

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

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

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

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

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

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

Table 4: Wyckoff site: 6d, site symmetry:  $.m'$ .

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

Table 5: Wyckoff site: 12e, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x - y, z]$	$[2]$
3	$[-x + y, -x, z]$	$[3]$
4	$[-x + y, y, z + \frac{1}{2}]$	$[4]$
5	$[-y, -x, z + \frac{1}{2}]$	$[5]$
6	$[x, x - y, z + \frac{1}{2}]$	$[6]$

*continued ...*

Table 5

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