

Table 1: Wyckoff site: 4a, site symmetry: $..-3'$.

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

Table 2: Wyckoff site: 4b, site symmetry: $..-3'$.

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

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

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

Table 4: Wyckoff site: 24d, site symmetry: 1

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

continued ...

Table 4

No.	position	mapping
10	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[10]
11	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[11]
12	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[12]
13	$[-x, -y, -z]$	[13]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[14]
15	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[15]
16	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[16]
17	$[-z, -x, -y]$	[17]
18	$[-y, -z, -x]$	[18]
19	$[y, \frac{1}{2} - z, x + \frac{1}{2}]$	[19]
20	$[z + \frac{1}{2}, x, \frac{1}{2} - y]$	[20]
21	$[y + \frac{1}{2}, z, \frac{1}{2} - x]$	[21]
22	$[\frac{1}{2} - z, x + \frac{1}{2}, y]$	[22]
23	$[\frac{1}{2} - y, z + \frac{1}{2}, x]$	[23]
24	$[z, \frac{1}{2} - x, y + \frac{1}{2}]$	[24]