

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: 12e, site symmetry: .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: 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	$[-x + y, y, z]$	[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]