{1}m$.

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

Table 12: Wyckoff site: 241, 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	$[-x, -y, -z]$	[7]
8	$[y, -x + y, -z]$	[8]
9	$[x - y, x, -z]$	[9]
10	$[-x + y, y, z]$	[10]
11	$[-y, -x, z]$	[11]
12	$[x, x - y, z]$	[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	$[-x + y, -x, \frac{1}{2} - z]$	[19]
20	$[x, y, \frac{1}{2} - z]$	[20]
21	$[-y, x - y, \frac{1}{2} - z]$	[21]
22	$[-x, -x + y, z + \frac{1}{2}]$	[22]
23	$[x - y, -y, z + \frac{1}{2}]$	[23]
24	$[y, x, z + \frac{1}{2}]$	[24]