

Table 1: Wyckoff site: 4a, site symmetry:  $\overline{4}m'$ .

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

Table 2: Wyckoff site: 4b, site symmetry:  $\overline{4}m'2$ 

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

Table 3: Wyckoff site: 4c, site symmetry:  $\overline{4}m'$ .

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

Table 4: Wyckoff site: 4d, site symmetry:  $\overline{4}m'2'$ 

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

Table 5: Wyckoff site: 8e, site symmetry:  $2.22$ 

No.	position	mapping
1	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	$[1, 8, 22, 23]$
2	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[2, 4, 19, 21]$

*continued ...*

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry:  $2'/m$ .

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

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

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

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

No.	position	mapping
1	$[0, 0, z]$	[1, 6, 28, 29]
2	$[0, 0, z + \frac{1}{2}]$	[2, 3, 31, 32]
3	$[\frac{1}{2}, \frac{1}{2}, -z]$	[4, 5, 25, 30]
4	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[7, 8, 26, 27]
5	$[0, 0, -z]$	[9, 14, 20, 21]

*continued ...*

Table 8

No.	position	mapping
6	$[0, 0, \frac{1}{2} - z]$	$[10, 11, 23, 24]$
7	$[\frac{1}{2}, \frac{1}{2}, z]$	$[12, 13, 17, 22]$
8	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[15, 16, 18, 19]$

Table 9: Wyckoff site: 8i, site symmetry:  $\text{mm}'2'$ .

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

Table 10: Wyckoff site: 8j, site symmetry:  $\text{mm}'2'$ .

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

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

No.	position	mapping
1	$[\frac{3}{4}, \frac{3}{4}, z]$	$[1, 22]$
2	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	$[2, 19]$
3	$[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$	$[3, 18]$
4	$[\frac{1}{4}, \frac{3}{4}, -z]$	$[4, 21]$
5	$[\frac{3}{4}, \frac{1}{4}, -z]$	$[5, 20]$
6	$[\frac{1}{4}, \frac{1}{4}, z]$	$[6, 17]$
7	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - z]$	$[7, 24]$
8	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	$[8, 23]$

continued ...

Table 11

No.	position	mapping
9	$[\frac{1}{4}, \frac{1}{4}, -z]$	[9,30]
10	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[10,27]
11	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[11,26]
12	$[\frac{3}{4}, \frac{1}{4}, z]$	[12,29]
13	$[\frac{1}{4}, \frac{3}{4}, z]$	[13,28]
14	$[\frac{3}{4}, \frac{3}{4}, -z]$	[14,25]
15	$[\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[15,32]
16	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[16,31]

Table 12: Wyckoff site: 16l, site symmetry:  $\dots 2$ 

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

Table 13: Wyckoff site: 16m, site symmetry:  $\dots 2'$ 

No.	position	mapping
1	$[x, x, \frac{1}{4}]$	[1,23]
2	$[-x, x, \frac{3}{4}]$	[2,21]
3	$[x, -x, \frac{3}{4}]$	[3,20]
4	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	[4,19]
5	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}]$	[5,18]
6	$[-x, -x, \frac{1}{4}]$	[6,24]
7	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[7,17]
8	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{4}]$	[8,22]
9	$[-x, -x, \frac{3}{4}]$	[9,31]
10	$[x, -x, \frac{1}{4}]$	[10,29]

*continued ...*

Table 13

No.	position	mapping
11	$[-x, x, \frac{1}{4}]$	[11,28]
12	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{4}]$	[12,27]
13	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$	[13,26]
14	$[x, x, \frac{3}{4}]$	[14,32]
15	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{3}{4}]$	[15,25]
16	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}]$	[16,30]

Table 14: Wyckoff site: 16n, site symmetry:  $\bar{m}$ .

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

Table 15: Wyckoff site: 16o, site symmetry:  $\bar{m}'$ .

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

*continued ...*

Table 15

No.	position	mapping
13	$[\frac{1}{2}, \frac{1}{2} - y, z]$	[13, 22]
14	$[0, y, -z]$	[14, 21]
15	$[\frac{1}{2} - y, \frac{1}{2}, z + \frac{1}{2}]$	[15, 18]
16	$[y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[16, 19]

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

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