

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

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$

Table 2: Wyckoff site: 1b, site symmetry:  $-6m'2'$

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

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

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

Table 4: Wyckoff site: 1d, site symmetry:  $-6m'2'$

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

Table 5: Wyckoff site: 1e, site symmetry:  $-6m'2'$

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

Table 6: Wyckoff site: 1f, site symmetry:  $-6m'2'$

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

Table 7: Wyckoff site: 2g, site symmetry:  $3\bar{m}'$ .

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 10, 11, 12]$
2	$[0, 0, -z]$	$[4, 5, 6, 7, 8, 9]$

Table 8: Wyckoff site: 2h, site symmetry:  $3\bar{m}'$ .

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

Table 9: Wyckoff site: 2i, site symmetry:  $3\bar{m}'$ .

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

Table 10: Wyckoff site: 3j, site symmetry:  $\bar{m}\bar{m}'2'$ .

No.	position	mapping
1	$[x, -x, 0]$	$[1, 5, 9, 11]$
2	$[x, 2x, 0]$	$[2, 6, 7, 12]$
3	$[-2x, -x, 0]$	$[3, 4, 8, 10]$

Table 11: Wyckoff site: 3k, site symmetry:  $\bar{m}\bar{m}'2'$ .

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

Table 12: Wyckoff site: 6l, site symmetry:  $\bar{m}..$ .

No.	position	mapping
1	$[x, y, 0]$	$[1, 5]$
2	$[-y, x - y, 0]$	$[2, 6]$

*continued ...*

Table 12

No.	position	mapping
3	$[-x + y, -x, 0]$	[3,4]
4	$[x, x - y, 0]$	[7,12]
5	$[-x + y, y, 0]$	[8,10]
6	$[-y, -x, 0]$	[9,11]

Table 13: Wyckoff site:  $6\bar{\mathbf{m}}$ , site symmetry:  $\mathbf{m} \cdot \cdot$ 

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

Table 14: Wyckoff site:  $6\mathbf{n}$ , site symmetry:  $\cdot \mathbf{m}' \cdot$ 

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

Table 15: Wyckoff site:  $12\mathbf{o}$ , site symmetry:  $\mathbf{1}$ 

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

*continued ...*

Table 15

No.	position	mapping
12	$[x, x - y, z]$	[12]