

Table 1: Wyckoff site: 8a, site symmetry: $\bar{3}$.

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

Table 2: Wyckoff site: 12b, site symmetry: $2..$

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

Table 3: Wyckoff site: 24c, site symmetry: 1

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

continued ...

Table 3

No.	position	mapping
12	$[\frac{1}{2} - z, x, -y]$	[12]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[14]
15	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[15]
16	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[16]
17	$[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$	[17]
18	$[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[18]
19	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[19]
20	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[20]
21	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[21]
22	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[22]
23	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[23]
24	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[24]