

Table 1: Wyckoff site: **4a**, site symmetry: -1

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

Table 2: Wyckoff site: **4b**, site symmetry: -1

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

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

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

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

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