

SG No. 212  $O^6$   $P4_332$  [ cubic ]

 \* plus set:  $+ [0, 0, 0]$ 

 Table 1: Wyckoff site: 4a, site symmetry:  $.32$ 

| No. | position                                  | mapping           |
|-----|-------------------------------------------|-------------------|
| 1   | $[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$ | [1,5,9,14,19,24]  |
| 2   | $[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}]$ | [2,7,12,13,17,21] |
| 3   | $[\frac{7}{8}, \frac{5}{8}, \frac{3}{8}]$ | [3,8,10,15,20,22] |
| 4   | $[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}]$ | [4,6,11,16,18,23] |

 Table 2: Wyckoff site: 4b, site symmetry:  $.32$ 

| No. | position                                  | mapping           |
|-----|-------------------------------------------|-------------------|
| 1   | $[\frac{5}{8}, \frac{5}{8}, \frac{5}{8}]$ | [1,5,9,14,19,24]  |
| 2   | $[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}]$ | [2,7,12,13,17,21] |
| 3   | $[\frac{3}{8}, \frac{1}{8}, \frac{7}{8}]$ | [3,8,10,15,20,22] |
| 4   | $[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}]$ | [4,6,11,16,18,23] |

 Table 3: Wyckoff site: 8c, site symmetry:  $.3$ 

| No. | position                                              | mapping    |
|-----|-------------------------------------------------------|------------|
| 1   | $[x, x, x]$                                           | [1,5,9]    |
| 2   | $[\frac{1}{2} - x, -x, x + \frac{1}{2}]$              | [2,7,12]   |
| 3   | $[-x, x + \frac{1}{2}, \frac{1}{2} - x]$              | [3,8,10]   |
| 4   | $[x + \frac{1}{2}, \frac{1}{2} - x, -x]$              | [4,6,11]   |
| 5   | $[x + \frac{1}{4}, x + \frac{3}{4}, \frac{3}{4} - x]$ | [13,17,21] |
| 6   | $[\frac{1}{4} - x, \frac{1}{4} - x, \frac{1}{4} - x]$ | [14,19,24] |
| 7   | $[x + \frac{3}{4}, \frac{3}{4} - x, x + \frac{1}{4}]$ | [15,20,22] |
| 8   | $[\frac{3}{4} - x, x + \frac{1}{4}, x + \frac{3}{4}]$ | [16,18,23] |

 Table 4: Wyckoff site: 12d, site symmetry:  $..2$ 

| No. | position                                          | mapping |
|-----|---------------------------------------------------|---------|
| 1   | $[\frac{1}{8}, y, \frac{1}{4} - y]$               | [1,19]  |
| 2   | $[\frac{3}{8}, -y, \frac{3}{4} - y]$              | [2,17]  |
| 3   | $[\frac{7}{8}, y + \frac{1}{2}, y + \frac{1}{4}]$ | [3,20]  |
| 4   | $[\frac{5}{8}, \frac{1}{2} - y, y + \frac{3}{4}]$ | [4,18]  |
| 5   | $[\frac{1}{4} - y, \frac{1}{8}, y]$               | [5,14]  |
| 6   | $[\frac{3}{4} - y, \frac{3}{8}, -y]$              | [6,16]  |
| 7   | $[y + \frac{1}{4}, \frac{7}{8}, y + \frac{1}{2}]$ | [7,13]  |
| 8   | $[y + \frac{3}{4}, \frac{5}{8}, \frac{1}{2} - y]$ | [8,15]  |

continued ...

Table 4

| No. | position                                          | mapping |
|-----|---------------------------------------------------|---------|
| 9   | $[y, \frac{1}{4} - y, \frac{1}{8}]$               | [9,24]  |
| 10  | $[-y, \frac{3}{4} - y, \frac{3}{8}]$              | [10,22] |
| 11  | $[y + \frac{1}{2}, y + \frac{1}{4}, \frac{7}{8}]$ | [11,23] |
| 12  | $[\frac{1}{2} - y, y + \frac{3}{4}, \frac{5}{8}]$ | [12,21] |

Table 5: Wyckoff site: 24e, site symmetry: 1

| No. | position                                              | mapping |
|-----|-------------------------------------------------------|---------|
| 1   | $[x, y, z]$                                           | [1]     |
| 2   | $[\frac{1}{2} - x, -y, z + \frac{1}{2}]$              | [2]     |
| 3   | $[-x, y + \frac{1}{2}, \frac{1}{2} - z]$              | [3]     |
| 4   | $[x + \frac{1}{2}, \frac{1}{2} - y, -z]$              | [4]     |
| 5   | $[z, x, y]$                                           | [5]     |
| 6   | $[z + \frac{1}{2}, \frac{1}{2} - x, -y]$              | [6]     |
| 7   | $[\frac{1}{2} - z, -x, y + \frac{1}{2}]$              | [7]     |
| 8   | $[-z, x + \frac{1}{2}, \frac{1}{2} - y]$              | [8]     |
| 9   | $[y, z, x]$                                           | [9]     |
| 10  | $[-y, z + \frac{1}{2}, \frac{1}{2} - x]$              | [10]    |
| 11  | $[y + \frac{1}{2}, \frac{1}{2} - z, -x]$              | [11]    |
| 12  | $[\frac{1}{2} - y, -z, x + \frac{1}{2}]$              | [12]    |
| 13  | $[y + \frac{1}{4}, x + \frac{3}{4}, \frac{3}{4} - z]$ | [13]    |
| 14  | $[\frac{1}{4} - y, \frac{1}{4} - x, \frac{1}{4} - z]$ | [14]    |
| 15  | $[y + \frac{3}{4}, \frac{3}{4} - x, z + \frac{1}{4}]$ | [15]    |
| 16  | $[\frac{3}{4} - y, x + \frac{1}{4}, z + \frac{3}{4}]$ | [16]    |
| 17  | $[x + \frac{1}{4}, z + \frac{3}{4}, \frac{3}{4} - y]$ | [17]    |
| 18  | $[\frac{3}{4} - x, z + \frac{1}{4}, y + \frac{3}{4}]$ | [18]    |
| 19  | $[\frac{1}{4} - x, \frac{1}{4} - z, \frac{1}{4} - y]$ | [19]    |
| 20  | $[x + \frac{3}{4}, \frac{3}{4} - z, y + \frac{1}{4}]$ | [20]    |
| 21  | $[z + \frac{1}{4}, y + \frac{3}{4}, \frac{3}{4} - x]$ | [21]    |
| 22  | $[z + \frac{3}{4}, \frac{3}{4} - y, x + \frac{1}{4}]$ | [22]    |
| 23  | $[\frac{3}{4} - z, y + \frac{1}{4}, x + \frac{3}{4}]$ | [23]    |
| 24  | $[\frac{1}{4} - z, \frac{1}{4} - y, \frac{1}{4} - x]$ | [24]    |