We establish quantitative correlations between pressure and temperature (PT) changes, and the degree of symmetry and of chirality of the main molecular building blocks of low quartz that these PT changes induce. The distortion from ideal tetrahedral symmetry, from helicity (deviation from $C_2$ symmetry), and the level of chirality are evaluated quantitatively using the continuous-symmetry and chirality-measures approach. These measures are global and reflect all changes in bond angles and bond lengths. The specific molecular building blocks analyzed are the SiO$_4$ elementary building block (which is found to be chiral!), the Si(OSi)$_4$ unit, the second-shell SiSi$_4$ tetrahedron [composed of the five Si atoms of Si(OSi)$_4$] and the four-tetrahedra helix fragment, $-$O(SiO$_3$)$_4$$. The temperature and pressure effects on symmetry and chirality were found to mirror each other in all building blocks. By employing this quantitative approach to symmetry and chirality we were able to combine the pressure effects and temperature effects into a unified picture. Furthermore, the global nature of the symmetry measure allows the comparison of the behavior of isostructural materials such as germania and quartz. For these crystals it has been shown that the symmetry/chirality behavior of germania at low pressures is a predictor for the behavior of these structural properties in quartz at higher pressures. Finally, given that the rigid SiO$_4$ unit undergoes only minor structural changes, it has been a useful observation that the symmetry/chirality of the small SiSi$_4$ tetrahedron is a very sensitive probe for the symmetry and chirality changes in quartz as a whole.

1. Background

Motto: ‘If you know a thing only qualitatively, you know it no more than vaguely. If you know it quantitatively – grasping some numerical measure that distinguishes it from an infinite number of other possibilities – you are beginning to know it deeply. You comprehend some of its beauty and you gain access to its power and the understanding it provides’ (Sagan, 1997).

1.1. The aim of this study

We are interested in the question of how changes in pressure and temperature (PT) affect the symmetry and chirality of the molecular building blocks of crystalline extended structures. We approach this question by treating symmetry and chirality as quantitative structural parameters, which change continuously. Our model material for this study is...