

Table 1: Wyckoff site: 4a, site symmetry:  $\dots 2$

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

Table 2: Wyckoff site: 4b, site symmetry:  $\dots 2$

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

Table 3: Wyckoff site: 4c, site symmetry:  $\dots m'$

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

Table 4: Wyckoff site: 8d, site symmetry: 1

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