

MSG No. 79.25 *I*4 [Type I, tetragonal]

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

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

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

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

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

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