

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

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

Table 2: Wyckoff site: 4b, site symmetry: $\bar{4}'2'm$

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

Table 3: Wyckoff site: 4c, 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	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[17, 18, 19, 22, 25, 26, 27, 30]$
4	$[0, 0, \frac{1}{2}]$	$[20, 21, 23, 24, 28, 29, 31, 32]$

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	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[17, 22, 23, 24, 25, 30, 31, 32]$
4	$[0, \frac{1}{2}, \frac{1}{2}]$	$[18, 19, 20, 21, 26, 27, 28, 29]$

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, 15, 23, 25]$
2	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[2, 13, 21, 26]$

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, 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]
3	[0, 0, -z]	[9, 10, 11, 14]
4	$[\frac{1}{2}, \frac{1}{2}, z]$	[12, 13, 15, 16]
5	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[17, 18, 19, 22]
6	$[0, 0, \frac{1}{2} - z]$	[20, 21, 23, 24]
7	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[25, 26, 27, 30]
8	$[0, 0, z + \frac{1}{2}]$	[28, 29, 31, 32]

Table 7: Wyckoff site: 8g, 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	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[17, 22, 31, 32]
6	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[18, 19, 28, 29]
7	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[20, 21, 26, 27]
8	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[23, 24, 25, 30]

Table 8: Wyckoff site: 8h, 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	$[x + \frac{1}{2}, x, \frac{1}{2}]$	[17, 23, 30, 32]

continued ...

Table 8

No.	position	mapping
6	$[-x, x + \frac{1}{2}, \frac{1}{2}]$	[18, 21, 27, 28]
7	$[x, \frac{1}{2} - x, \frac{1}{2}]$	[19, 20, 26, 29]
8	$[\frac{1}{2} - x, -x, \frac{1}{2}]$	[22, 24, 25, 31]

Table 9: Wyckoff site: 16i, 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	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	[4, 19]
5	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}]$	[5, 18]
6	$[-x, -x, \frac{1}{4}]$	[6, 24]
7	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}]$	[7, 17]
8	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{3}{4}]$	[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	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{4}]$	[12, 27]
13	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$	[13, 26]
14	$[x, x, \frac{3}{4}]$	[14, 32]
15	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{4}]$	[15, 25]
16	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[16, 30]

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

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

continued ...

Table 10

No.	position	mapping
16	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[16, 27]

Table 11: Wyckoff site: 16k, 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	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[17, 30]
10	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2}]$	[18, 27]
11	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[19, 26]
12	$[x, -y, \frac{1}{2}]$	[20, 29]
13	$[-x, y, \frac{1}{2}]$	[21, 28]
14	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2}]$	[22, 25]
15	$[y, x, \frac{1}{2}]$	[23, 32]
16	$[-y, -x, \frac{1}{2}]$	[24, 31]

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

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	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	[17, 32]
10	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	[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	$[-x, x + \frac{1}{2}, \frac{1}{2} - z]$	[21, 27]
14	$[\frac{1}{2} - x, -x, z + \frac{1}{2}]$	[22, 31]
15	$[x + \frac{1}{2}, x, \frac{1}{2} - z]$	[23, 30]
16	$[\frac{1}{2} - x, -x, \frac{1}{2} - z]$	[24, 25]

Table 13: Wyckoff site: **32m**, 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	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[17]
18	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[18]
19	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[19]
20	$[x, -y, \frac{1}{2} - z]$	[20]
21	$[-x, y, \frac{1}{2} - z]$	[21]
22	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[22]
23	$[y, x, \frac{1}{2} - z]$	[23]
24	$[-y, -x, \frac{1}{2} - z]$	[24]
25	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[25]
26	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[26]
27	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[27]
28	$[-x, y, z + \frac{1}{2}]$	[28]
29	$[x, -y, z + \frac{1}{2}]$	[29]
30	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[30]
31	$[-y, -x, z + \frac{1}{2}]$	[31]
32	$[y, x, z + \frac{1}{2}]$	[32]