

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

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

Table 2: Wyckoff site: 4b, site symmetry: $2mm$.

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

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

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

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

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

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	$[-x, y, z]$	[5]
6	$[x, -y, z]$	[6]
7	$[-y, -x, z + \frac{1}{2}]$	[7]
8	$[y, x, z + \frac{1}{2}]$	[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	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[13]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[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]