

MSG No. 45.237 $Ib'a2'$ [Type III, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: 1

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