

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

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

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

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

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

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

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

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