

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $2..$

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

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

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