

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $2/m..$

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

Table 4: Wyckoff site: 4d, site symmetry: $-4'..$

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

Table 5: Wyckoff site: 4e, site symmetry: $2.mm$

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

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

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

Table 7: Wyckoff site: 4g, site symmetry: $m.m2$

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: $m..$

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

Table 10: Wyckoff site: 8j, site symmetry: $\cdot \cdot m$

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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