

Table 1: Wyckoff site: 4a, site symmetry:  $4'2'2$ 

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

Table 2: Wyckoff site: 4b, site symmetry:  $-42'm'$ 

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

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

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

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

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

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

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

*continued ...*

Table 5

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

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

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

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

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

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

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

*continued ...*

Table 8

No.	position	mapping
6	$[-x, -x, 0]$	$[6, 9, 24, 31]$
7	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	$[7, 16, 17, 30]$
8	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	$[8, 15, 22, 25]$

Table 9: Wyckoff site: 16i, site symmetry:  $\cdot \cdot 2$ 

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

Table 10: Wyckoff site: 16j, site symmetry:  $\cdot 2'$ 

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

*continued ...*

Table 10

No.	position	mapping
16	$[\frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}]$	[16, 27]

Table 11: Wyckoff site: 16k, site symmetry:  $m..$ 

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

Table 12: Wyckoff site: 16l, site symmetry:  $..m'$ 

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

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

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