

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

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

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

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

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

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

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

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