

Table 1: Wyckoff site: 2a, site symmetry: $32.$

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

Table 2: Wyckoff site: 2b, site symmetry: $-6..$

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

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

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

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

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

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

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

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

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	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[7,8,9]
4	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[10,11,12]

Table 7: Wyckoff site: **6g**, site symmetry: **.2**.

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

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

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

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

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

continued ...

Table 9

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