

Table 1: Wyckoff site: **1a**, site symmetry:  $6'/\mathfrak{m}' \dots$

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:  $6'/\mathfrak{m}' \dots$

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: **2c**, site symmetry:  $-6' \dots$

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

Table 4: Wyckoff site: **2d**, site symmetry:  $-6' \dots$

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

Table 5: Wyckoff site: **2e**, site symmetry:  $6' \dots$

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

Table 6: Wyckoff site: **3f**, site symmetry:  $2'/\mathfrak{m}' \dots$

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

Table 7: Wyckoff site:  $3g$ , site symmetry:  $2'/m' \dots$ 

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

Table 8: Wyckoff site:  $4h$ , site symmetry:  $3 \dots$ 

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

Table 9: Wyckoff site:  $6i$ , site symmetry:  $2' \dots$ 

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

Table 10: Wyckoff site:  $6j$ , site symmetry:  $m' \dots$ 

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

Table 11: Wyckoff site:  $6k$ , site symmetry:  $m' \dots$ 

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	$[1, 11]$

*continued ...*

Table 11

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

Table 12: Wyckoff site: 121, site symmetry: 1

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