

Table 1: Wyckoff site: 6a, site symmetry: $3\bar{m}'$.

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

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

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

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	$[-x + y, y, z + \frac{1}{2}]$	$[4]$
5	$[-y, -x, z + \frac{1}{2}]$	$[5]$
6	$[x, x - y, z + \frac{1}{2}]$	$[6]$
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	$[-x + y + \frac{2}{3}, y + \frac{1}{3}, z + \frac{5}{6}]$	[10]
11	$[\frac{2}{3} - y, \frac{1}{3} - x, z + \frac{5}{6}]$	[11]
12	$[x + \frac{2}{3}, x - y + \frac{1}{3}, z + \frac{5}{6}]$	[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	$[-x + y + \frac{1}{3}, y + \frac{2}{3}, z + \frac{1}{6}]$	[16]
17	$[\frac{1}{3} - y, \frac{2}{3} - x, z + \frac{1}{6}]$	[17]
18	$[x + \frac{1}{3}, x - y + \frac{2}{3}, z + \frac{1}{6}]$	[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	$[-x + y, y, z]$	[22]
23	$[-y, -x, z]$	[23]
24	$[x, x - y, z]$	[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	$[-x + y + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	[28]
29	$[\frac{2}{3} - y, \frac{1}{3} - x, z + \frac{1}{3}]$	[29]
30	$[x + \frac{2}{3}, x - y + \frac{1}{3}, z + \frac{1}{3}]$	[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	$[-x + y + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	[34]
35	$[\frac{1}{3} - y, \frac{2}{3} - x, z + \frac{2}{3}]$	[35]
36	$[x + \frac{1}{3}, x - y + \frac{2}{3}, z + \frac{2}{3}]$	[36]