

Table 1: Wyckoff site: 1a, site symmetry: $4/mm'm'$

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

Table 2: Wyckoff site: 1b, site symmetry: $4/mm'm'$

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

Table 3: Wyckoff site: 1c, site symmetry: $4/mm'm'$

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

Table 4: Wyckoff site: 1d, site symmetry: $4/mm'm'$

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

Table 5: Wyckoff site: 2e, site symmetry: $mm'm'$.

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

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

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

Table 7: Wyckoff site: $2g$, site symmetry: $4m'm'$

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

Table 8: Wyckoff site: $2h$, site symmetry: $4m'm'$

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

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

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

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

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

Table 11: Wyckoff site: $4k$, site symmetry: $m.2'm'$

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

Table 12: Wyckoff site: $4\mathbf{l}$, site symmetry: $\mathbf{m}2'\mathbf{m}'$.

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

Table 13: Wyckoff site: $4\mathbf{m}$, site symmetry: $\mathbf{m}2'\mathbf{m}'$.

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

Table 14: Wyckoff site: $4\mathbf{n}$, site symmetry: $\mathbf{m}2'\mathbf{m}'$.

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

Table 15: Wyckoff site: $4\mathbf{o}$, site symmetry: $\mathbf{m}2'\mathbf{m}'$.

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

Table 16: Wyckoff site: $8\mathbf{p}$, site symmetry: $\mathbf{m} . .$

No.	position	mapping
1	$[x, y, 0]$	$[1, 8]$
2	$[-y, x, 0]$	$[2, 7]$
3	$[y, -x, 0]$	$[3, 6]$
4	$[-x, -y, 0]$	$[4, 5]$

continued ...

Table 16

No.	position	mapping
5	$[x, -y, 0]$	$[9, 14]$
6	$[-x, y, 0]$	$[10, 13]$
7	$[y, x, 0]$	$[11, 16]$
8	$[-y, -x, 0]$	$[12, 15]$

Table 17: Wyckoff site: $8q$, site symmetry: $m..$

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

Table 18: Wyckoff site: $8r$, site symmetry: $..m'$

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

Table 19: Wyckoff site: $8s$, site symmetry: $.m'$

No.	position	mapping
1	$[x, 0, z]$	$[1, 14]$
2	$[0, x, z]$	$[2, 16]$
3	$[0, -x, z]$	$[3, 15]$
4	$[-x, 0, z]$	$[4, 13]$
5	$[-x, 0, -z]$	$[5, 10]$
6	$[0, -x, -z]$	$[6, 12]$
7	$[0, x, -z]$	$[7, 11]$

continued ...

Table 19

No.	position	mapping
8	$[x, 0, -z]$	$[8, 9]$

Table 20: Wyckoff site: $8\mathbf{t}$, site symmetry: $.m'$.

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

Table 21: Wyckoff site: $16\mathbf{u}$, site symmetry: 1

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