

MSG No. 55.355 *Pb'am* [ Type III, orthorhombic ]

Table 1: Wyckoff site: **2a**, site symmetry:  $\dots 2'/\text{m}$

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

Table 2: Wyckoff site: **2b**, site symmetry:  $\dots 2'/\text{m}$

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

Table 3: Wyckoff site: **2c**, site symmetry:  $\dots 2'/\text{m}$

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

Table 4: Wyckoff site: **2d**, site symmetry:  $\dots 2'/\text{m}$

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

Table 5: Wyckoff site: **4e**, site symmetry:  $\dots 2'$

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

Table 6: Wyckoff site: 4f, site symmetry: ...2'

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

Table 7: Wyckoff site: 4g, site symmetry: ...m

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

Table 8: Wyckoff site: 4h, site symmetry: ...m

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

Table 9: Wyckoff site: 8i, site symmetry: 1

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