

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

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

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

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

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	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[4, 5, 15, 16, 23, 24, 28, 29]
4	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[7, 8, 12, 13, 20, 21, 31, 32]

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

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

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

No.	position	mapping
1	$[0, \frac{1}{2}, 0]$	[1, 7, 9, 15]
2	$[0, 0, \frac{1}{2}]$	[2, 5, 10, 13]

continued ...

Table 5

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

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	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[4, 5, 23, 24]
4	$[\frac{3}{4}, \frac{1}{4}, -z]$	[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	$[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[12, 13, 31, 32]
8	$[\frac{1}{4}, \frac{3}{4}, z]$	[15, 16, 28, 29]

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

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

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

No.	position	mapping
1	$[x, x, \frac{3}{4}]$	[1, 16, 23, 30]
2	$[\frac{1}{2} - x, x, \frac{1}{4}]$	[2, 12, 21, 27]
3	$[x, \frac{1}{2} - x, \frac{1}{4}]$	[3, 13, 20, 26]
4	$[x + \frac{1}{2}, -x, \frac{3}{4}]$	[4, 10, 19, 29]
5	$[-x, x + \frac{1}{2}, \frac{3}{4}]$	[5, 11, 18, 28]

continued ...

Table 8

No.	position	mapping
6	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{3}{4}]$	[6, 15, 24, 25]
7	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[7, 14, 17, 32]
8	$[-x, -x, \frac{1}{4}]$	[8, 9, 22, 31]

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

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

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

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

continued ...

Table 10

No.	position	mapping
16	$[\frac{1}{4}, x, 0]$	[16,27]

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

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	$[x + \frac{1}{2}, -y, \frac{3}{4}]$	[4,29]
5	$[-x, y + \frac{1}{2}, \frac{3}{4}]$	[5,28]
6	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{3}{4}]$	[6,25]
7	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[7,32]
8	$[-y, -x, \frac{1}{4}]$	[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	$[\frac{1}{2} - x, y, \frac{1}{4}]$	[12,21]
13	$[x, \frac{1}{2} - y, \frac{1}{4}]$	[13,20]
14	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}]$	[14,17]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{3}{4}]$	[15,24]
16	$[y, x, \frac{3}{4}]$	[16,23]

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

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

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	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[4]
5	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[5]
6	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[6]
7	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[7]
8	$[-y, -x, -z]$	[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	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[12]
13	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[13]
14	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[14]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[15]
16	$[y, x, z]$	[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	$[x, \frac{1}{2} - y, -z]$	[20]
21	$[\frac{1}{2} - x, y, -z]$	[21]
22	$[-x, -y, z + \frac{1}{2}]$	[22]
23	$[y, x, \frac{1}{2} - z]$	[23]
24	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[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	$[-x, y + \frac{1}{2}, z]$	[28]
29	$[x + \frac{1}{2}, -y, z]$	[29]
30	$[x, y, \frac{1}{2} - z]$	[30]
31	$[-y, -x, z + \frac{1}{2}]$	[31]
32	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[32]