

Table 1: Wyckoff site: **2a**, site symmetry:  $4m'm'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 13, 14, 15, 16]$
2	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[5, 6, 7, 8, 9, 10, 11, 12]$

Table 2: Wyckoff site: **4b**, site symmetry:  $2m'm'$

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 4, 13, 14]$
2	$[\frac{1}{2}, 0, z]$	$[2, 3, 15, 16]$
3	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[5, 6, 9, 12]$
4	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[7, 8, 10, 11]$

Table 3: Wyckoff site: **8c**, site symmetry:  $.m'$

No.	position	mapping
1	$[x, x, z]$	$[1, 16]$
2	$[-x, x, z]$	$[2, 13]$
3	$[x, -x, z]$	$[3, 14]$
4	$[-x, -x, z]$	$[4, 15]$
5	$[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]$	$[5, 10]$
6	$[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	$[6, 11]$
7	$[\frac{1}{2} - x, \frac{1}{2} - x, z + \frac{1}{2}]$	$[7, 12]$
8	$[x + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	$[8, 9]$

Table 4: Wyckoff site: **8d**, site symmetry:  $.m'$

No.	position	mapping
1	$[x, 0, z]$	$[1, 14]$
2	$[0, x, z]$	$[2, 16]$
3	$[0, -x, z]$	$[3, 15]$
4	$[-x, 0, z]$	$[4, 13]$
5	$[\frac{1}{2} - x, \frac{1}{2}, z + \frac{1}{2}]$	$[5, 12]$
6	$[x + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[6, 9]$
7	$[\frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	$[7, 11]$
8	$[\frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	$[8, 10]$

Table 5: Wyckoff site: **16e**, site symmetry: **1**

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x, z]$	[2]
3	$[y, -x, z]$	[3]
4	$[-x, -y, z]$	[4]
5	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[6]
7	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[7]
8	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[10]
11	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[11]
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[12]
13	$[-x, y, z]$	[13]
14	$[x, -y, z]$	[14]
15	$[-y, -x, z]$	[15]
16	$[y, x, z]$	[16]