

Table 1: Wyckoff site: 3a, site symmetry:  $\bar{3}2$ .

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{3}]$	$[7, 8, 9, 10, 11, 12]$
3	$[\frac{1}{3}, \frac{2}{3}, \frac{2}{3}]$	$[13, 14, 15, 16, 17, 18]$

Table 2: Wyckoff site: 3b, site symmetry:  $\bar{3}2$ .

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{5}{6}]$	$[7, 8, 9, 10, 11, 12]$
3	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{6}]$	$[13, 14, 15, 16, 17, 18]$

Table 3: Wyckoff site: 6c, site symmetry:  $\bar{3}$ .

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3]$
2	$[0, 0, -z]$	$[4, 5, 6]$
3	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}]$	$[7, 8, 9]$
4	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{3} - z]$	$[10, 11, 12]$
5	$[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}]$	$[13, 14, 15]$
6	$[\frac{1}{3}, \frac{2}{3}, \frac{2}{3} - z]$	$[16, 17, 18]$

Table 4: Wyckoff site: 9d, site symmetry:  $\bar{3}2$ .

No.	position	mapping
1	$[x, 0, 0]$	$[1, 4]$
2	$[0, x, 0]$	$[2, 5]$
3	$[-x, -x, 0]$	$[3, 6]$
4	$[x + \frac{2}{3}, \frac{1}{3}, \frac{1}{3}]$	$[7, 10]$
5	$[\frac{2}{3}, x + \frac{1}{3}, \frac{1}{3}]$	$[8, 11]$
6	$[\frac{2}{3} - x, \frac{1}{3} - x, \frac{1}{3}]$	$[9, 12]$
7	$[x + \frac{1}{3}, \frac{2}{3}, \frac{2}{3}]$	$[13, 16]$
8	$[\frac{1}{3}, x + \frac{2}{3}, \frac{2}{3}]$	$[14, 17]$
9	$[\frac{1}{3} - x, \frac{2}{3} - x, \frac{2}{3}]$	$[15, 18]$

Table 5: Wyckoff site:  $9\mathbf{e}$ , site symmetry:  $.2.$ 

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	[1,4]
2	$[0, x, \frac{1}{2}]$	[2,5]
3	$[-x, -x, \frac{1}{2}]$	[3,6]
4	$[x + \frac{2}{3}, \frac{1}{3}, \frac{5}{6}]$	[7,10]
5	$[\frac{2}{3}, x + \frac{1}{3}, \frac{5}{6}]$	[8,11]
6	$[\frac{2}{3} - x, \frac{1}{3} - x, \frac{5}{6}]$	[9,12]
7	$[x + \frac{1}{3}, \frac{2}{3}, \frac{1}{6}]$	[13,16]
8	$[\frac{1}{3}, x + \frac{2}{3}, \frac{1}{6}]$	[14,17]
9	$[\frac{1}{3} - x, \frac{2}{3} - x, \frac{1}{6}]$	[15,18]

Table 6: Wyckoff site:  $18\mathbf{f}$ , site symmetry:  $1$ 

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x - y, z]$	[2]
3	$[-x + y, -x, z]$	[3]
4	$[x - y, -y, -z]$	[4]
5	$[y, x, -z]$	[5]
6	$[-x, -x + y, -z]$	[6]
7	$[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	[7]
8	$[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{1}{3}]$	[8]
9	$[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$	[9]
10	$[x - y + \frac{2}{3}, \frac{1}{3} - y, \frac{1}{3} - z]$	[10]
11	$[y + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{3} - z]$	[11]
12	$[\frac{2}{3} - x, -x + y + \frac{1}{3}, \frac{1}{3} - z]$	[12]
13	$[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	[13]
14	$[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{2}{3}]$	[14]
15	$[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$	[15]
16	$[x - y + \frac{1}{3}, \frac{2}{3} - y, \frac{2}{3} - z]$	[16]
17	$[y + \frac{1}{3}, x + \frac{2}{3}, \frac{2}{3} - z]$	[17]
18	$[\frac{1}{3} - x, -x + y + \frac{2}{3}, \frac{2}{3} - z]$	[18]