

Table 1: Wyckoff site: 4a, site symmetry:  $.32'$ 

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

 Table 2: Wyckoff site: 4b, site symmetry:  $.32'$ 

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

 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	$[x + \frac{1}{4}, \frac{1}{4} - x, x + \frac{3}{4}]$	[13,18,23]
6	$[x + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{4} - x]$	[14,15,19]
7	$[\frac{1}{4} - x, x + \frac{3}{4}, x + \frac{1}{4}]$	[16,17,21]
8	$[\frac{3}{4} - x, \frac{3}{4} - x, \frac{3}{4} - x]$	[20,22,24]

 Table 4: Wyckoff site: 12d, site symmetry:  $. .2'$ 

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

*continued ...*

Table 4

No.	position	mapping
10	$[y + \frac{3}{4}, \frac{3}{8}, -y]$	[10,19]
11	$[y + \frac{1}{2}, \frac{1}{4} - y, \frac{7}{8}]$	[11,23]
12	$[\frac{3}{4} - y, \frac{5}{8}, \frac{1}{2} - y]$	[12,20]

Table 5: Wyckoff site: 24e, 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]
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	$[x + \frac{1}{4}, \frac{1}{4} - z, y + \frac{3}{4}]$	[13]
14	$[x + \frac{3}{4}, z + \frac{1}{4}, \frac{1}{4} - y]$	[14]
15	$[z + \frac{3}{4}, y + \frac{1}{4}, \frac{1}{4} - x]$	[15]
16	$[\frac{1}{4} - z, y + \frac{3}{4}, x + \frac{1}{4}]$	[16]
17	$[\frac{1}{4} - y, x + \frac{3}{4}, z + \frac{1}{4}]$	[17]
18	$[y + \frac{1}{4}, \frac{1}{4} - x, z + \frac{3}{4}]$	[18]
19	$[y + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{4} - z]$	[19]
20	$[\frac{3}{4} - y, \frac{3}{4} - x, \frac{3}{4} - z]$	[20]
21	$[\frac{1}{4} - x, z + \frac{3}{4}, y + \frac{1}{4}]$	[21]
22	$[\frac{3}{4} - x, \frac{3}{4} - z, \frac{3}{4} - y]$	[22]
23	$[z + \frac{1}{4}, \frac{1}{4} - y, x + \frac{3}{4}]$	[23]
24	$[\frac{3}{4} - z, \frac{3}{4} - y, \frac{3}{4} - x]$	[24]