

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

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

Table 2: Wyckoff site: 8b, site symmetry: $.m$.

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

Table 3: Wyckoff site: 16c, site symmetry: 1

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