

MSG No. 148.19 $R\bar{3}'$ [Type III, trigonal]

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

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

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

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

Table 3: Wyckoff site: 6c, site symmetry: 3 ..

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

Table 4: Wyckoff site: 9d, site symmetry: $-1'$

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

Table 5: Wyckoff site: $9\mathbf{e}$, site symmetry: $-1'$

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

Table 6: Wyckoff site: $18\mathbf{f}$, site symmetry: 1

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