

Table 1: Wyckoff site: **4a**, site symmetry: 422

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

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

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

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

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

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

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

Table 5: Wyckoff site: **8e**, site symmetry:  $..2/m'$ 

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, 7, 25, 31]$
2	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[2, 5, 26, 29]$

*continued ...*

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 4..

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

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

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

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

No.	position	mapping
1	$[x, x + \frac{1}{2}, 0]$	[1, 14, 23, 32]
2	$[\frac{1}{2} - x, x, 0]$	[2, 11, 21, 28]
3	$[x + \frac{1}{2}, -x, 0]$	[3, 10, 20, 29]
4	$[x, \frac{1}{2} - x, \frac{1}{2}]$	[4, 13, 19, 26]
5	$[-x, x + \frac{1}{2}, \frac{1}{2}]$	[5, 12, 18, 27]

*continued ...*

Table 8

No.	position	mapping
6	$[-x, \frac{1}{2} - x, 0]$	[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 9: Wyckoff site: 16i, site symmetry: .2

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

Table 10: Wyckoff site: 16j, site symmetry: .2.

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

*continued ...*

Table 10

No.	position	mapping
16	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[29,30]

Table 11: Wyckoff site: 16k, site symmetry:  $m\ldots$ 

No.	position	mapping
1	$[x, y, 0]$	[1,14]
2	$[-y, x, 0]$	[2,11]
3	$[y, -x, 0]$	[3,10]
4	$[x, -y, \frac{1}{2}]$	[4,13]
5	$[-x, y, \frac{1}{2}]$	[5,12]
6	$[-x, -y, 0]$	[6,9]
7	$[y, x, \frac{1}{2}]$	[7,16]
8	$[-y, -x, \frac{1}{2}]$	[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	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	[20,29]
13	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	[21,28]
14	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2}]$	[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 12: Wyckoff site: 16l, site symmetry:  $\ldots m'$ 

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

Table 13: Wyckoff site: 32m, site symmetry: 1

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