

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

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

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

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

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

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