

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 10: Wyckoff site: 4j, site symmetry: $m2'm'$.

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

Table 11: Wyckoff site: 4k, site symmetry: $m2'm'$.

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

Table 12: Wyckoff site: $4l$, site symmetry: $m2'm'$.

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

Table 13: Wyckoff site: $4m$, site symmetry: $m2'm'$.

No.	position	mapping
1	$[x, \frac{1}{2}, 0]$	$[1, 8, 9, 14]$
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	$[-x, \frac{1}{2}, 0]$	$[4, 5, 10, 13]$

Table 14: Wyckoff site: $8n$, 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	$[-x, -x, \frac{3}{4}]$	$[5, 15]$
6	$[x, -x, \frac{1}{4}]$	$[6, 14]$
7	$[-x, x, \frac{1}{4}]$	$[7, 13]$
8	$[x, x, \frac{3}{4}]$	$[8, 16]$

Table 15: Wyckoff site: $8o$, site symmetry: $.m'$.

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

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

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

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

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

Table 18: Wyckoff site: $16r$, site symmetry: 1

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