

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: $2m'm'$.

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

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

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

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

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

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

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