

Table 1: Wyckoff site: 6a, site symmetry: $\bar{3}2$.

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

Table 2: Wyckoff site: 6b, site symmetry: $\bar{3}2'$.

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

Table 3: Wyckoff site: 12c, site symmetry: $\bar{3}..$

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

Table 4: Wyckoff site: 18d, site symmetry: $.2$.

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

Table 5: Wyckoff site: 18e, site symmetry: $.2'$.

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

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