

MSG No. 75.5 P_C4 [Type IV, 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]	[5,6,7,8]

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

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

Table 3: Wyckoff site: 4c, site symmetry: 2'..

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

Table 4: Wyckoff site: 8d, 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]	[5]
6	[\frac{1}{2} - y, x + \frac{1}{2}, z]	[6]
7	[y + \frac{1}{2}, \frac{1}{2} - x, z]	[7]
8	[\frac{1}{2} - x, \frac{1}{2} - y, z]	[8]