

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

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

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

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

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

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

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

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