

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $-42'm'$

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{4}]$	$[1, 6, 10, 11, 20, 21, 31, 32]$
2	$[0, \frac{1}{2}, \frac{3}{4}]$	$[2, 3, 9, 14, 23, 24, 28, 29]$

*continued ...*

Table 5

No.	position	mapping
3	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[4, 5, 15, 16, 17, 22, 26, 27]$
4	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[7, 8, 12, 13, 18, 19, 25, 30]$

Table 6: Wyckoff site: 4f, site symmetry:  $-4'2'm$ 

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, x + \frac{1}{2}, \frac{1}{2}]$	$[1, 14, 23, 32]$
2	$[-x, x + \frac{1}{2}, 0]$	$[2, 11, 21, 28]$
3	$[x, \frac{1}{2} - x, 0]$	$[3, 10, 20, 29]$

*continued ...*

Table 12

No.	position	mapping
4	$[x + \frac{1}{2}, -x, 0]$	[4, 13, 19, 26]
5	$[\frac{1}{2} - x, x, 0]$	[5, 12, 18, 27]
6	$[-x, \frac{1}{2} - x, \frac{1}{2}]$	[6, 9, 24, 31]
7	$[x + \frac{1}{2}, x, \frac{1}{2}]$	[7, 16, 17, 30]
8	$[\frac{1}{2} - x, -x, \frac{1}{2}]$	[8, 15, 22, 25]

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

No.	position	mapping
1	$[x, x, 0]$	[1, 7, 14, 16]
2	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]$	[2, 5, 11, 12]
3	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[3, 4, 10, 13]
4	$[-x, -x, 0]$	[6, 8, 9, 15]
5	$[x + \frac{1}{2}, x + \frac{1}{2}, 0]$	[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	$[\frac{1}{2} - x, \frac{1}{2} - x, 0]$	[22, 24, 25, 31]

Table 14: Wyckoff site: 16n, site symmetry: .2'.

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

Table 15: Wyckoff site: 16o, site symmetry:  $\bar{3}m'$ 

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

Table 16: Wyckoff site: 16p, site symmetry:  $\bar{3}m$ 

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

Table 17: Wyckoff site: 16q, site symmetry:  $m\bar{3}$ 

No.	position	mapping
1	$[x, y, 0]$	[1,14]

continued ...

Table 17

No.	position	mapping
2	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2}]$	[2,11]
3	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[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	$[-x, -y, 0]$	[6,9]
7	$[y, x, 0]$	[7,16]
8	$[-y, -x, 0]$	[8,15]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, 0]$	[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	$[\frac{1}{2} - x, \frac{1}{2} - y, 0]$	[22,25]
15	$[y + \frac{1}{2}, x + \frac{1}{2}, 0]$	[23,32]
16	$[\frac{1}{2} - y, \frac{1}{2} - x, 0]$	[24,31]

Table 18: Wyckoff site: **32r**, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[2]
3	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[3]
4	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[4]
5	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[5]
6	$[-x, -y, z]$	[6]
7	$[y, x, -z]$	[7]
8	$[-y, -x, -z]$	[8]
9	$[-x, -y, -z]$	[9]
10	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[10]
11	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[12]
13	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[13]
14	$[x, y, -z]$	[14]
15	$[-y, -x, z]$	[15]
16	$[y, x, z]$	[16]
17	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[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	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[22]
23	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[23]
24	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[24]
25	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[25]

continued ...

Table 18

No.	position	mapping
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	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[30]
31	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[31]
32	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[32]