

Table 1: Wyckoff site: 4a, site symmetry:  $42'2'$

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

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

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

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

No.	position	mapping
1	[0, 0, 0]	[1, 2, 3, 4, 5, 6, 7, 8]
2	$[0, 0, \frac{1}{2}]$	[9, 10, 11, 12, 13, 14, 15, 16]
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[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 4: Wyckoff site: 4d, site symmetry:  $m.m'm'$

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

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[1, 11, 21, 31]
2	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[2, 10, 22, 30]

*continued ...*

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$[x, x + \frac{1}{2}, 0]$	[1, 8, 27, 32]
2	$[\frac{1}{2} - x, x, 0]$	[2, 7, 26, 29]
3	$[x + \frac{1}{2}, -x, 0]$	[3, 6, 25, 30]
4	$[-x, \frac{1}{2} - x, 0]$	[4, 5, 28, 31]
5	$[x, \frac{1}{2} - x, \frac{1}{2}]$	[9, 14, 19, 22]

continued ...

Table 8

No.	position	mapping
6	$[-x, x + \frac{1}{2}, \frac{1}{2}]$	[10,13,18,23]
7	$[x + \frac{1}{2}, x, \frac{1}{2}]$	[11,16,17,24]
8	$[\frac{1}{2} - x, -x, \frac{1}{2}]$	[12,15,20,21]

Table 9: Wyckoff site: 16i, site symmetry:  $. . 2'$ 

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

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

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

continued ...

Table 10

No.	position	mapping
16	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[24,30]

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

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

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

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