

Table 1: Wyckoff site: 2a, site symmetry: $4/mmm$

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: $4/mmm$

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

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

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

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

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

Table 6: Wyckoff site: 4f, site symmetry: mmm .

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

Table 7: Wyckoff site: 4g, site symmetry: 4mm

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

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

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

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

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

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

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

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

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

Table 12: Wyckoff site: $8l$, site symmetry: $m2m.$

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

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

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	$[1, 13, 20, 30]$
2	$[0, x, \frac{1}{4}]$	$[2, 16, 23, 27]$
3	$[0, -x, \frac{1}{4}]$	$[3, 15, 24, 26]$

continued ...

Table 13

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

Table 14: Wyckoff site: $8n$, site symmetry: $m2m$.

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

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

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

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	$[x, -y, 0]$	$[4, 13]$
5	$[-x, y, 0]$	$[5, 12]$
6	$[-x, -y, 0]$	$[6, 9]$

continued ...

Table 16

No.	position	mapping
7	$[y, x, 0]$	$[7, 16]$
8	$[-y, -x, 0]$	$[8, 15]$
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	$[x, -y, \frac{1}{2}]$	$[20, 29]$
13	$[-x, y, \frac{1}{2}]$	$[21, 28]$
14	$[-x, -y, \frac{1}{2}]$	$[22, 25]$
15	$[y, x, \frac{1}{2}]$	$[23, 32]$
16	$[-y, -x, \frac{1}{2}]$	$[24, 31]$

Table 17: Wyckoff site: 16q, 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	$[x, -y, \frac{3}{4}]$	$[4, 29]$
5	$[-x, y, \frac{3}{4}]$	$[5, 28]$
6	$[-x, -y, \frac{1}{4}]$	$[6, 25]$
7	$[y, x, \frac{3}{4}]$	$[7, 32]$
8	$[-y, -x, \frac{3}{4}]$	$[8, 31]$
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	$[-x, y, \frac{1}{4}]$	$[12, 21]$
13	$[x, -y, \frac{1}{4}]$	$[13, 20]$
14	$[x, y, \frac{3}{4}]$	$[14, 17]$
15	$[-y, -x, \frac{1}{4}]$	$[15, 24]$
16	$[y, x, \frac{1}{4}]$	$[16, 23]$

Table 18: Wyckoff site: 16r, site symmetry: $..m$

No.	position	mapping
1	$[x, x, z]$	$[1, 16]$
2	$[-x, x, z]$	$[2, 12]$
3	$[x, -x, z]$	$[3, 13]$
4	$[x, -x, -z]$	$[4, 10]$
5	$[-x, x, -z]$	$[5, 11]$
6	$[-x, -x, z]$	$[6, 15]$
7	$[x, x, -z]$	$[7, 14]$
8	$[-x, -x, -z]$	$[8, 9]$

continued ...

Table 18

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

Table 19: Wyckoff site: $16s$, site symmetry: $.m$.

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

Table 20: Wyckoff site: $16t$, site symmetry: $.m$.

No.	position	mapping
1	$[x, \frac{1}{2}, z]$	[1, 13]
2	$[\frac{1}{2}, x, z]$	[2, 16]
3	$[\frac{1}{2}, -x, z]$	[3, 15]
4	$[x, \frac{1}{2}, -z]$	[4, 14]
5	$[-x, \frac{1}{2}, -z]$	[5, 9]
6	$[-x, \frac{1}{2}, z]$	[6, 12]
7	$[\frac{1}{2}, x, -z]$	[7, 11]
8	$[\frac{1}{2}, -x, -z]$	[8, 10]
9	$[x, \frac{1}{2}, z + \frac{1}{2}]$	[17, 29]
10	$[\frac{1}{2}, x, z + \frac{1}{2}]$	[18, 32]

continued ...

Table 20

No.	position	mapping
11	$[\frac{1}{2}, -x, z + \frac{1}{2}]$	[19,31]
12	$[x, \frac{1}{2}, \frac{1}{2} - z]$	[20,30]
13	$[-x, \frac{1}{2}, \frac{1}{2} - z]$	[21,25]
14	$[-x, \frac{1}{2}, z + \frac{1}{2}]$	[22,28]
15	$[\frac{1}{2}, x, \frac{1}{2} - z]$	[23,27]
16	$[\frac{1}{2}, -x, \frac{1}{2} - z]$	[24,26]

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	$[x, -y, -z]$	[4]
5	$[-x, y, -z]$	[5]
6	$[-x, -y, z]$	[6]
7	$[y, x, -z]$	[7]
8	$[-y, -x, -z]$	[8]
9	$[-x, -y, -z]$	[9]
10	$[y, -x, -z]$	[10]
11	$[-y, x, -z]$	[11]
12	$[-x, y, z]$	[12]
13	$[x, -y, z]$	[13]
14	$[x, y, -z]$	[14]
15	$[-y, -x, z]$	[15]
16	$[y, x, z]$	[16]
17	$[x, y, z + \frac{1}{2}]$	[17]
18	$[-y, x, z + \frac{1}{2}]$	[18]
19	$[y, -x, z + \frac{1}{2}]$	[19]
20	$[x, -y, \frac{1}{2} - z]$	[20]
21	$[-x, y, \frac{1}{2} - z]$	[21]
22	$[-x, -y, z + \frac{1}{2}]$	[22]
23	$[y, x, \frac{1}{2} - z]$	[23]
24	$[-y, -x, \frac{1}{2} - z]$	[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	$[-x, y, z + \frac{1}{2}]$	[28]
29	$[x, -y, z + \frac{1}{2}]$	[29]
30	$[x, y, \frac{1}{2} - z]$	[30]
31	$[-y, -x, z + \frac{1}{2}]$	[31]
32	$[y, x, z + \frac{1}{2}]$	[32]