

Table 1: Wyckoff site: 2a, site symmetry: $32.1'$

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

Table 2: Wyckoff site: 2b, site symmetry: $3.21'$

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

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

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

Table 4: Wyckoff site: 2d, site symmetry: $3.21'$

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

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	$[0, 0, -z]$	$[7, 8, 9, 19, 20, 21]$
4	$[0, 0, \frac{1}{2} - z]$	$[10, 11, 12, 22, 23, 24]$

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	$[\frac{2}{3}, \frac{1}{3}, -z]$	$[7, 8, 9, 19, 20, 21]$
4	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	$[10, 11, 12, 22, 23, 24]$

Table 7: Wyckoff site: **6g**, site symmetry: $..2.1'$

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

Table 8: Wyckoff site: **6h**, site symmetry: $..21'$

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

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	$[x - y, -y, -z]$	$[7, 19]$
8	$[y, x, -z]$	$[8, 20]$
9	$[-x, -x + y, -z]$	$[9, 21]$
10	$[x, x - y, \frac{1}{2} - z]$	$[10, 22]$
11	$[-x + y, y, \frac{1}{2} - z]$	$[11, 23]$

continued ...

Table 9

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