

Table 1: Wyckoff site: 16a, site symmetry: $\dots 2$

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

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

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

Table 3: Wyckoff site: 32c, site symmetry: 1

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