

MSG No. 77.14 $P4_21'$ [Type II, tetragonal]

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

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

Table 2: Wyckoff site: 2b, site symmetry: 2..1'

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

Table 3: Wyckoff site: 2c, site symmetry: 2..1'

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

Table 4: Wyckoff site: 4d, site symmetry: 11'

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