

MSG No. 91.104 $P4_1221'$ [Type II, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: .2.1'

No.	position	mapping
1	[0, y, 0]	[1,5,9,13]
2	[-y, 0, $\frac{1}{4}$]	[2,8,10,16]
3	[y, 0, $\frac{3}{4}$]	[3,7,11,15]
4	[0, -y, $\frac{1}{2}$]	[4,6,12,14]

Table 2: Wyckoff site: 4b, site symmetry: .2.1'

No.	position	mapping
1	[\mathbf{\frac{1}{2}}, y, 0]	[1,5,9,13]
2	[-y, \mathbf{\frac{1}{2}}, \mathbf{\frac{1}{4}}]	[2,8,10,16]
3	[y, \mathbf{\frac{1}{2}}, \mathbf{\frac{3}{4}}]	[3,7,11,15]
4	[\mathbf{\frac{1}{2}}, -y, \mathbf{\frac{1}{2}}]	[4,6,12,14]

Table 3: Wyckoff site: 4c, site symmetry: ..21'

No.	position	mapping
1	[x, x, $\frac{3}{8}$]	[1,7,9,15]
2	[-x, x, $\frac{5}{8}$]	[2,5,10,13]
3	[x, -x, $\frac{1}{8}$]	[3,4,11,12]
4	[-x, -x, $\frac{7}{8}$]	[6,8,14,16]

Table 4: Wyckoff site: 8d, site symmetry: 11'

No.	position	mapping
1	[x, y, z]	[1,9]
2	[-y, x, z + $\frac{1}{4}$]	[2,10]
3	[y, -x, z + $\frac{3}{4}$]	[3,11]
4	[x, -y, $\frac{1}{2}$ - z]	[4,12]
5	[-x, y, -z]	[5,13]
6	[-x, -y, z + $\frac{1}{2}$]	[6,14]
7	[y, x, $\frac{3}{4}$ - z]	[7,15]
8	[-y, -x, $\frac{1}{4}$ - z]	[8,16]