

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: $.m$

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

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

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

Table 5: Wyckoff site: **16e**, 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	$[-y, x, z]$	[5]
6	$[y, -x, z]$	[6]
7	$[-x, y, z]$	[7]
8	$[x, -y, z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[10]
11	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[11]
12	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[12]
13	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[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]