

Table 1: Wyckoff site: 4a, site symmetry:  $-4m2$ 

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

Table 2: Wyckoff site: 4b, site symmetry:  $-4m2$ 

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

Table 3: Wyckoff site: 8c, site symmetry:  $.2/m.$ 

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

Table 4: Wyckoff site: 8d, site symmetry:  $.2/m.$ 

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

Table 5: Wyckoff site: **8e**, site symmetry: **2mm**.

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

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

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

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

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

*continued ...*

Table 7

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

Table 8: Wyckoff site: **16h**, site symmetry: **.m**.

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

Table 9: Wyckoff site: **32i**, 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	$[x, -y, -z]$	[4]
5	$[-x, y + \frac{1}{2}, -z]$	[5]
6	$[-x, \frac{1}{2} - y, z]$	[6]
7	$[y + \frac{3}{4}, x + \frac{1}{4}, \frac{3}{4} - z]$	[7]
8	$[\frac{1}{4} - y, \frac{1}{4} - x, \frac{3}{4} - z]$	[8]
9	$[-x, -y, -z]$	[9]
10	$[y + \frac{3}{4}, \frac{1}{4} - x, \frac{3}{4} - z]$	[10]
11	$[\frac{1}{4} - y, x + \frac{1}{4}, \frac{3}{4} - z]$	[11]

*continued ...*

Table 9

No.	position	mapping
12	$[-x, y, z]$	[12]
13	$[x, \frac{1}{2} - y, z]$	[13]
14	$[x, y + \frac{1}{2}, -z]$	[14]
15	$[\frac{1}{4} - y, \frac{3}{4} - x, z + \frac{1}{4}]$	[15]
16	$[y + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}]$	[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	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[20]
21	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[21]
22	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[22]
23	$[y + \frac{1}{4}, x + \frac{3}{4}, \frac{1}{4} - z]$	[23]
24	$[\frac{3}{4} - y, \frac{3}{4} - x, \frac{1}{4} - z]$	[24]
25	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[25]
26	$[y + \frac{1}{4}, \frac{3}{4} - x, \frac{1}{4} - z]$	[26]
27	$[\frac{3}{4} - y, x + \frac{3}{4}, \frac{1}{4} - z]$	[27]
28	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[28]
29	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[29]
30	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[30]
31	$[\frac{3}{4} - y, \frac{1}{4} - x, z + \frac{3}{4}]$	[31]
32	$[y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{3}{4}]$	[32]