

Table 1: Wyckoff site: 3a, site symmetry: $2221'$

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

Table 2: Wyckoff site: 3b, site symmetry: $2221'$

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

Table 3: Wyckoff site: 3c, site symmetry: $2221'$

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

Table 4: Wyckoff site: 3d, site symmetry: $2221'$

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

Table 5: Wyckoff site: 6e, site symmetry: $2..1'$

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

Table 6: Wyckoff site: $6\mathbf{f}$, site symmetry: $2..1'$

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

Table 7: Wyckoff site: $6\mathbf{g}$, site symmetry: $..2.1'$

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

Table 8: Wyckoff site: $6\mathbf{h}$, site symmetry: $..2.1'$

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

Table 9: Wyckoff site: $6\mathbf{i}$, site symmetry: $..21'$

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

Table 10: Wyckoff site: 6j, site symmetry: $\cdot\cdot 21'$

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

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

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