

Table 1: Wyckoff site: **8a**, site symmetry: $2..1'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 17, 20]$
2	$[0, \frac{1}{2}, z + \frac{1}{4}]$	$[2, 3, 18, 19]$
3	$[0, 0, z + \frac{1}{2}]$	$[5, 6, 21, 22]$
4	$[\frac{1}{2}, 0, z + \frac{1}{4}]$	$[7, 8, 23, 24]$
5	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[9, 12, 25, 28]$
6	$[\frac{1}{2}, 0, z + \frac{3}{4}]$	$[10, 11, 26, 27]$
7	$[\frac{1}{2}, \frac{1}{2}, z]$	$[13, 14, 29, 30]$
8	$[0, \frac{1}{2}, z + \frac{3}{4}]$	$[15, 16, 31, 32]$

Table 2: Wyckoff site: **16b**, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 17]$
2	$[-y, x + \frac{1}{2}, z + \frac{1}{4}]$	$[2, 18]$
3	$[y, \frac{1}{2} - x, z + \frac{1}{4}]$	$[3, 19]$
4	$[-x, -y, z]$	$[4, 20]$
5	$[-x, y, z + \frac{1}{2}]$	$[5, 21]$
6	$[x, -y, z + \frac{1}{2}]$	$[6, 22]$
7	$[\frac{1}{2} - y, -x, z + \frac{1}{4}]$	$[7, 23]$
8	$[y + \frac{1}{2}, x, z + \frac{1}{4}]$	$[8, 24]$
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	$[9, 25]$
10	$[\frac{1}{2} - y, x, z + \frac{3}{4}]$	$[10, 26]$
11	$[y + \frac{1}{2}, -x, z + \frac{3}{4}]$	$[11, 27]$
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	$[12, 28]$
13	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	$[13, 29]$
14	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	$[14, 30]$
15	$[-y, \frac{1}{2} - x, z + \frac{3}{4}]$	$[15, 31]$
16	$[y, x + \frac{1}{2}, z + \frac{3}{4}]$	$[16, 32]$