THE RAMAN FREQUENCY SHIFTS RELATED TO THE THERMODYNAMIC QUANTITIES CLOSE TO THE PHASE I - PHASE II TRANSITION IN NH_4Br

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We establish here the modified Pippard relations by relating the specific heat C_p to the frequency shifts $\frac{1}{\nu}\left(\frac{\partial\nu}{\partial T}\right)_P$ and also the thermal expansivity α_p to the $\frac{1}{\nu}\left(\frac{\partial\nu}{\partial P}\right)_T$ for the ν (140 cm^{-1}) Raman mode of NH_4Br close to its phase I- phase II transition. From our linear plots of C_p vs. $\frac{1}{\nu}\left(\frac{\partial\nu}{\partial T}\right)_P$ and α_p vs. α_p to the $\frac{1}{\nu}\left(\frac{\partial\nu}{\partial P}\right)_T$, we extract the values of the slope DP/dT, which are close to the experimental value of 28.2 bar/°C near the phase I-phase II transition in NH_4Br.