

Table 1: Wyckoff site: 4a, site symmetry:  $4'22'$ 

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0, \frac{1}{2}, 0]$	[1, 9, 23, 31]
2	$[0, 0, \frac{1}{2}]$	[2, 10, 21, 29]

*continued ...*

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$[x, x, \frac{3}{4}]$	[1, 7, 30, 32]
2	$[\frac{1}{2} - x, x, \frac{1}{4}]$	[2, 5, 27, 28]
3	$[x, \frac{1}{2} - x, \frac{1}{4}]$	[3, 4, 26, 29]
4	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{3}{4}]$	[6, 8, 25, 31]
5	$[-x, -x, \frac{1}{4}]$	[9, 15, 22, 24]

continued ...

Table 8

No.	position	mapping
6	$[x + \frac{1}{2}, -x, \frac{3}{4}]$	[10, 13, 19, 20]
7	$[-x, x + \frac{1}{2}, \frac{3}{4}]$	[11, 12, 18, 21]
8	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[14, 16, 17, 23]

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

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

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

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

*continued ...*

Table 10

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

Table 11: Wyckoff site: **16k**, site symmetry:  $m'\bar{1}$ 

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

Table 12: Wyckoff site: **16l**, site symmetry:  $\bar{1}m'$ 

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