

Table 1: Wyckoff site: **6a**, site symmetry: $3m$.

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 5, 6]$
2	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}]$	$[7, 8, 9, 10, 11, 12]$
3	$[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}]$	$[13, 14, 15, 16, 17, 18]$
4	$[0, 0, z + \frac{1}{2}]$	$[19, 20, 21, 22, 23, 24]$
5	$[\frac{2}{3}, \frac{1}{3}, z + \frac{5}{6}]$	$[25, 26, 27, 28, 29, 30]$
6	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{6}]$	$[31, 32, 33, 34, 35, 36]$

Table 2: Wyckoff site: **18b**, site symmetry: $\bar{6}m$.

No.	position	mapping
1	$[x, -x, z]$	$[1, 5]$
2	$[x, 2x, z]$	$[2, 6]$
3	$[-2x, -x, z]$	$[3, 4]$
4	$[x + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$	$[7, 11]$
5	$[x + \frac{2}{3}, 2x + \frac{1}{3}, z + \frac{1}{3}]$	$[8, 12]$
6	$[\frac{2}{3} - 2x, \frac{1}{3} - x, z + \frac{1}{3}]$	$[9, 10]$
7	$[x + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$	$[13, 17]$
8	$[x + \frac{1}{3}, 2x + \frac{2}{3}, z + \frac{2}{3}]$	$[14, 18]$
9	$[\frac{1}{3} - 2x, \frac{2}{3} - x, z + \frac{2}{3}]$	$[15, 16]$
10	$[x, -x, z + \frac{1}{2}]$	$[19, 23]$
11	$[x, 2x, z + \frac{1}{2}]$	$[20, 24]$
12	$[-2x, -x, z + \frac{1}{2}]$	$[21, 22]$
13	$[x + \frac{2}{3}, \frac{1}{3} - x, z + \frac{5}{6}]$	$[25, 29]$
14	$[x + \frac{2}{3}, 2x + \frac{1}{3}, z + \frac{5}{6}]$	$[26, 30]$
15	$[\frac{2}{3} - 2x, \frac{1}{3} - x, z + \frac{5}{6}]$	$[27, 28]$
16	$[x + \frac{1}{3}, \frac{2}{3} - x, z + \frac{1}{6}]$	$[31, 35]$
17	$[x + \frac{1}{3}, 2x + \frac{2}{3}, z + \frac{1}{6}]$	$[32, 36]$
18	$[\frac{1}{3} - 2x, \frac{2}{3} - x, z + \frac{1}{6}]$	$[33, 34]$

Table 3: Wyckoff site: **36c**, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x - y, z]$	$[2]$
3	$[-x + y, -x, z]$	$[3]$
4	$[-x + y, y, z]$	$[4]$
5	$[-y, -x, z]$	$[5]$
6	$[x, x - y, z]$	$[6]$
7	$[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	$[7]$

continued ...

Table 3

No.	position	mapping
8	$[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{1}{3}]$	[8]
9	$[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$	[9]
10	$[-x + y + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	[10]
11	$[\frac{2}{3} - y, \frac{1}{3} - x, z + \frac{1}{3}]$	[11]
12	$[x + \frac{2}{3}, x - y + \frac{1}{3}, z + \frac{1}{3}]$	[12]
13	$[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	[13]
14	$[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{2}{3}]$	[14]
15	$[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$	[15]
16	$[-x + y + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	[16]
17	$[\frac{1}{3} - y, \frac{2}{3} - x, z + \frac{2}{3}]$	[17]
18	$[x + \frac{1}{3}, x - y + \frac{2}{3}, z + \frac{2}{3}]$	[18]
19	$[x, y, z + \frac{1}{2}]$	[19]
20	$[-y, x - y, z + \frac{1}{2}]$	[20]
21	$[-x + y, -x, z + \frac{1}{2}]$	[21]
22	$[-x + y, y, z + \frac{1}{2}]$	[22]
23	$[-y, -x, z + \frac{1}{2}]$	[23]
24	$[x, x - y, z + \frac{1}{2}]$	[24]
25	$[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{5}{6}]$	[25]
26	$[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{5}{6}]$	[26]
27	$[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{5}{6}]$	[27]
28	$[-x + y + \frac{2}{3}, y + \frac{1}{3}, z + \frac{5}{6}]$	[28]
29	$[\frac{2}{3} - y, \frac{1}{3} - x, z + \frac{5}{6}]$	[29]
30	$[x + \frac{2}{3}, x - y + \frac{1}{3}, z + \frac{5}{6}]$	[30]
31	$[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{1}{6}]$	[31]
32	$[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{1}{6}]$	[32]
33	$[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{1}{6}]$	[33]
34	$[-x + y + \frac{1}{3}, y + \frac{2}{3}, z + \frac{1}{6}]$	[34]
35	$[\frac{1}{3} - y, \frac{2}{3} - x, z + \frac{1}{6}]$	[35]
36	$[x + \frac{1}{3}, x - y + \frac{2}{3}, z + \frac{1}{6}]$	[36]