

Table 1: Wyckoff site: 8a, site symmetry: $-4..$

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

Table 2: Wyckoff site: 8b, site symmetry: $2.2'2'$

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

Table 3: Wyckoff site: 16c, site symmetry: -1

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

continued ...

Table 3

No.	position	mapping
16	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[28,32]

Table 4: Wyckoff site: 16d, site symmetry: $2..$

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

Table 5: Wyckoff site: 16e, site symmetry: $.2'$

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

Table 6: Wyckoff site: 16f, site symmetry: $\dots 2'$

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

Table 7: Wyckoff site: 32g, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[\frac{1}{4} - y, x + \frac{3}{4}, z + \frac{1}{4}]$	[2]
3	$[y + \frac{3}{4}, \frac{3}{4} - x, z + \frac{1}{4}]$	[3]
4	$[-x, \frac{1}{2} - y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[y + \frac{3}{4}, \frac{1}{4} - x, \frac{3}{4} - z]$	[6]
7	$[\frac{1}{4} - y, x + \frac{1}{4}, \frac{3}{4} - z]$	[7]
8	$[x, y + \frac{1}{2}, -z]$	[8]
9	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[9]
10	$[\frac{1}{2} - x, y, -z]$	[10]
11	$[y + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{4} - z]$	[11]
12	$[\frac{1}{4} - y, \frac{1}{4} - x, \frac{1}{4} - z]$	[12]
13	$[-x, y, z + \frac{1}{2}]$	[13]
14	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[14]
15	$[\frac{3}{4} - y, \frac{1}{4} - x, z + \frac{1}{4}]$	[15]
16	$[y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}]$	[16]
17	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[17]
18	$[\frac{3}{4} - y, x + \frac{1}{4}, z + \frac{3}{4}]$	[18]
19	$[y + \frac{1}{4}, \frac{1}{4} - x, z + \frac{3}{4}]$	[19]
20	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[20]
21	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[21]
22	$[y + \frac{1}{4}, \frac{3}{4} - x, \frac{1}{4} - z]$	[22]
23	$[\frac{3}{4} - y, x + \frac{3}{4}, \frac{1}{4} - z]$	[23]

continued ...

Table 7

No.	position	mapping
24	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[24]
25	$[x, -y, \frac{1}{2} - z]$	[25]
26	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[26]
27	$[y + \frac{1}{4}, x + \frac{3}{4}, \frac{3}{4} - z]$	[27]
28	$[\frac{3}{4} - y, \frac{3}{4} - x, \frac{3}{4} - z]$	[28]
29	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[29]
30	$[x + \frac{1}{2}, -y, z]$	[30]
31	$[\frac{1}{4} - y, \frac{3}{4} - x, z + \frac{3}{4}]$	[31]
32	$[y + \frac{3}{4}, x + \frac{3}{4}, z + \frac{3}{4}]$	[32]