

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry:  $\dots 2/m$ 

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 8, 12, 13]$
2	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	$[2, 7, 11, 14]$

*continued ...*

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry:  $\dots 2/m'$ 

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

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

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

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

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	[1, 2, 23, 24]
2	$[-x, 0, \frac{1}{4}]$	[3, 4, 21, 22]
3	$[-x, 0, \frac{3}{4}]$	[5, 6, 19, 20]
4	$[x, 0, \frac{3}{4}]$	[7, 8, 17, 18]
5	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[9, 10, 31, 32]

*continued ...*

Table 8

No.	position	mapping
6	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{4}]$	[11, 12, 29, 30]
7	$[\frac{1}{2} - x, \frac{1}{2}, \frac{3}{4}]$	[13, 14, 27, 28]
8	$[x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[15, 16, 25, 26]

Table 9: Wyckoff site: 8i, site symmetry:  $m'2'm$ 

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

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

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

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

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

Table 12: Wyckoff site: 8l, site symmetry:  $m'm'2$ 

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

Table 13: Wyckoff site: 16m, site symmetry:  $..2$ 

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

Table 14: Wyckoff site: 16n, site symmetry:  $m'..$ 

No.	position	mapping
1	$[0, y, z]$	$[1, 22]$
2	$[0, -y, \frac{1}{2} - z]$	$[2, 21]$
3	$[0, y, \frac{1}{2} - z]$	$[3, 24]$
4	$[0, -y, z]$	$[4, 23]$
5	$[0, -y, -z]$	$[5, 18]$
6	$[0, y, z + \frac{1}{2}]$	$[6, 17]$
7	$[0, -y, z + \frac{1}{2}]$	$[7, 20]$
8	$[0, y, -z]$	$[8, 19]$
9	$[\frac{1}{2}, y + \frac{1}{2}, z]$	$[9, 30]$

*continued ...*

Table 14

No.	position	mapping
10	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[10, 29]
11	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[11, 32]
12	$[\frac{1}{2}, \frac{1}{2} - y, z]$	[12, 31]
13	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	[13, 26]
14	$[\frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[14, 25]
15	$[\frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[15, 28]
16	$[\frac{1}{2}, y + \frac{1}{2}, -z]$	[16, 27]

Table 15: Wyckoff site: 16o, site symmetry:  $.m'$ .

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

Table 16: Wyckoff site: 16p, site symmetry:  $.m$ 

No.	position	mapping
1	$[x, y, 0]$	[1, 8]
2	$[x, -y, \frac{1}{2}]$	[2, 7]
3	$[-x, y, \frac{1}{2}]$	[3, 6]
4	$[-x, -y, 0]$	[4, 5]
5	$[x + \frac{1}{2}, y + \frac{1}{2}, 0]$	[9, 16]
6	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[10, 15]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	[11, 14]
8	$[\frac{1}{2} - x, \frac{1}{2} - y, 0]$	[12, 13]
9	$[x, y, \frac{1}{2}]$	[17, 24]
10	$[x, -y, 0]$	[18, 23]
11	$[-x, y, 0]$	[19, 22]

*continued ...*

Table 16

No.	position	mapping
12	$[-x, -y, \frac{1}{2}]$	[20, 21]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[25, 32]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	[26, 31]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	[27, 30]
16	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2}]$	[28, 29]

Table 17: Wyckoff site:  $16\mathbf{q}$ , site symmetry:  $\bar{6}m'$ 

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

Table 18: Wyckoff site:  $32\mathbf{r}$ , site symmetry:  $1$ 

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

*continued ...*

Table 18

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