

MSG No. 27.83 $P_{acc}2$ [Type IV, orthorhombic]

Table 1: Wyckoff site: **4a**, site symmetry: $\dots 2$

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

Table 2: Wyckoff site: **4b**, site symmetry: $\dots 2$

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

Table 3: Wyckoff site: **4c**, site symmetry: $\dots 2'$

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

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

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

Table 5: Wyckoff site: **8e**, site symmetry: 1

| No. | position | mapping |
|-----|---------------|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[-x, -y, z]$ | [2] |

continued ...

Table 5

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