

Table 1: Wyckoff site: 4a, site symmetry:  $-1'$

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

Table 2: Wyckoff site: 4b, site symmetry:  $-1'$

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

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

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

Table 4: Wyckoff site: 8d, site symmetry: 1

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