

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $..2$

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

Table 4: Wyckoff site: 4d, site symmetry: $..2$

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

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

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

continued ...

Table 5

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