

Table 1: Wyckoff site: 3a, site symmetry: $3m.1'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 5, 6, 19, 20, 21, 22, 23, 24]$
2	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}]$	$[7, 8, 9, 10, 11, 12, 25, 26, 27, 28, 29, 30]$
3	$[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}]$	$[13, 14, 15, 16, 17, 18, 31, 32, 33, 34, 35, 36]$

 Table 2: Wyckoff site: 9b, site symmetry: $.m.1'$

No.	position	mapping
1	$[x, -x, z]$	$[1, 5, 19, 23]$
2	$[x, 2x, z]$	$[2, 6, 20, 24]$
3	$[-2x, -x, z]$	$[3, 4, 21, 22]$
4	$[x + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$	$[7, 11, 25, 29]$
5	$[x + \frac{2}{3}, 2x + \frac{1}{3}, z + \frac{1}{3}]$	$[8, 12, 26, 30]$
6	$[\frac{2}{3} - 2x, \frac{1}{3} - x, z + \frac{1}{3}]$	$[9, 10, 27, 28]$
7	$[x + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$	$[13, 17, 31, 35]$
8	$[x + \frac{1}{3}, 2x + \frac{2}{3}, z + \frac{2}{3}]$	$[14, 18, 32, 36]$
9	$[\frac{1}{3} - 2x, \frac{2}{3} - x, z + \frac{2}{3}]$	$[15, 16, 33, 34]$

 Table 3: Wyckoff site: 18c, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 19]$
2	$[-y, x - y, z]$	$[2, 20]$
3	$[-x + y, -x, z]$	$[3, 21]$
4	$[-x + y, y, z]$	$[4, 22]$
5	$[-y, -x, z]$	$[5, 23]$
6	$[x, x - y, z]$	$[6, 24]$
7	$[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	$[7, 25]$
8	$[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{1}{3}]$	$[8, 26]$
9	$[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$	$[9, 27]$
10	$[-x + y + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	$[10, 28]$
11	$[\frac{2}{3} - y, \frac{1}{3} - x, z + \frac{1}{3}]$	$[11, 29]$
12	$[x + \frac{2}{3}, x - y + \frac{1}{3}, z + \frac{1}{3}]$	$[12, 30]$
13	$[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	$[13, 31]$
14	$[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{2}{3}]$	$[14, 32]$
15	$[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$	$[15, 33]$
16	$[-x + y + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	$[16, 34]$
17	$[\frac{1}{3} - y, \frac{2}{3} - x, z + \frac{2}{3}]$	$[17, 35]$
18	$[x + \frac{1}{3}, x - y + \frac{2}{3}, z + \frac{2}{3}]$	$[18, 36]$