

MSG No. 160.65 $R3m$ [Type I, trigonal]

Table 1: Wyckoff site: **3a**, site symmetry: $3m$.

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

Table 2: Wyckoff site: **9b**, site symmetry: $\bar{3}m$.

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

Table 3: Wyckoff site: **18c**, site symmetry: 1

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