

MSG No. 60.425 $Pb'c'n'$ [Type III, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry: **.2.**

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