

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	$[0, \frac{1}{2}, 0]$	[5,7]
4	$[0, \frac{1}{2}, \frac{1}{2}]$	[6,8]

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

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	[1,3]
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	[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 3: Wyckoff site: 4c, site symmetry: $2'..$

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

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

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

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

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

continued ...

Table 5

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