

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: 3 . .

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

Table 6: Wyckoff site: **4f**, site symmetry: **3.**.

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

Table 7: Wyckoff site: **6g**, site symmetry: **-1'**

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

Table 8: Wyckoff site: **6h**, site symmetry: **m'**.

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

Table 9: Wyckoff site: **12i**, site symmetry: **1**

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

continued ...

Table 9

No.	position	mapping
12	$[-y, x - y, \frac{1}{2} - z]$	[12]