

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

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

Table 2: Wyckoff site: 4b, site symmetry: $.-3'$.

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

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: $.3$.

No.	position	mapping
1	$[x, x, x]$	$[1, 5, 6]$
2	$[x, \frac{1}{2} - x, \frac{1}{2} - x]$	$[2, 10, 11]$

continued ...

Table 5

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

Table 6: Wyckoff site: 12f, site symmetry: 2..

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

Table 7: Wyckoff site: 12g, site symmetry: 2..

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

Table 8: Wyckoff site: $24h$, site symmetry: 1

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