

Table 1: Wyckoff site: 1a, site symmetry:  $432$ 

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

Table 2: Wyckoff site: 1b, site symmetry:  $432$ 

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

Table 3: Wyckoff site: 3c, site symmetry:  $42.2$ 

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

Table 4: Wyckoff site: 3d, site symmetry:  $42.2$ 

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

Table 5: Wyckoff site: 6e, site symmetry:  $4. .$ 

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

Table 6: Wyckoff site: **6f**, site symmetry:  $4.$ .

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

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

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

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

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

Table 9: Wyckoff site: 12i, site symmetry:  $\dots 2$ 

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

Table 10: Wyckoff site: 12j, site symmetry:  $\dots 2$ 

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

Table 11: Wyckoff site: 24k, site symmetry: 1

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

*continued ...*

Table 11

No.	position	mapping
10	$[-x, -y, z]$	[10]
11	$[y, x, -z]$	[11]
12	$[-y, -x, -z]$	[12]
13	$[-x, z, y]$	[13]
14	$[-x, -z, -y]$	[14]
15	$[z, -y, x]$	[15]
16	$[-z, -y, -x]$	[16]
17	$[z, x, y]$	[17]
18	$[y, z, x]$	[18]
19	$[-y, z, -x]$	[19]
20	$[-z, -x, y]$	[20]
21	$[-y, -z, x]$	[21]
22	$[z, -x, -y]$	[22]
23	$[y, -z, -x]$	[23]
24	$[-z, x, -y]$	[24]