

Table 1: Wyckoff site: 2a, site symmetry: $m' .mm$

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

Table 2: Wyckoff site: 2b, site symmetry: $-42m$

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

Table 3: Wyckoff site: 2c, site symmetry: $m' .mm$

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

Table 4: Wyckoff site: 2d, site symmetry: $-42m$

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

Table 5: Wyckoff site: 4e, site symmetry: $222.$

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

Table 6: Wyckoff site: 4f, site symmetry: $2/m'$.

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

Table 7: Wyckoff site: 4g, site symmetry: $2.mm$

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

Table 8: Wyckoff site: 4h, site symmetry: $2.mm$

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

Table 9: Wyckoff site: 4i, site symmetry: $m'.2'm$

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

Table 10: Wyckoff site: 4j, site symmetry: $m'.2'm$

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

Table 11: Wyckoff site: $8k$, site symmetry: $2..$

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

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

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

Table 13: Wyckoff site: $8m$, site symmetry: $.2.$

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

Table 14: Wyckoff site: $8n$, site symmetry: $m'..$

No.	position	mapping
1	$[x, y, 0]$	$[1, 16]$
2	$[x, -y, \frac{1}{2}]$	$[2, 15]$
3	$[-x, y, \frac{1}{2}]$	$[3, 14]$

continued ...

Table 14

No.	position	mapping
4	$[-x, -y, 0]$	$[4, 13]$
5	$[y, -x, \frac{1}{2}]$	$[5, 10]$
6	$[-y, x, \frac{1}{2}]$	$[6, 9]$
7	$[-y, -x, 0]$	$[7, 12]$
8	$[y, x, 0]$	$[8, 11]$

Table 15: Wyckoff site: $8o$, site symmetry: $\bar{3}m$

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

Table 16: Wyckoff site: $16p$, site symmetry: 1

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