CALCULATION OF RAMAN FREQUENCIES AS FUNCTIONS OF TEMPERATURE AND PRESSURE IN PHASES OF SOLID I, II AND III (III') OF BENZENE

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The Raman frequencies of the lattice modes (A,B and C) are calculated as a function of temperature at constant pressures of 0, 1.4 and 3.05 GPa in the solid phase I of benzene using the volume data through the mode Grüneisen parameter. The Raman frequencies of those lattice modes (A, B and C) are also calculated as a function of pressure at constant temperatures of 274 and 294K in the solid phase I of benzene using the volume data.

Finally, calculation of the Raman frequencies of the lattice modes (A, B and C) studied here are calculated at various pressures (T=294 K) in the solid phases of II, III and III' of benzene using the volume data from the values of the Grüneisen parameter of the lattice modes. Our calculated frequencies of the Raman modes studied decrease with increasing temperature and they increase with increasing pressure in phase I, as observed experimentally. The calculated Raman frequencies of the lattice modes A, B and C also increase as the pressure increases in the phases II, III and III', as reported experimentally. This shows that our method of calculating the Raman frequencies from the volume data is satisfactory to predict the observed behavior in the solid phases of I, II, III and III' in benzene.