

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

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

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	$[\frac{2}{3}, \frac{1}{3}, z]$	$[2, 4, 6, 14, 16, 18]$
3	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	$[7, 8, 9, 19, 20, 21]$
4	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	$[10, 11, 12, 22, 23, 24]$

Table 3: Wyckoff site: 6c, site symmetry:  $2..1'$

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

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

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