

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

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

Table 2: Wyckoff site: 3b, site symmetry:  $-3..1'$

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

Table 3: Wyckoff site: 6c, site symmetry:  $3..1'$

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

Table 4: Wyckoff site: 9d, site symmetry:  $-11'$

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

Table 5: Wyckoff site: 9e, site symmetry:  $-11'$ 

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

Table 6: Wyckoff site: 18f, 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	$[-x, -y, -z]$	[4,22]
5	$[y, -x + y, -z]$	[5,23]
6	$[x - y, x, -z]$	[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	$[\frac{2}{3} - x, \frac{1}{3} - y, \frac{1}{3} - z]$	[10,28]
11	$[y + \frac{2}{3}, -x + y + \frac{1}{3}, \frac{1}{3} - z]$	[11,29]
12	$[x - y + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{3} - z]$	[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	$[\frac{1}{3} - x, \frac{2}{3} - y, \frac{2}{3} - z]$	[16,34]
17	$[y + \frac{1}{3}, -x + y + \frac{2}{3}, \frac{2}{3} - z]$	[17,35]
18	$[x - y + \frac{1}{3}, x + \frac{2}{3}, \frac{2}{3} - z]$	[18,36]