

MSG No. 103.198 $P4'cc'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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