

MSG No. 37.183 $Cc'c'2$ [Type III, 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 | $[\frac{1}{2}, \frac{1}{2}, z]$ | $[5, 6]$ |
| 4 | $[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$ | $[7, 8]$ |

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 | $[\frac{1}{2}, 0, z]$ | $[5, 6]$ |
| 4 | $[\frac{1}{2}, 0, z + \frac{1}{2}]$ | $[7, 8]$ |

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

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

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

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