

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: $4/mm'm'$

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $m.mm'$

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

Table 6: Wyckoff site: $4f$, site symmetry: $m.mm'$

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

Table 7: Wyckoff site: $4g$, site symmetry: $4'm'm$

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

Table 8: Wyckoff site: $4h$, site symmetry: $4m'm'$

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

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

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

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

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

Table 11: Wyckoff site: 8k, site symmetry: $mm'2'$.

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

Table 12: Wyckoff site: 8l, 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	$[x + \frac{1}{2}, x, 0]$	$[17, 23, 30, 32]$
6	$[-x, x + \frac{1}{2}, 0]$	$[18, 21, 27, 28]$
7	$[x, \frac{1}{2} - x, 0]$	$[19, 20, 26, 29]$
8	$[\frac{1}{2} - x, -x, 0]$	$[22, 24, 25, 31]$

Table 13: Wyckoff site: 8m, site symmetry: $m.2m$

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

continued ...

Table 13

No.	position	mapping
4	$[-x, \frac{1}{2} - x, \frac{1}{2}]$	[6, 8, 9, 15]
5	$[x + \frac{1}{2}, x, \frac{1}{2}]$	[17, 23, 30, 32]
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 14: Wyckoff site: 8n, site symmetry: $m.2'm'$

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

Table 15: Wyckoff site: 8o, site symmetry: $m.2'm'$

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

Table 16: Wyckoff site: 16p, 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]

continued ...

Table 16

No.	position	mapping
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	$[x + \frac{1}{2}, y + \frac{1}{2}, 0]$	[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	$[x, -y, 0]$	[20,29]
13	$[-x, y, 0]$	[21,28]
14	$[\frac{1}{2} - x, \frac{1}{2} - y, 0]$	[22,25]
15	$[y, x, 0]$	[23,32]
16	$[-y, -x, 0]$	[24,31]

Table 17: Wyckoff site: 16q, site symmetry: $m..$

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	[1,14]
2	$[-y, x, \frac{1}{2}]$	[2,11]
3	$[y, -x, \frac{1}{2}]$	[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	$[-x, -y, \frac{1}{2}]$	[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	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[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 18: Wyckoff site: 16r, site symmetry: $.m'$.

No.	position	mapping
1	$[0, y, z]$	[1,28]
2	$[-y, 0, z]$	[2,31]
3	$[y, 0, z]$	[3,32]
4	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	[4,25]
5	$[\frac{1}{2}, y + \frac{1}{2}, -z]$	[5,30]
6	$[0, -y, z]$	[6,29]
7	$[y + \frac{1}{2}, \frac{1}{2}, -z]$	[7,26]
8	$[\frac{1}{2} - y, \frac{1}{2}, -z]$	[8,27]

continued ...

Table 18

No.	position	mapping
9	$[0, -y, -z]$	[9,20]
10	$[y, 0, -z]$	[10,23]
11	$[-y, 0, -z]$	[11,24]
12	$[\frac{1}{2}, y + \frac{1}{2}, z]$	[12,17]
13	$[\frac{1}{2}, \frac{1}{2} - y, z]$	[13,22]
14	$[0, y, -z]$	[14,21]
15	$[\frac{1}{2} - y, \frac{1}{2}, z]$	[15,18]
16	$[y + \frac{1}{2}, \frac{1}{2}, z]$	[16,19]

Table 19: Wyckoff site: $16s$, site symmetry: $\dots m$

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

Table 20: Wyckoff site: $16t$, site symmetry: $\dots m'$

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

continued ...

Table 20

No.	position	mapping
11	$[-x, x, -z]$	[11, 21]
12	$[\frac{1}{2} - x, x + \frac{1}{2}, z]$	[12, 18]
13	$[x + \frac{1}{2}, \frac{1}{2} - x, z]$	[13, 19]
14	$[x, x, -z]$	[14, 23]
15	$[\frac{1}{2} - x, \frac{1}{2} - x, z]$	[15, 22]
16	$[x + \frac{1}{2}, x + \frac{1}{2}, z]$	[16, 17]

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