

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

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

Table 2: Wyckoff site: 2b, site symmetry: $m'm'm'$.

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

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

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

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

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

Table 5: Wyckoff site: 2e, site symmetry: $-4m'2'$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 14: Wyckoff site: $8\mathbf{n}$, site symmetry: $. . 2'$

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

Table 15: Wyckoff site: $8\mathbf{o}$, site symmetry: $.m'$.

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

Table 16: Wyckoff site: $8p$, site symmetry: $.m'$.

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

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

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

Table 18: Wyckoff site: $16r$, 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	$[y, -x, \frac{1}{2} - z]$	$[5]$
6	$[-y, x, \frac{1}{2} - z]$	$[6]$
7	$[-y, -x, z + \frac{1}{2}]$	$[7]$
8	$[y, x, z + \frac{1}{2}]$	$[8]$
9	$[-y, x, z + \frac{1}{2}]$	$[9]$
10	$[y, -x, z + \frac{1}{2}]$	$[10]$
11	$[y, x, \frac{1}{2} - z]$	$[11]$
12	$[-y, -x, \frac{1}{2} - z]$	$[12]$
13	$[-x, -y, -z]$	$[13]$
14	$[-x, y, z]$	$[14]$
15	$[x, -y, z]$	$[15]$
16	$[x, y, -z]$	$[16]$