

Table 1: Wyckoff site: 4a, site symmetry: $-4m2$

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

Table 2: Wyckoff site: 4b, site symmetry: $-4'm2'$

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

Table 3: Wyckoff site: 4c, site symmetry: $4mm$

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

Table 4: Wyckoff site: 8d, site symmetry: $. . 2/m$

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

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

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

Table 6: Wyckoff site: **8f**, site symmetry: $2mm$.

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

Table 7: Wyckoff site: **16g**, site symmetry: $\dots 2$

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

Table 8: Wyckoff site: 16h, site symmetry: $\dots 2'$

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

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

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

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

No.	position	mapping
1	$[x, x, z]$	[1, 16]

continued ...

Table 10

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

Table 11: Wyckoff site: **32k**, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[\frac{1}{2} - y, x, z]$	[2]
3	$[y, \frac{1}{2} - x, z]$	[3]
4	$[x + \frac{1}{2}, -y, -z]$	[4]
5	$[-x, y + \frac{1}{2}, -z]$	[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	$[y + \frac{1}{2}, -x, -z]$	[10]
11	$[-y, x + \frac{1}{2}, -z]$	[11]
12	$[\frac{1}{2} - x, y, z]$	[12]
13	$[x, \frac{1}{2} - y, z]$	[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	$[x, y, z + \frac{1}{2}]$	[17]
18	$[\frac{1}{2} - y, x, z + \frac{1}{2}]$	[18]
19	$[y, \frac{1}{2} - x, z + \frac{1}{2}]$	[19]
20	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[20]
21	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[21]
22	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[22]
23	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[23]
24	$[-y, -x, \frac{1}{2} - z]$	[24]
25	$[-x, -y, \frac{1}{2} - z]$	[25]

continued ...

Table 11

No.	position	mapping
26	$[y + \frac{1}{2}, -x, \frac{1}{2} - z]$	[26]
27	$[-y, x + \frac{1}{2}, \frac{1}{2} - z]$	[27]
28	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[28]
29	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[29]
30	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[30]
31	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[31]
32	$[y, x, z + \frac{1}{2}]$	[32]