

Table 1: Wyckoff site: 8a, site symmetry:  $.3.1'$ 

| No. | position  | mapping                    |
|-----|---|----------------------------|
| 1   | $[x, x, x]$   | $[1, 5, 6, 25, 29, 30]$    |
| 2   | $[x, -x, \frac{1}{2} - x]$                            | $[2, 10, 11, 26, 34, 35]$  |
| 3   | $[\frac{1}{2} - x, x, -x]$                            | $[3, 7, 12, 27, 31, 36]$   |
| 4   | $[-x, \frac{1}{2} - x, x]$                            | $[4, 8, 9, 28, 32, 33]$    |
| 5   | $[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$ | $[13, 17, 18, 37, 41, 42]$ |
| 6   | $[x + \frac{1}{2}, \frac{1}{2} - x, -x]$              | $[14, 22, 23, 38, 46, 47]$ |
| 7   | $[-x, x + \frac{1}{2}, \frac{1}{2} - x]$              | $[15, 19, 24, 39, 43, 48]$ |
| 8   | $[\frac{1}{2} - x, -x, x + \frac{1}{2}]$              | $[16, 20, 21, 40, 44, 45]$ |

Table 2: Wyckoff site: 12b, site symmetry:  $2..1'$ 

| No. | position                                      | mapping            |
|-----|---|--------------------|
| 1   | $[x, 0, \frac{1}{4}]$                         | $[1, 2, 25, 26]$   |
| 2   | $[\frac{1}{2} - x, 0, \frac{3}{4}]$           | $[3, 16, 27, 40]$  |
| 3   | $[-x, \frac{1}{2}, \frac{1}{4}]$              | $[4, 15, 28, 39]$  |
| 4   | $[\frac{1}{4}, x, 0]$                         | $[5, 12, 29, 36]$  |
| 5   | $[0, \frac{1}{4}, x]$                         | $[6, 9, 30, 33]$   |
| 6   | $[\frac{1}{2}, \frac{1}{4}, -x]$              | $[7, 23, 31, 47]$  |
| 7   | $[\frac{3}{4}, \frac{1}{2} - x, 0]$           | $[8, 22, 32, 46]$  |
| 8   | $[\frac{1}{4}, -x, \frac{1}{2}]$              | $[10, 20, 34, 44]$ |
| 9   | $[0, \frac{3}{4}, \frac{1}{2} - x]$           | $[11, 19, 35, 43]$ |
| 10  | $[x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$ | $[13, 14, 37, 38]$ |
| 11  | $[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2}]$ | $[17, 24, 41, 48]$ |
| 12  | $[\frac{1}{2}, \frac{3}{4}, x + \frac{1}{2}]$ | $[18, 21, 42, 45]$ |

Table 3: Wyckoff site: 24c, site symmetry:  $11'$ 

| No. | position                   | mapping    |
|-----|----------------------------|------------|
| 1   | $[x, y, z]$                | $[1, 25]$  |
| 2   | $[x, -y, \frac{1}{2} - z]$ | $[2, 26]$  |
| 3   | $[\frac{1}{2} - x, y, -z]$ | $[3, 27]$  |
| 4   | $[-x, \frac{1}{2} - y, z]$ | $[4, 28]$  |
| 5   | $[z, x, y]$                | $[5, 29]$  |
| 6   | $[y, z, x]$                | $[6, 30]$  |
| 7   | $[\frac{1}{2} - y, z, -x]$ | $[7, 31]$  |
| 8   | $[-z, \frac{1}{2} - x, y]$ | $[8, 32]$  |
| 9   | $[-y, \frac{1}{2} - z, x]$ | $[9, 33]$  |
| 10  | $[z, -x, \frac{1}{2} - y]$ | $[10, 34]$ |
| 11  | $[y, -z, \frac{1}{2} - x]$ | $[11, 35]$ |

*continued ...*

Table 3

| No. | position  | mapping |
|-----|---|---------|
| 12  | $[\frac{1}{2} - z, x, -y]$                            | [12,36] |
| 13  | $[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$ | [13,37] |
| 14  | $[x + \frac{1}{2}, \frac{1}{2} - y, -z]$              | [14,38] |
| 15  | $[-x, y + \frac{1}{2}, \frac{1}{2} - z]$              | [15,39] |
| 16  | $[\frac{1}{2} - x, -y, z + \frac{1}{2}]$              | [16,40] |
| 17  | $[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$ | [17,41] |
| 18  | $[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$ | [18,42] |
| 19  | $[-y, z + \frac{1}{2}, \frac{1}{2} - x]$              | [19,43] |
| 20  | $[\frac{1}{2} - z, -x, y + \frac{1}{2}]$              | [20,44] |
| 21  | $[\frac{1}{2} - y, -z, x + \frac{1}{2}]$              | [21,45] |
| 22  | $[z + \frac{1}{2}, \frac{1}{2} - x, -y]$              | [22,46] |
| 23  | $[y + \frac{1}{2}, \frac{1}{2} - z, -x]$              | [23,47] |
| 24  | $[-z, x + \frac{1}{2}, \frac{1}{2} - y]$              | [24,48] |