

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

No.	position	mapping
1	$[0, 0, z]$	[1,2,5,6]
2	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[3,4,7,8]

Table 2: Wyckoff site: 4b, site symmetry: $2..$

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	[1,2]
2	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[3,4]
3	$[\frac{1}{2}, 0, z]$	[5,6]
4	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[7,8]

Table 3: Wyckoff site: 8c, site symmetry: 1

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