

Table 1: Wyckoff site: 4a, site symmetry:  $2.2'2'$

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

Table 2: Wyckoff site: 4b, site symmetry:  $-4..$

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

Table 3: Wyckoff site: 4c, site symmetry:  $-4'..$

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

Table 4: Wyckoff site: 4d, site symmetry:  $2.22$

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

Table 5: Wyckoff site: 8e, site symmetry:  $..2'$

| No. | position                | mapping |
|-----|-------------------------|---------|
| 1   | $[x, x, \frac{1}{4}]$   | [1,11]  |
| 2   | $[-x, -x, \frac{1}{4}]$ | [2,12]  |

*continued ...*

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 2..

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

Table 7: Wyckoff site: 8g, site symmetry: 2..

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

Table 8: Wyckoff site: 8h, site symmetry: ..2

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

continued ...

Table 8

| No. | position                             | mapping |
|-----|--------------------------------------|---------|
| 6   | $[\frac{1}{2} - x, -x, \frac{1}{2}]$ | [10,12] |
| 7   | $[x, \frac{1}{2} - x, \frac{1}{2}]$  | [13,16] |
| 8   | $[-x, x + \frac{1}{2}, \frac{1}{2}]$ | [14,15] |

Table 9: Wyckoff site: 16i, site symmetry: 1

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