LATTICE DYNAMICS OF DEUTERATED BROMOFORM IN THE SOLID PHASE

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The crystal structure of solid phases of deuterated bromoform ($CDBr_3$) were determined using neutron techniques/1/. The alpha phase is stable between 8°C and -5°C; the beta phase is stable between -5°C and -175°C and the gamma phase is formed by rapid cooling of the liquid $CDBr_3$ to liquid nitrogen temperature. The crystal structure of $CHBr_3$ were reported by by Kawaguchi et al/2/ and it was concluded that /3/ they observed only the alpha phase of $CHBr_3$. Raman and IR data were reported in these systems /3,4/. The lattice dynamical calculations in alpha phase of $CHBr_3$ /5,6/ showed satisfactory results. Along these lines the present work reports the phonon calculations in gamma phase of $CDBr_3$ employing the external mode formalism in complex crystals/7/. Employing suitable potential parameters/2/ the static and dynamic equilibrium conditions are verified. The vanishing of forces at atoms and torques at molecules suggests the validity of these potential parameters. In the harmonic rigid molecular approximation for external modes the secular equation

$$| B(q) - w^2(q)\, m | = 0$$

is set up and the phonons are calculated at the zone centre for gamma phase of $CDBr_3$. In the above equation m is the diagonal matrix of masses and principal moments of inertia and the dynamical matrix B(q) is estimated using the non bonded atom-atom interactions/7/. The calculated phonons are 57, 48,47,43,35, 27,24,15,10 cm^{-1}, whereas the experimental Raman data /4/ are 52, 44,39 cm^{-1} . Low frequency spectra of polycrystalline $CHBr_3$ at 20 K consists of Raman active peaks at 53, 48, 39, 34,30cm^{-1} and IR absorption bands at 55,39 cm^{-1}. Hence our calculations in gamma phase of $CDBr_3$ are satisfactory and extensive calculations in all allowed q vectors in the first Brillouin Zone are under progress. Comparative studies of the phonons in all the three phases of $CDBr_3$ and $CHBr_3$ will remove speculations in assignments of vibrational frequencies in these systems.

References

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