

Table 1: Wyckoff site: 4a, site symmetry: 2.22

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

Table 2: Wyckoff site: 4b, site symmetry: 2.2'2'

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

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

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

Table 4: Wyckoff site: 8d, site symmetry: 2..

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

Table 5: Wyckoff site:  $8e$ , site symmetry:  $\dots 2$ 

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

Table 6: Wyckoff site:  $8f$ , site symmetry:  $\dots 2'$ 

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

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

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