

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

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

Table 2: Wyckoff site: 2b, site symmetry: $-3..1'$

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $3..1'$

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

Table 6: Wyckoff site: 4f, site symmetry: $3..1'$

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

Table 7: Wyckoff site: 6g, site symmetry: $-11'$

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

Table 8: Wyckoff site: 6h, site symmetry: $m..1'$

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

Table 9: Wyckoff site: 12i, site symmetry: $11'$

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

continued ...

Table 9

No.	position	mapping
12	$[-y, x - y, \frac{1}{2} - z]$	[12, 24]