

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

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: $4/mm'm'$

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: $mm'm'$.

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

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

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

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

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

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, 21, 28]
2	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[2, 13, 22, 25]
3	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[3, 14, 23, 26]
4	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[4, 15, 24, 27]
5	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[5, 12, 17, 32]
6	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[6, 9, 18, 29]
7	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[7, 10, 19, 30]
8	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[8, 11, 20, 31]

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

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: $m2'm'$

No.	position	mapping
1	$[x, 0, 0]$	[1, 8, 9, 14]
2	$[0, x, 0]$	[2, 7, 11, 16]
3	$[0, -x, 0]$	[3, 6, 12, 15]

continued ...

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry: $m2'm'$.

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0, y, z]$	$[1, 13]$

continued ...

Table 14

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

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	$[y, -x, -z]$	[6]
7	$[-y, x, -z]$	[7]
8	$[x, y, -z]$	[8]
9	$[x, -y, -z]$	[9]
10	$[-x, y, -z]$	[10]
11	$[y, x, -z]$	[11]
12	$[-y, -x, -z]$	[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	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[20]
21	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[21]
22	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[22]
23	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[23]
24	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[24]
25	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[25]

continued ...

Table 15

No.	position	mapping
26	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[26]
27	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[27]
28	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[28]
29	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[29]
30	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[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]