

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

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

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

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

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

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

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

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

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

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

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

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