# Glass-forming ability of $TeO_2$ and temperature induced changes on the structure of the glassy, supercooled and molten state

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**Abstract**

Polarized (VV) and depolarized (VH) Raman spectra are obtained for glassy, supercooled, and molten $TeO_2$ at temperatures up to 1000 K in order to elucidate the temperature evolution of the pertinent structural and vibrational properties. The intrinsic tendency of the system for crystallization is avoided by means of a newly applied protocol, thereby enabling the recording of Raman spectra of pure $TeO_2$ on going from the molten to the supercooled liquid and to the room temperature glass states. Following an appropriate fitting procedure, the revealed bands are assigned to specific modes of structural polymorphs. A weak polarised band at ~880 $cm^{-1}$ is assigned to Te=O terminal stretching in agreement with literature *ab initio* molecular orbital calculations. Subtle changes to the relative band intensities within the 550-900 $cm^{-1}$ stretching region are caused by temperature increase. The network-like structure of the glass/melt is composed by $TeO_4$ trigonal bipyramid and $TeO_3$ trigonal pyramid units. With increasing temperature $TeO_4$ units convert to $TeO_3$ units with a concurrent increase in the number of Te=O sites resulting from cleavages within the network structure. The fraction of such terminal oxygen atoms has been directly estimated from the

spectroscopic data. The relative populations of the basic building blocks and the average number of O atoms around Te have been estimated for a wide temperature range directly from the Raman spectra, implying a gradual transformation of $TeO_{4/2}$ to $TeO_{2/2}(=O)$ trigonal pyramid units. The results are discussed in the context of the current phenomenological and theoretical status of the field.

**Θεματική περιοχή: Φυσικοχημεία - Θερμοδυναμική**