

Table 1: Wyckoff site: 8a, site symmetry: $2mm$.

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

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

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

Table 3: Wyckoff site: 16c, site symmetry: $.m$.

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

continued ...

Table 3

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

Table 4: Wyckoff site: 32d, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x + \frac{1}{2}, z + \frac{1}{4}]$	[2]
3	$[y, \frac{1}{2} - x, z + \frac{1}{4}]$	[3]
4	$[-x, -y, z]$	[4]
5	$[-x, y, z]$	[5]
6	$[x, -y, z]$	[6]
7	$[-y, \frac{1}{2} - x, z + \frac{1}{4}]$	[7]
8	$[y, x + \frac{1}{2}, z + \frac{1}{4}]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[\frac{1}{2} - y, x, z + \frac{3}{4}]$	[10]
11	$[y + \frac{1}{2}, -x, z + \frac{3}{4}]$	[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	$[\frac{1}{2} - y, -x, z + \frac{3}{4}]$	[15]
16	$[y + \frac{1}{2}, x, z + \frac{3}{4}]$	[16]
17	$[x, y, z + \frac{1}{2}]$	[17]
18	$[-y, x + \frac{1}{2}, z + \frac{3}{4}]$	[18]
19	$[y, \frac{1}{2} - x, z + \frac{3}{4}]$	[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	$[-y, \frac{1}{2} - x, z + \frac{3}{4}]$	[23]
24	$[y, x + \frac{1}{2}, z + \frac{3}{4}]$	[24]
25	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[25]
26	$[\frac{1}{2} - y, x, z + \frac{1}{4}]$	[26]
27	$[y + \frac{1}{2}, -x, z + \frac{1}{4}]$	[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	$[\frac{1}{2} - y, -x, z + \frac{1}{4}]$	[31]

continued ...

Table 4

No.	position	mapping
32	$[y + \frac{1}{2}, x, z + \frac{1}{4}]$	[32]