

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]