

Table 1: Wyckoff site: 2a, site symmetry: 6mm

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

Table 2: Wyckoff site: 4b, site symmetry: 3m.

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

Table 3: Wyckoff site: 6c, site symmetry: 2mm

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

Table 4: Wyckoff site: 12d, site symmetry: . . m

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

Table 5: Wyckoff site: $12\mathbf{e}$, site symmetry: $\bar{6}m$.

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

Table 6: Wyckoff site: $24\mathbf{f}$, site symmetry: $\bar{6}m$.

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