Structure of liquid GeO2 from a computer simulation model

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The structural properties of liquid GeO2 were investigated using molecular dynamics simulation. A comparison of the obtained pair correlation functions, coordination number, angular distribution, and both the neutron and x-ray static structure with those of liquid silica was presented. It was found that in the liquid state the short range order was dominated by the presence of slightly distorted Ge(O1/2)4 tetrahedra. The results of simulation of systems at higher densities indicated a volume collapse in the pressure-volume curve in the range 4-8 GPa, which suggested the possibility of liquid-liquid phase transition to occur.