

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

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

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

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

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

continued ...

Table 5

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