

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

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

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

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

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

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

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

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

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

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

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

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