

MSG No. 85.60  $P4/n1'$  [ Type II, tetragonal ]

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry:  $4..1'$

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

Table 4: Wyckoff site: 4d, site symmetry:  $-11'$

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

Table 5: Wyckoff site: 4e, site symmetry:  $-11'$

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

Table 6: Wyckoff site:  $4\mathbf{f}$ , site symmetry:  $2..1'$ 

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

Table 7: Wyckoff site:  $8\mathbf{g}$ , site symmetry:  $11'$ 

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