

Table 1: Wyckoff site: 4a, site symmetry: $2\mathbf{m}'\mathbf{m}'$.

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	$[\frac{1}{2}, 0, z]$	$[5, 6, 9, 12]$
4	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[7, 8, 10, 11]$

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

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

Table 3: Wyckoff site: 8c, site symmetry: $2'\dots$

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

Table 4: Wyckoff site: 8d, site symmetry: $\dots\mathbf{m}'$.

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	$[\frac{1}{2}, y + \frac{1}{2}, z]$	$[5, 9]$
6	$[\frac{1}{2}, \frac{1}{2} - y, z]$	$[6, 12]$
7	$[\frac{1}{2} - y, \frac{1}{2}, z + \frac{1}{2}]$	$[7, 10]$
8	$[y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[8, 11]$

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