

Table 1: Wyckoff site: 4a, site symmetry: $42'2'$

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

Table 2: Wyckoff site: 4b, site symmetry: 422

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

Table 3: Wyckoff site: 4c, site symmetry: $-42'm'$

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: $..2'/m'$

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	[1, 9, 23, 31]
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	[2, 10, 21, 29]

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: 8g, site symmetry: $4\dots$

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

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

No.	position	mapping
1	$[\frac{3}{4}, \frac{1}{4}, z]$	[1, 6, 31, 32]
2	$[\frac{1}{4}, \frac{3}{4}, z]$	[2, 3, 28, 29]
3	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[4, 5, 26, 27]
4	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[7, 8, 25, 30]
5	$[\frac{1}{4}, \frac{3}{4}, -z]$	[9, 14, 23, 24]

continued ...

Table 8

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

Table 9: Wyckoff site: 16i, site symmetry: $\dots 2'$

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

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

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

continued ...

Table 10

No.	position	mapping
16	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}]$	[30, 32]

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

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

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

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

Table 13: Wyckoff site: **16m**, site symmetry: $\cdot \cdot m$

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

Table 14: Wyckoff site: **32n**, site symmetry: 1

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

continued ...

Table 14

No.	position	mapping
24	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[24]
25	$[-x, -y, \frac{1}{2} - z]$	[25]
26	$[y + \frac{1}{2}, -x, \frac{1}{2} - z]$	[26]
27	$[-y, x + \frac{1}{2}, \frac{1}{2} - z]$	[27]
28	$[-x, y + \frac{1}{2}, z]$	[28]
29	$[x + \frac{1}{2}, -y, z]$	[29]
30	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[30]
31	$[-y, -x, z]$	[31]
32	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[32]