

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

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

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	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	$[2, 4, 6, 10, 11, 12]$
3	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	$[13, 15, 17, 19, 20, 21]$
4	$[\frac{2}{3}, \frac{1}{3}, z]$	$[14, 16, 18, 22, 23, 24]$

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

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

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

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

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

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

Table 6: Wyckoff site: $24\mathbf{f}$, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[x - y, x, z + \frac{1}{2}]$	$[2]$
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	$[-x, -x + y, z + \frac{1}{2}]$	$[10]$
11	$[x - y, -y, z + \frac{1}{2}]$	$[11]$
12	$[y, x, z + \frac{1}{2}]$	$[12]$
13	$[x, y, z + \frac{1}{2}]$	$[13]$
14	$[x - y, x, z]$	$[14]$
15	$[-y, x - y, z + \frac{1}{2}]$	$[15]$
16	$[-x, -y, z]$	$[16]$
17	$[-x + y, -x, z + \frac{1}{2}]$	$[17]$
18	$[y, -x + y, z]$	$[18]$
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	$[-x, -x + y, z]$	$[22]$
23	$[x - y, -y, z]$	$[23]$
24	$[y, x, z]$	$[24]$