

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 10: Wyckoff site: **8j**, site symmetry: $\bar{3}m'$

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

Table 11: Wyckoff site: **16k**, site symmetry: $\bar{1}$

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