# MSG No. 166.99 $R\bar{3}'m$ [ Type III, trigonal ]

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

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

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

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

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

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

Table 4: Wyckoff site: `9d`, site symmetry: `.2'/m`.

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

Table 5: Wyckoff site: `9e`, site symmetry: `.2'/m.`

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

Table 6: Wyckoff site: `18f`, site symmetry: `.2'.`

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

Table 7: Wyckoff site: `18g`, site symmetry: `.2'.`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x, 0, \frac{1}{2}\right]$ | `[1,7]` |
| 2 | $\left[0, x, \frac{1}{2}\right]$ | `[2,8]` |
| 3 | $\left[-x, -x, \frac{1}{2}\right]$ | `[3,9]` |
| 4 | $\left[-x, 0, \frac{1}{2}\right]$ | `[4,10]` |
| 5 | $\left[0, -x, \frac{1}{2}\right]$ | `[5,11]` |
| 6 | $\left[x, x, \frac{1}{2}\right]$ | `[6,12]` |

*continued ...*

Table 7

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

Table 8: Wyckoff site: 18h, site symmetry: .m.

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

Table 9: Wyckoff site: 36i, 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] |

*continued ...*

Table 9

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