

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

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

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

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

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

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

Table 4: Wyckoff site: 8d, site symmetry:  $-1'$

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

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

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

Table 6: Wyckoff site: **8f**, site symmetry:  $..2'$ 

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

Table 7: Wyckoff site: **16g**, site symmetry:  $1$ 

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