

Table 1: Wyckoff site: **8a**, site symmetry: $\dots 21'$

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

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

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