

Table 1: Wyckoff site: 2a, site symmetry: 2.mm

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

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

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

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

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

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

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