

MSG No. 77.16  $P_c4_2$  [ Type IV, tetragonal ]

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

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

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

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

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

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

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

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