

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[1, 7, 22, 24]
2	$[0, \frac{1}{2}, \frac{1}{4}]$	[2, 5, 19, 20]

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

No.	position	mapping
6	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[10, 11, 23, 24]
7	$[\frac{1}{4}, \frac{1}{4}, z]$	[12, 13, 17, 22]
8	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[15, 16, 18, 19]

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, z]$	[1, 22]
2	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[2, 19]
3	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[3, 18]
4	$[\frac{1}{2}, 0, -z]$	[4, 21]
5	$[0, \frac{1}{2}, -z]$	[5, 20]
6	$[0, 0, z]$	[6, 17]
7	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[7, 24]
8	$[0, 0, \frac{1}{2} - z]$	[8, 23]

continued ...

Table 11

No.	position	mapping
9	$[\frac{1}{2}, \frac{1}{2}, -z]$	[9,30]
10	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[10,27]
11	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[11,26]
12	$[\frac{1}{2}, 0, z]$	[12,29]
13	$[0, \frac{1}{2}, z]$	[13,28]
14	$[0, 0, -z]$	[14,25]
15	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[15,32]
16	$[0, 0, z + \frac{1}{2}]$	[16,31]

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

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

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

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

continued ...

Table 13

No.	position	mapping
11	$[x + \frac{1}{2}, -x, \frac{1}{4}]$	[19,20]
12	$[-x, -x, \frac{3}{4}]$	[22,24]
13	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{4}]$	[25,31]
14	$[x, \frac{1}{2} - x, \frac{3}{4}]$	[26,29]
15	$[\frac{1}{2} - x, x, \frac{3}{4}]$	[27,28]
16	$[x, x, \frac{1}{4}]$	[30,32]

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

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

Table 15: Wyckoff site: 16o, site symmetry: $.m'$.

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

continued ...

Table 15

No.	position	mapping
13	$[\frac{1}{4}, -y, z]$	[13,22]
14	$[\frac{1}{4}, y + \frac{1}{2}, -z]$	[14,21]
15	$[-y, \frac{1}{4}, z + \frac{1}{2}]$	[15,18]
16	$[y + \frac{1}{2}, \frac{1}{4}, z + \frac{1}{2}]$	[16,19]

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

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