

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: $2'..$

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]