

Table 1: Wyckoff site: 2a, site symmetry: 23 .

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $.32'$

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

Table 4: Wyckoff site: 6d, site symmetry: $222..$

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

Table 5: Wyckoff site: 6e, site symmetry: $2.2'2'$

No.	position	mapping
1	$[\frac{1}{4}, 0, \frac{1}{2}]$	$[1, 2, 21, 22]$
2	$[\frac{3}{4}, 0, \frac{1}{2}]$	$[3, 4, 13, 14]$

continued ...

Table 5

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

Table 6: Wyckoff site: 6f, site symmetry: $2.2'2'$

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

Table 7: Wyckoff site: 8g, site symmetry: $.3.$

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

Table 8: Wyckoff site: 12h, site symmetry: $2..$

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

continued ...

Table 8

No.	position	mapping
10	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[17, 19]
11	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[18, 20]
12	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[21, 22]

Table 9: Wyckoff site: 12i, site symmetry: 2. .

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

Table 10: Wyckoff site: 12j, site symmetry: 2. .

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

Table 11: Wyckoff site: 12k, site symmetry: $\dots 2'$

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

Table 12: Wyckoff site: 12l, site symmetry: $\dots 2'$

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

Table 13: Wyckoff site: 24m, site symmetry: 1

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

continued ...

Table 13

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