

Table 1: Wyckoff site:  $1\mathbf{o}$ , site symmetry:  $42'2'$ 

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

 Table 2: Wyckoff site:  $2\mathbf{a}$ , site symmetry:  $4..$ 

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

 Table 3: Wyckoff site:  $4\mathbf{b}$ , site symmetry:  $..2'$ 

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

 Table 4: Wyckoff site:  $4\mathbf{c}$ , site symmetry:  $..2'$ 

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

 Table 5: Wyckoff site:  $8\mathbf{d}$ , site symmetry:  $1$ 

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

*continued ...*

Table 5

No.	position	mapping
8	$[-y, -x, -z]$	[7]