

Relationships between C_{ij} and S_{ij} in the orthorhombic system (Belikov et al 70 reported in Oganov et al 02):

$$S_{11} = (C_{22}C_{33} - C_{23}^2) / D \quad (1)$$

$$S_{22} = (C_{11}C_{33} - C_{13}^2) / D \quad (2)$$

$$S_{33} = (C_{11}C_{22} - C_{12}^2) / D \quad (3)$$

$$S_{44} = 1/C_{44} \quad (4)$$

$$S_{55} = 1/C_{55} \quad (5)$$

$$S_{66} = 1/C_{66} \quad (6)$$

$$S_{12} = -(C_{12}C_{33} - C_{13}C_{23}) / D \quad (7)$$

$$S_{13} = (C_{12}C_{23} - C_{13}C_{22}) / D \quad (8)$$

$$S_{23} = -(C_{11}C_{23} - C_{13}C_{12}) / D \quad (9)$$

Where

$$D = C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} - C_{23}^2C_{11} - C_{12}^2C_{33} - C_{13}^2C_{22} \quad (10)$$