

MSG No. 102.191 $P4_2n'm'$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 2..m'm'

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

Table 2: Wyckoff site: 4b, site symmetry: 2..

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

Table 3: Wyckoff site: 4c, site symmetry: ..m'

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

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

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