

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: **12e**, site symmetry: $.m'$.

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

Table 6: Wyckoff site: **24f**, 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	$[-x + y, y, z + \frac{1}{2}]$	$[7]$
8	$[-y, -x, z + \frac{1}{2}]$	$[8]$
9	$[x, x - y, z + \frac{1}{2}]$	$[9]$
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	$[x - y, x, z]$	$[14]$
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	$[-x + y, y, z]$	$[19]$
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	$[y, x, z + \frac{1}{2}]$	$[24]$