

Table 1: Wyckoff site: 2a, site symmetry:  $4/m'm'm'$ 

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

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

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

Table 3: Wyckoff site: 4c, site symmetry:  $m'm'm'$ .

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

Table 4: Wyckoff site: 4d, site symmetry:  $-4'm'2$ 

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

Table 5: Wyckoff site: 4e, site symmetry:  $4m'm'$ 

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, 0, 0]$	[1, 4, 13, 14]
2	$[0, x, 0]$	[2, 7, 11, 16]
3	$[0, -x, 0]$	[3, 8, 10, 15]

*continued ...*

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry:  $m'2m'$ .

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

Table 11: Wyckoff site: 16k, site symmetry:  $\dots 2$ 

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

Table 12: Wyckoff site:  $16\bar{1}$ , site symmetry:  $m'..$ 

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

Table 13: Wyckoff site:  $16\bar{m}$ , site symmetry:  $..m'$ 

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

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

No.	position	mapping
1	$[0, y, z]$	$[1, 12]$

*continued ...*

Table 14

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

Table 15: Wyckoff site: **32o**, site symmetry: 1

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

continued ...

Table 15

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