

MSG No. 104.205 $P4'n'c$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4' ..

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

Table 2: Wyckoff site: 4b, site symmetry: 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: 8c, site symmetry: 1

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