

Table 1: Wyckoff site: **2a**, site symmetry:  $2.\mathbf{m}'\mathbf{m}'$

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry:  $..\mathbf{m}'$

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

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

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