

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]