

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

| No. | position | mapping |
|-----|---|--|
| 1 | $[0, 0, 0]$ | $[1, 2, 3, 4, 5, 6, 19, 20, 21, 22, 23, 24]$ |
| 2 | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{3}]$ | $[7, 8, 9, 10, 11, 12, 25, 26, 27, 28, 29, 30]$ |
| 3 | $[\frac{1}{3}, \frac{2}{3}, \frac{2}{3}]$ | $[13, 14, 15, 16, 17, 18, 31, 32, 33, 34, 35, 36]$ |

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

| No. | position | mapping |
|-----|---|--|
| 1 | $[0, 0, \frac{1}{2}]$ | $[1, 2, 3, 4, 5, 6, 19, 20, 21, 22, 23, 24]$ |
| 2 | $[\frac{2}{3}, \frac{1}{3}, \frac{5}{6}]$ | $[7, 8, 9, 10, 11, 12, 25, 26, 27, 28, 29, 30]$ |
| 3 | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{6}]$ | $[13, 14, 15, 16, 17, 18, 31, 32, 33, 34, 35, 36]$ |

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

| No. | position | mapping |
|-----|---|----------------------------|
| 1 | $[0, 0, z]$ | $[1, 2, 3, 19, 20, 21]$ |
| 2 | $[0, 0, -z]$ | $[4, 5, 6, 22, 23, 24]$ |
| 3 | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}]$ | $[7, 8, 9, 25, 26, 27]$ |
| 4 | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{3} - z]$ | $[10, 11, 12, 28, 29, 30]$ |
| 5 | $[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}]$ | $[13, 14, 15, 31, 32, 33]$ |
| 6 | $[\frac{1}{3}, \frac{2}{3}, \frac{2}{3} - z]$ | $[16, 17, 18, 34, 35, 36]$ |

Table 4: Wyckoff site: 9d, site symmetry: $-11'$

| No. | position | mapping |
|-----|---|--------------------|
| 1 | $[\frac{1}{2}, 0, \frac{1}{2}]$ | $[1, 4, 19, 22]$ |
| 2 | $[0, \frac{1}{2}, \frac{1}{2}]$ | $[2, 5, 20, 23]$ |
| 3 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | $[3, 6, 21, 24]$ |
| 4 | $[\frac{1}{6}, \frac{1}{3}, \frac{5}{6}]$ | $[7, 10, 25, 28]$ |
| 5 | $[\frac{2}{3}, \frac{5}{6}, \frac{5}{6}]$ | $[8, 11, 26, 29]$ |
| 6 | $[\frac{1}{6}, \frac{5}{6}, \frac{5}{6}]$ | $[9, 12, 27, 30]$ |
| 7 | $[\frac{5}{6}, \frac{2}{3}, \frac{1}{6}]$ | $[13, 16, 31, 34]$ |
| 8 | $[\frac{1}{3}, \frac{1}{6}, \frac{1}{6}]$ | $[14, 17, 32, 35]$ |
| 9 | $[\frac{5}{6}, \frac{1}{6}, \frac{1}{6}]$ | $[15, 18, 33, 36]$ |

Table 5: Wyckoff site: 9e, site symmetry: $-11'$

| No. | position | mapping |
|-----|---|--------------------|
| 1 | $[\frac{1}{2}, 0, 0]$ | $[1, 4, 19, 22]$ |
| 2 | $[0, \frac{1}{2}, 0]$ | $[2, 5, 20, 23]$ |
| 3 | $[\frac{1}{2}, \frac{1}{2}, 0]$ | $[3, 6, 21, 24]$ |
| 4 | $[\frac{1}{6}, \frac{1}{3}, \frac{1}{3}]$ | $[7, 10, 25, 28]$ |
| 5 | $[\frac{2}{3}, \frac{5}{6}, \frac{1}{3}]$ | $[8, 11, 26, 29]$ |
| 6 | $[\frac{1}{6}, \frac{5}{6}, \frac{1}{3}]$ | $[9, 12, 27, 30]$ |
| 7 | $[\frac{5}{6}, \frac{2}{3}, \frac{2}{3}]$ | $[13, 16, 31, 34]$ |
| 8 | $[\frac{1}{3}, \frac{1}{6}, \frac{2}{3}]$ | $[14, 17, 32, 35]$ |
| 9 | $[\frac{5}{6}, \frac{1}{6}, \frac{2}{3}]$ | $[15, 18, 33, 36]$ |

Table 6: Wyckoff site: 18f, site symmetry: $11'$

| No. | position | mapping |
|-----|--|------------|
| 1 | $[x, y, z]$ | $[1, 19]$ |
| 2 | $[-y, x - y, z]$ | $[2, 20]$ |
| 3 | $[-x + y, -x, z]$ | $[3, 21]$ |
| 4 | $[-x, -y, -z]$ | $[4, 22]$ |
| 5 | $[y, -x + y, -z]$ | $[5, 23]$ |
| 6 | $[x - y, x, -z]$ | $[6, 24]$ |
| 7 | $[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$ | $[7, 25]$ |
| 8 | $[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{1}{3}]$ | $[8, 26]$ |
| 9 | $[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$ | $[9, 27]$ |
| 10 | $[\frac{2}{3} - x, \frac{1}{3} - y, \frac{1}{3} - z]$ | $[10, 28]$ |
| 11 | $[y + \frac{2}{3}, -x + y + \frac{1}{3}, \frac{1}{3} - z]$ | $[11, 29]$ |
| 12 | $[x - y + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{3} - z]$ | $[12, 30]$ |
| 13 | $[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$ | $[13, 31]$ |
| 14 | $[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{2}{3}]$ | $[14, 32]$ |
| 15 | $[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$ | $[15, 33]$ |
| 16 | $[\frac{1}{3} - x, \frac{2}{3} - y, \frac{2}{3} - z]$ | $[16, 34]$ |
| 17 | $[y + \frac{1}{3}, -x + y + \frac{2}{3}, \frac{2}{3} - z]$ | $[17, 35]$ |
| 18 | $[x - y + \frac{1}{3}, x + \frac{2}{3}, \frac{2}{3} - z]$ | $[18, 36]$ |