

Table 1: Wyckoff site: **2a**, site symmetry: $4/m'$. .

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

Table 2: Wyckoff site: **2b**, site symmetry: $4/m'$. .

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

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

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

Table 4: Wyckoff site: **4d**, site symmetry: 2.22

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

Table 5: Wyckoff site: **4e**, site symmetry: 4 . .

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

Table 6: Wyckoff site: **8f**, site symmetry: $2..$

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

Table 7: Wyckoff site: **8g**, site symmetry: $..2$

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

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

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

Table 9: Wyckoff site: **16i**, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x, z]$	$[2]$
3	$[y, -x, z]$	$[3]$

continued ...

Table 9

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