

Table 1: Wyckoff site: 8a, site symmetry: 222

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

Table 2: Wyckoff site: 8b, site symmetry: 222

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

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

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

*continued ...*

Table 3

No.	position	mapping
16	$[\frac{1}{2}, \frac{1}{2}, 0]$	[25, 29]

Table 4: Wyckoff site: 16d, site symmetry:  $-1'$ 

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

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

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

Table 6: Wyckoff site: 16f, site symmetry:  $.2.$ 

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

Table 7: Wyckoff site: 16g, site symmetry:  $..2$ 

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

Table 8: Wyckoff site: 32h, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]

*continued ...*

Table 8

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