

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $42'2'$

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

Table 4: Wyckoff site: 4d, site symmetry: $4/m..$

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

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

No.	position	mapping
1	$[\frac{3}{4}, \frac{3}{4}, 0]$	[1, 14, 22, 25]
2	$[\frac{1}{4}, \frac{3}{4}, 0]$	[2, 11, 19, 26]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 2.22

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

Table 7: Wyckoff site: 8g, site symmetry: 4' . .

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

Table 8: Wyckoff site: 8h, site symmetry: 4. .

No.	position	mapping
1	$[0, 0, z]$	[1, 2, 3, 6]
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[4, 5, 7, 8]
3	$[0, 0, -z]$	[9, 10, 11, 14]
4	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[12, 13, 15, 16]
5	$[\frac{1}{2}, \frac{1}{2}, z]$	[17, 18, 19, 22]

continued ...

Table 8

No.	position	mapping
6	$[0, 0, \frac{1}{2} - z]$	$[20, 21, 23, 24]$
7	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[25, 26, 27, 30]$
8	$[0, 0, z + \frac{1}{2}]$	$[28, 29, 31, 32]$

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

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

Table 10: Wyckoff site: $16j$, site symmetry: $.2'.$

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

continued ...

Table 10

No.	position	mapping
16	$[y + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[16,26]

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

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

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

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

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

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

Table 14: Wyckoff site: $32\mathbf{n}$, site symmetry: $\mathbf{1}$

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

continued ...

Table 14

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