

Table 1: Wyckoff site: **1a**, site symmetry:  $4'mm'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 5, 6, 7, 8]$

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

No.	position	mapping
1	$[x, x, z]$	$[1, 3]$
2	$[-x, -x, z]$	$[2, 4]$
3	$[-x, x, z]$	$[5, 7]$
4	$[x, -x, z]$	$[6, 8]$

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

No.	position	mapping
1	$[x, 0, z]$	$[1, 8]$
2	$[-x, 0, z]$	$[2, 7]$
3	$[0, x, z]$	$[3, 5]$
4	$[0, -x, z]$	$[4, 6]$

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

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