

Table 1: Wyckoff site: 4a, site symmetry: $\dots 2'$

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

Table 2: Wyckoff site: 4b, site symmetry: $\dots 2$

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

Table 3: Wyckoff site: 4c, site symmetry: $\mathfrak{m}' \dots$

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

Table 4: Wyckoff site: 8d, site symmetry: 1

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