

Table 1: Wyckoff site: 2a, site symmetry: $6'..$

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

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

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

Table 3: Wyckoff site: 6c, site symmetry: $2'..$

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

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	$[-x, -x + y, z + \frac{1}{2}]$	$[4]$
5	$[x - y, -y, z + \frac{1}{2}]$	$[5]$
6	$[y, x, z + \frac{1}{2}]$	$[6]$
7	$[x - y, x, z]$	$[7]$
8	$[-x, -y, z]$	$[8]$
9	$[y, -x + y, z]$	$[9]$
10	$[-x + y, y, z + \frac{1}{2}]$	$[10]$
11	$[-y, -x, z + \frac{1}{2}]$	$[11]$
12	$[x, x - y, z + \frac{1}{2}]$	$[12]$