

Table 1: Wyckoff site: 2a, site symmetry:  $mm'2'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $mm'2'$

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

Table 3: Wyckoff site: 4c, site symmetry:  $.m'$

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $m..$

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

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

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