

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

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry:  $\dots 2'$ 

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

Table 4: Wyckoff site: **4d**, site symmetry:  $2' \dots$ 

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

Table 5: Wyckoff site: **8e**, site symmetry:  $1$ 

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	$[2]$

*continued ...*

Table 5

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