

Table 1: Wyckoff site:  $1o$ , site symmetry:  $-42'm'$ 

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

Table 2: Wyckoff site:  $2a$ , site symmetry:  $2.m'm'$ 

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

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

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

Table 5: Wyckoff site:  $8d$ , 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]