

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

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

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	$[\frac{2}{3}, \frac{1}{3}, z]$	$[2, 4, 6, 22, 23, 24]$
3	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	$[7, 8, 9, 13, 15, 17]$
4	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	$[10, 11, 12, 14, 16, 18]$

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

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

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

No.	position	mapping
1	$[x, 0, z]$	$[1, 23]$
2	$[x, x, z]$	$[2, 21]$
3	$[0, x, z]$	$[3, 24]$
4	$[-x, 0, z]$	$[4, 19]$
5	$[-x, -x, z]$	$[5, 22]$
6	$[0, -x, z]$	$[6, 20]$
7	$[-x, 0, z + \frac{1}{2}]$	$[7, 16]$
8	$[0, -x, z + \frac{1}{2}]$	$[8, 18]$
9	$[x, x, z + \frac{1}{2}]$	$[9, 14]$
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:  $12e$ , site symmetry:  $.m'$ .

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

Table 6: Wyckoff site:  $24f$ , site symmetry:  $1$ 

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	$[-x + y, y, z + \frac{1}{2}]$	[7]
8	$[-y, -x, z + \frac{1}{2}]$	[8]
9	$[x, x - y, z + \frac{1}{2}]$	[9]
10	$[-x, -x + y, z + \frac{1}{2}]$	[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	$[x - y, x, z + \frac{1}{2}]$	[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	$[-x + y, y, z]$	[19]
20	$[-y, -x, z]$	[20]
21	$[x, x - y, z]$	[21]
22	$[-x, -x + y, z]$	[22]
23	$[x - y, -y, z]$	[23]
24	$[y, x, z]$	[24]