

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

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

Table 2: Wyckoff site: 4b, site symmetry:  $mmm$ 

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 8, 28, 29]$
2	$[\frac{1}{4}, \frac{3}{4}, 0]$	$[2, 7, 27, 30]$

*continued ...*

Table 5

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

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

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

Table 7: Wyckoff site: 8g, site symmetry:  $2mm$ 

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

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

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	[1, 7, 18, 24]
2	$[x, 0, \frac{3}{4}]$	[2, 8, 17, 23]
3	$[-x, 0, \frac{3}{4}]$	[3, 5, 20, 22]
4	$[-x, 0, \frac{1}{4}]$	[4, 6, 19, 21]
5	$[x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[9, 15, 26, 32]

*continued ...*

Table 8

No.	position	mapping
6	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[10, 16, 25, 31]
7	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{4}]$	[11, 13, 28, 30]
8	$[\frac{1}{2} - x, \frac{1}{2}, \frac{3}{4}]$	[12, 14, 27, 29]

Table 9: Wyckoff site: 8i, site symmetry: m2m

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

Table 10: Wyckoff site: 8j, site symmetry: m2'm'

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

Table 11: Wyckoff site: 8k, site symmetry: mm2

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

Table 12: Wyckoff site:  $81$ , site symmetry:  $mm2$ 

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

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

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

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

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

*continued ...*

Table 14

No.	position	mapping
10	$[0, -y, \frac{1}{2} - z]$	[18, 21]
11	$[0, y, \frac{1}{2} - z]$	[19, 24]
12	$[0, -y, z + \frac{1}{2}]$	[20, 23]
13	$[\frac{1}{2}, y + \frac{1}{2}, z]$	[25, 30]
14	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	[26, 29]
15	$[\frac{1}{2}, y + \frac{1}{2}, -z]$	[27, 32]
16	$[\frac{1}{2}, \frac{1}{2} - y, z]$	[28, 31]

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

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

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

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

continued ...

Table 16

No.	position	mapping
12	$[-x, -y, \frac{1}{2}]$	[20, 21]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, 0]$	[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	$[\frac{1}{2} - x, \frac{1}{2} - y, 0]$	[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	$[x, -y, \frac{3}{4}]$	[2, 23]
3	$[-x, y, \frac{3}{4}]$	[3, 22]
4	$[-x, -y, \frac{1}{4}]$	[4, 21]
5	$[-x, -y, \frac{3}{4}]$	[5, 20]
6	$[-x, y, \frac{1}{4}]$	[6, 19]
7	$[x, -y, \frac{1}{4}]$	[7, 18]
8	$[x, y, \frac{3}{4}]$	[8, 17]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[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	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{3}{4}]$	[12, 29]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{4}]$	[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	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}]$	[16, 25]

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

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