

Table 1: Wyckoff site: **8a**, site symmetry:  $.3.$ 

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]