

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	$[0, \frac{1}{2}, 0]$	$[1, 2, 3, 4, 13, 14, 15, 16]$
2	$[\frac{1}{2}, 0, 0]$	$[5, 6, 7, 8, 9, 10, 11, 12]$
3	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[17, 18, 19, 20, 29, 30, 31, 32]$
4	$[0, \frac{1}{2}, \frac{1}{2}]$	$[21, 22, 23, 24, 25, 26, 27, 28]$

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

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

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

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

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

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

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

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

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, 5, 10, 15]
3	$[-x, x, 0]$	[3, 6, 9, 14]
4	$[-x, -x, 0]$	[4, 7, 12, 13]
5	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[17, 24, 27, 32]
6	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[18, 21, 26, 31]
7	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]$	[19, 22, 25, 30]
8	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[20, 23, 28, 29]

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

No.	position	mapping
1	$[x, 0, 0]$	[1, 2, 15, 16]
2	$[-x, 0, 0]$	[3, 4, 13, 14]
3	$[0, -x, 0]$	[5, 7, 10, 12]

continued ...

Table 9

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

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

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

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

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

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

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

Table 13: Wyckoff site: $16m$, site symmetry: $\bar{1}..m$.

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

Table 14: Wyckoff site: $16n$, site symmetry: $\bar{1}.m'$.

No.	position	mapping
1	$[0, y, z]$	$[1, 14]$

continued ...

Table 14

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

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

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

continued ...

Table 15

No.	position	mapping
26	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[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	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[29]
30	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[30]
31	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[31]
32	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[32]