

Table 1: Wyckoff site: 2a, site symmetry:  $3.m1'$ 

No.	position	mapping
1	$[0, 0, z]$	$[1, 3, 5, 10, 11, 12, 13, 15, 17, 22, 23, 24]$
2	$[0, 0, z + \frac{1}{2}]$	$[2, 4, 6, 7, 8, 9, 14, 16, 18, 19, 20, 21]$

Table 2: Wyckoff site: 4b, site symmetry:  $3..1'$ 

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 3, 5, 13, 15, 17]$
2	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	$[2, 4, 6, 14, 16, 18]$
3	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	$[7, 8, 9, 19, 20, 21]$
4	$[\frac{2}{3}, \frac{1}{3}, z]$	$[10, 11, 12, 22, 23, 24]$

Table 3: Wyckoff site: 6c, site symmetry:  $..m1'$ 

No.	position	mapping
1	$[x, 0, z]$	$[1, 11, 13, 23]$
2	$[x, x, z + \frac{1}{2}]$	$[2, 9, 14, 21]$
3	$[0, x, z]$	$[3, 12, 15, 24]$
4	$[-x, 0, z + \frac{1}{2}]$	$[4, 7, 16, 19]$
5	$[-x, -x, z]$	$[5, 10, 17, 22]$
6	$[0, -x, z + \frac{1}{2}]$	$[6, 8, 18, 20]$

Table 4: Wyckoff site: 12d, site symmetry:  $11'$ 

No.	position	mapping
1	$[x, y, z]$	$[1, 13]$
2	$[x - y, x, z + \frac{1}{2}]$	$[2, 14]$
3	$[-y, x - y, z]$	$[3, 15]$
4	$[-x, -y, z + \frac{1}{2}]$	$[4, 16]$
5	$[-x + y, -x, z]$	$[5, 17]$
6	$[y, -x + y, z + \frac{1}{2}]$	$[6, 18]$
7	$[-x + y, y, z + \frac{1}{2}]$	$[7, 19]$
8	$[-y, -x, z + \frac{1}{2}]$	$[8, 20]$
9	$[x, x - y, z + \frac{1}{2}]$	$[9, 21]$
10	$[-x, -x + y, z]$	$[10, 22]$
11	$[x - y, -y, z]$	$[11, 23]$
12	$[y, x, z]$	$[12, 24]$