

Table 1: Wyckoff site: 2a, site symmetry:  $4mm1'$ 

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 5, 6, 7, 8, 17, 18, 19, 20, 21, 22, 23, 24]$
2	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[9, 10, 11, 12, 13, 14, 15, 16, 25, 26, 27, 28, 29, 30, 31, 32]$

Table 2: Wyckoff site: 4b, site symmetry:  $2mm.1'$ 

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 4, 5, 6, 17, 20, 21, 22]$
2	$[\frac{1}{2}, 0, z]$	$[2, 3, 7, 8, 18, 19, 23, 24]$
3	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[9, 12, 13, 14, 25, 28, 29, 30]$
4	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[10, 11, 15, 16, 26, 27, 31, 32]$

Table 3: Wyckoff site: 8c, site symmetry:  $.m1'$ 

No.	position	mapping
1	$[x, x, z]$	$[1, 8, 17, 24]$
2	$[-x, x, z]$	$[2, 5, 18, 21]$
3	$[x, -x, z]$	$[3, 6, 19, 22]$
4	$[-x, -x, z]$	$[4, 7, 20, 23]$
5	$[x + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	$[9, 16, 25, 32]$
6	$[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]$	$[10, 13, 26, 29]$
7	$[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	$[11, 14, 27, 30]$
8	$[\frac{1}{2} - x, \frac{1}{2} - x, z + \frac{1}{2}]$	$[12, 15, 28, 31]$

Table 4: Wyckoff site: 8d, site symmetry:  $.m.1'$ 

No.	position	mapping
1	$[x, 0, z]$	$[1, 6, 17, 22]$
2	$[0, x, z]$	$[2, 8, 18, 24]$
3	$[0, -x, z]$	$[3, 7, 19, 23]$
4	$[-x, 0, z]$	$[4, 5, 20, 21]$
5	$[x + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[9, 14, 25, 30]$
6	$[\frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	$[10, 16, 26, 32]$
7	$[\frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	$[11, 15, 27, 31]$
8	$[\frac{1}{2} - x, \frac{1}{2}, z + \frac{1}{2}]$	$[12, 13, 28, 29]$

Table 5: Wyckoff site:  $16e$ , site symmetry:  $11'$ 

No.	position	mapping
1	$[x, y, z]$	$[1, 17]$
2	$[-y, x, z]$	$[2, 18]$
3	$[y, -x, z]$	$[3, 19]$
4	$[-x, -y, z]$	$[4, 20]$
5	$[-x, y, z]$	$[5, 21]$
6	$[x, -y, z]$	$[6, 22]$
7	$[-y, -x, z]$	$[7, 23]$
8	$[y, x, z]$	$[8, 24]$
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	$[9, 25]$
10	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	$[10, 26]$
11	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	$[11, 27]$
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	$[12, 28]$
13	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	$[13, 29]$
14	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	$[14, 30]$
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	$[15, 31]$
16	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	$[16, 32]$