

Table 1: Wyckoff site: 2a, site symmetry: $3.21'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 13, 14, 15, 16, 17, 18]$
2	$[0, 0, \frac{1}{2}]$	$[7, 8, 9, 10, 11, 12, 19, 20, 21, 22, 23, 24]$

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

No.	position	mapping
1	$[0, 0, \frac{1}{4}]$	$[1, 2, 3, 7, 8, 9, 13, 14, 15, 19, 20, 21]$
2	$[0, 0, \frac{3}{4}]$	$[4, 5, 6, 10, 11, 12, 16, 17, 18, 22, 23, 24]$

Table 3: Wyckoff site: 2c, site symmetry: $3.21'$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1, 2, 3, 4, 5, 6, 13, 14, 15, 16, 17, 18]$
2	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[7, 8, 9, 10, 11, 12, 19, 20, 21, 22, 23, 24]$

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

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[1, 2, 3, 7, 8, 9, 13, 14, 15, 19, 20, 21]$
2	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[4, 5, 6, 10, 11, 12, 16, 17, 18, 22, 23, 24]$

Table 5: Wyckoff site: 2e, site symmetry: $3.21'$

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[1, 2, 3, 4, 5, 6, 13, 14, 15, 16, 17, 18]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[7, 8, 9, 10, 11, 12, 19, 20, 21, 22, 23, 24]$

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

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[1, 2, 3, 7, 8, 9, 13, 14, 15, 19, 20, 21]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[4, 5, 6, 10, 11, 12, 16, 17, 18, 22, 23, 24]$

Table 7: Wyckoff site: **4g**, site symmetry: $3..1'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 13, 14, 15]$
2	$[0, 0, -z]$	$[4, 5, 6, 16, 17, 18]$
3	$[0, 0, \frac{1}{2} - z]$	$[7, 8, 9, 19, 20, 21]$
4	$[0, 0, z + \frac{1}{2}]$	$[10, 11, 12, 22, 23, 24]$

Table 8: Wyckoff site: **4h**, site symmetry: $3..1'$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 2, 3, 13, 14, 15]$
2	$[\frac{1}{3}, \frac{2}{3}, -z]$	$[4, 5, 6, 16, 17, 18]$
3	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	$[7, 8, 9, 19, 20, 21]$
4	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	$[10, 11, 12, 22, 23, 24]$

Table 9: Wyckoff site: **4i**, site symmetry: $3..1'$

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, z]$	$[1, 2, 3, 13, 14, 15]$
2	$[\frac{2}{3}, \frac{1}{3}, -z]$	$[4, 5, 6, 16, 17, 18]$
3	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	$[7, 8, 9, 19, 20, 21]$
4	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	$[10, 11, 12, 22, 23, 24]$

Table 10: Wyckoff site: **6j**, site symmetry: $..21'$

No.	position	mapping
1	$[x, -x, 0]$	$[1, 6, 13, 18]$
2	$[x, 2x, 0]$	$[2, 4, 14, 16]$
3	$[-2x, -x, 0]$	$[3, 5, 15, 17]$
4	$[-2x, -x, \frac{1}{2}]$	$[7, 10, 19, 22]$
5	$[x, -x, \frac{1}{2}]$	$[8, 11, 20, 23]$
6	$[x, 2x, \frac{1}{2}]$	$[9, 12, 21, 24]$

Table 11: Wyckoff site: **6k**, site symmetry: $m..1'$

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	$[1, 8, 13, 20]$
2	$[-y, x - y, \frac{1}{4}]$	$[2, 9, 14, 21]$

continued ...

Table 11

No.	position	mapping
3	$[-x + y, -x, \frac{1}{4}]$	[3, 7, 15, 19]
4	$[x, x - y, \frac{3}{4}]$	[4, 12, 16, 24]
5	$[-x + y, y, \frac{3}{4}]$	[5, 10, 17, 22]
6	$[-y, -x, \frac{3}{4}]$	[6, 11, 18, 23]

Table 12: Wyckoff site: 121, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	[1, 13]
2	$[-y, x - y, z]$	[2, 14]
3	$[-x + y, -x, z]$	[3, 15]
4	$[x, x - y, -z]$	[4, 16]
5	$[-x + y, y, -z]$	[5, 17]
6	$[-y, -x, -z]$	[6, 18]
7	$[-x + y, -x, \frac{1}{2} - z]$	[7, 19]
8	$[x, y, \frac{1}{2} - z]$	[8, 20]
9	$[-y, x - y, \frac{1}{2} - z]$	[9, 21]
10	$[-x + y, y, z + \frac{1}{2}]$	[10, 22]
11	$[-y, -x, z + \frac{1}{2}]$	[11, 23]
12	$[x, x - y, z + \frac{1}{2}]$	[12, 24]