

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

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

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

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

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

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