

Table 1: Wyckoff site: 6a, site symmetry: $32'$.

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

Table 2: Wyckoff site: 6b, site symmetry: -3 .

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

Table 3: Wyckoff site: 12c, site symmetry: 3 .

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

Table 4: Wyckoff site: **18d**, site symmetry: -1

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

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

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

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	$[-x, -y, -z]$	[4]
5	$[y, -x + y, -z]$	[5]
6	$[x - y, x, -z]$	[6]
7	$[x - y, -y, \frac{1}{2} - z]$	[7]
8	$[y, x, \frac{1}{2} - z]$	[8]
9	$[-x, -x + y, \frac{1}{2} - z]$	[9]
10	$[-x + y, y, z + \frac{1}{2}]$	[10]
11	$[-y, -x, z + \frac{1}{2}]$	[11]
12	$[x, x - y, z + \frac{1}{2}]$	[12]
13	$[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	[13]
14	$[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{1}{3}]$	[14]
15	$[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$	[15]
16	$[\frac{2}{3} - x, \frac{1}{3} - y, \frac{1}{3} - z]$	[16]
17	$[y + \frac{2}{3}, -x + y + \frac{1}{3}, \frac{1}{3} - z]$	[17]
18	$[x - y + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{3} - z]$	[18]
19	$[x - y + \frac{2}{3}, \frac{1}{3} - y, \frac{5}{6} - z]$	[19]
20	$[y + \frac{2}{3}, x + \frac{1}{3}, \frac{5}{6} - z]$	[20]
21	$[\frac{2}{3} - x, -x + y + \frac{1}{3}, \frac{5}{6} - z]$	[21]
22	$[-x + y + \frac{2}{3}, y + \frac{1}{3}, z + \frac{5}{6}]$	[22]
23	$[\frac{2}{3} - y, \frac{1}{3} - x, z + \frac{5}{6}]$	[23]
24	$[x + \frac{2}{3}, x - y + \frac{1}{3}, z + \frac{5}{6}]$	[24]
25	$[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	[25]
26	$[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{2}{3}]$	[26]
27	$[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$	[27]
28	$[\frac{1}{3} - x, \frac{2}{3} - y, \frac{2}{3} - z]$	[28]
29	$[y + \frac{1}{3}, -x + y + \frac{2}{3}, \frac{2}{3} - z]$	[29]
30	$[x - y + \frac{1}{3}, x + \frac{2}{3}, \frac{2}{3} - z]$	[30]
31	$[x - y + \frac{1}{3}, \frac{2}{3} - y, \frac{1}{6} - z]$	[31]
32	$[y + \frac{1}{3}, x + \frac{2}{3}, \frac{1}{6} - z]$	[32]
33	$[\frac{1}{3} - x, -x + y + \frac{2}{3}, \frac{1}{6} - z]$	[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]