

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

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

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

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

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

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

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	$[-x + y, y, z]$	$[7, 19]$
8	$[-y, -x, z]$	$[8, 20]$
9	$[x, x - y, z]$	$[9, 21]$
10	$[-x, -x + y, z + \frac{1}{2}]$	$[10, 22]$
11	$[x - y, -y, z + \frac{1}{2}]$	$[11, 23]$
12	$[y, x, z + \frac{1}{2}]$	$[12, 24]$