

Table 1: Wyckoff site: 4a, site symmetry: $2.mm$

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

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

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

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

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

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

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

Table 5: Wyckoff site: **8e**, site symmetry: $\bar{3}m'$

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

Table 6: Wyckoff site: **16f**, 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	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[6]
7	$[-y, -x, z]$	[7]
8	$[y, x, z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[9]
10	$[-y, x, z + \frac{1}{2}]$	[10]
11	$[y, -x, z + \frac{1}{2}]$	[11]
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[12]
13	$[-x, y, z + \frac{1}{2}]$	[13]
14	$[x, -y, z + \frac{1}{2}]$	[14]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[15]
16	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[16]