

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

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

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

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

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

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

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

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

continued ...

Table 5

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

Table 6: Wyckoff site: **8f**, site symmetry: $2.\mathbf{m}'\mathbf{m}'$

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

Table 7: Wyckoff site: **8g**, site symmetry: $\mathbf{m}.2'\mathbf{m}'$

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

Table 8: Wyckoff site: **8h**, site symmetry: $\mathbf{m}'.2\mathbf{m}'$

No.	position	mapping
1	$[x, x + \frac{1}{2}, \frac{1}{4}]$	$[1, 7, 30, 32]$
2	$[\frac{1}{2} - x, x, \frac{1}{4}]$	$[2, 5, 27, 28]$
3	$[x + \frac{1}{2}, -x, \frac{1}{4}]$	$[3, 4, 26, 29]$
4	$[-x, \frac{1}{2} - x, \frac{1}{4}]$	$[6, 8, 25, 31]$
5	$[-x, \frac{1}{2} - x, \frac{3}{4}]$	$[9, 15, 22, 24]$

continued ...

Table 8

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

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

continued ...

Table 10

No.	position	mapping
16	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}]$	[16,23]

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

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

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	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[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	$[x, y, z + \frac{1}{2}]$	[17]

continued ...

Table 12

No.	position	mapping
18	$[-y, x, z + \frac{1}{2}]$	[18]
19	$[y, -x, z + \frac{1}{2}]$	[19]
20	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[20]
21	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[21]
22	$[-x, -y, z + \frac{1}{2}]$	[22]
23	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[23]
24	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[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	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[28]
29	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[29]
30	$[x, y, \frac{1}{2} - z]$	[30]
31	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[31]
32	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[32]