

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

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

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

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

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

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

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

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

continued ...

Table 4

No.	position	mapping
10	$[\frac{3}{4} - y, \frac{5}{8}, \frac{1}{2} - y]$	[12, 24]
11	$[y + \frac{1}{2}, \frac{1}{4} - y, \frac{7}{8}]$	[15, 23]
12	$[\frac{1}{2} - y, \frac{3}{4} - y, \frac{5}{8}]$	[16, 21]

Table 5: Wyckoff site: 24e, site symmetry: 1

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