

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: $4..$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 6]$
2	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[4, 5, 7, 8]$

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: $2.mm$

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

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

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

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

No.	position	mapping
1	$[x, x + \frac{1}{2}, \frac{1}{4}]$	$[1, 16, 23, 30]$
2	$[\frac{1}{2} - x, x, \frac{1}{4}]$	$[2, 12, 21, 27]$
3	$[x + \frac{1}{2}, -x, \frac{1}{4}]$	$[3, 13, 20, 26]$
4	$[x + \frac{1}{2}, -x, \frac{3}{4}]$	$[4, 10, 19, 29]$
5	$[\frac{1}{2} - x, x, \frac{3}{4}]$	$[5, 11, 18, 28]$

continued ...

Table 8

No.	position	mapping
6	$[-x, \frac{1}{2} - x, \frac{1}{4}]$	[6, 15, 24, 25]
7	$[x, x + \frac{1}{2}, \frac{3}{4}]$	[7, 14, 17, 32]
8	$[-x, \frac{1}{2} - x, \frac{3}{4}]$	[8, 9, 22, 31]

Table 9: Wyckoff site: 16i, site symmetry: $m..$

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

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

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

continued ...

Table 10

No.	position	mapping
16	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[16, 23]

Table 11: Wyckoff site: 16k, site symmetry: $\bar{3}m$

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

Table 12: Wyckoff site: 321, site symmetry: 1

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

continued ...

Table 12

No.	position	mapping
18	$[-y, x, z + \frac{1}{2}]$	[18]
19	$[y, -x, z + \frac{1}{2}]$	[19]
20	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[20]
21	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[21]
22	$[-x, -y, z + \frac{1}{2}]$	[22]
23	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[23]
24	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[24]
25	$[-x, -y, \frac{1}{2} - z]$	[25]
26	$[y, -x, \frac{1}{2} - z]$	[26]
27	$[-y, x, \frac{1}{2} - z]$	[27]
28	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[28]
29	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[29]
30	$[x, y, \frac{1}{2} - z]$	[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]