

Table 1: Wyckoff site: 2a, site symmetry: $3.m'$

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

Table 2: Wyckoff site: 4b, site symmetry: $3..$

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

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

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

Table 4: Wyckoff site: 12d, site symmetry: 1

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