

Table 1: Wyckoff site: 8a, site symmetry:  $2'2'2$

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

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

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

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

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

*continued ...*

Table 3

No.	position	mapping
16	$[\frac{1}{2}, \frac{1}{2}, 0]$	[25, 27]

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

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

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

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

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

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

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

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

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

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

*continued ...*

Table 8

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