

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

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

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

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

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

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

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

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