

Table 1: Wyckoff site: 4a, site symmetry: $4mm$

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

Table 2: Wyckoff site: 4b, site symmetry: $4'mm'$

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

Table 3: Wyckoff site: 8c, site symmetry: $2.mm$

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

Table 4: Wyckoff site: 16d, site symmetry: $.m.$

No.	position	mapping
1	$[0, y, z]$	$[1, 5]$
2	$[-y, 0, z]$	$[2, 7]$
3	$[y, 0, z]$	$[3, 8]$
4	$[0, -y, z]$	$[4, 6]$
5	$[\frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	$[9, 13]$
6	$[\frac{1}{2} - y, \frac{1}{2}, z + \frac{1}{2}]$	$[10, 15]$
7	$[y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[11, 16]$
8	$[\frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	$[12, 14]$
9	$[0, y, z + \frac{1}{2}]$	$[17, 21]$

continued ...

Table 4

No.	position	mapping
10	$[-y, 0, z + \frac{1}{2}]$	[18, 23]
11	$[y, 0, z + \frac{1}{2}]$	[19, 24]
12	$[0, -y, z + \frac{1}{2}]$	[20, 22]
13	$[\frac{1}{2}, y + \frac{1}{2}, z]$	[25, 29]
14	$[\frac{1}{2} - y, \frac{1}{2}, z]$	[26, 31]
15	$[y + \frac{1}{2}, \frac{1}{2}, z]$	[27, 32]
16	$[\frac{1}{2}, \frac{1}{2} - y, z]$	[28, 30]

Table 5: Wyckoff site: **16e**, site symmetry: $\dots m$

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

Table 6: Wyckoff site: **16f**, site symmetry: $\dots m'$

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	$[-x, x + \frac{1}{2}, z]$	[5, 26]
6	$[x, \frac{1}{2} - x, z]$	[6, 27]
7	$[\frac{1}{2} - x, -x, z]$	[7, 28]
8	$[x + \frac{1}{2}, x, z]$	[8, 25]
9	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	[9, 24]
10	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	[10, 21]
11	$[x, \frac{1}{2} - x, z + \frac{1}{2}]$	[11, 22]

continued ...

Table 6

No.	position	mapping
12	$[\frac{1}{2} - x, -x, z + \frac{1}{2}]$	[12, 23]
13	$[\frac{1}{2} - x, x, z + \frac{1}{2}]$	[13, 18]
14	$[x + \frac{1}{2}, -x, z + \frac{1}{2}]$	[14, 19]
15	$[-x, \frac{1}{2} - x, z + \frac{1}{2}]$	[15, 20]
16	$[x, x + \frac{1}{2}, z + \frac{1}{2}]$	[16, 17]

Table 7: Wyckoff site: 32g, 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	$[x, -y, z]$	[6]
7	$[-y, -x, z]$	[7]
8	$[y, x, z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[10]
11	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[11]
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[12]
13	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[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	$[x, y, z + \frac{1}{2}]$	[17]
18	$[-y, x, z + \frac{1}{2}]$	[18]
19	$[y, -x, z + \frac{1}{2}]$	[19]
20	$[-x, -y, z + \frac{1}{2}]$	[20]
21	$[-x, y, z + \frac{1}{2}]$	[21]
22	$[x, -y, z + \frac{1}{2}]$	[22]
23	$[-y, -x, z + \frac{1}{2}]$	[23]
24	$[y, x, z + \frac{1}{2}]$	[24]
25	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[25]
26	$[\frac{1}{2} - y, x + \frac{1}{2}, z]$	[26]
27	$[y + \frac{1}{2}, \frac{1}{2} - x, z]$	[27]
28	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[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]