

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

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry: -1

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

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

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

Table 5: Wyckoff site: **4e**, site symmetry: 2

No.	position	mapping
1	$[0, y, \frac{1}{4}]$	$[1, 2]$
2	$[0, -y, \frac{3}{4}]$	$[3, 4]$

continued ...

Table 5

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

Table 6: Wyckoff site: **8f**, site symmetry: **1**

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