

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

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

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

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

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

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

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

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

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

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

*continued ...*

Table 5

No.	position	mapping
7	$[-x, y, z]$	[7]
8	$[x, -y, z]$	[8]