

Table 1: Wyckoff site: 4a, site symmetry: $m'm'm$

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

Table 2: Wyckoff site: 4b, site symmetry: $m'm'm$

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

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: $\dots 2/m$

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

Table 6: Wyckoff site: 8f, site symmetry: 222

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

Table 7: Wyckoff site: 8g, site symmetry: $2'm'm$

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

Table 8: Wyckoff site: 8h, site symmetry: $m'2'm$

No.	position	mapping
1	$[\frac{3}{4}, y, 0]$	$[1, 8, 27, 30]$
2	$[\frac{3}{4}, -y, \frac{1}{2}]$	$[2, 7, 28, 29]$
3	$[\frac{1}{4}, y, \frac{1}{2}]$	$[3, 6, 25, 32]$

continued ...

Table 8

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

Table 9: Wyckoff site: 8i, site symmetry: $m'm'2$

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

Table 10: Wyckoff site: 16j, site symmetry: $\dots 2$

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

Table 11: Wyckoff site: 16k, site symmetry: .2.

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

Table 12: Wyckoff site: 16l, site symmetry: 2..

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

Table 13: Wyckoff site: 16m, site symmetry: m'..

No.	position	mapping
1	$[\frac{3}{4}, y, z]$	[1, 30]

continued ...

Table 13

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

Table 14: Wyckoff site: **16n**, site symmetry: $.m'$.

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

Table 15: Wyckoff site: **16o**, site symmetry: $..m$

No.	position	mapping
1	$[x, y, 0]$	[1,8]
2	$[x, -y, \frac{1}{2}]$	[2,7]
3	$[-x, y, \frac{1}{2}]$	[3,6]

continued ...

Table 15

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

Table 16: Wyckoff site: **32p**, site symmetry: **1**

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

continued ...

Table 16

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