Helical Lattice Vibrational Modes in DNA

A recent Letter by Grimm *et al.*[1] reported the observation of umklapp-phonon scattering at subterahertz frequencies in DNA by inelastic neutron scattering. They found that the nearly linear dispersion of their results did not extrapolate to zero frequency at zero wave vector as a simple acoustic mode should and that the data could be best fitted by a dispersion relation $\omega^2=\omega_0^2+v^2(\Delta Q)^2$ where $\omega_0/2\pi$ was 0.4 THz. On the other hand, in two earlier observations[2,3] carried out by Brillouin scattering, between 5 and 20 GHz, the acoustic mode is seen to behave normally and extrapolate to zero frequency at zone center. We explore a lattice-dynamics calculation that can account for the subterahertz observation and the lower-frequency acoustic results in a consistent way. We use refined bonded force constants and reasonable assumptions about unbalanced charges and dielectric behavior of the DNA helix.

The lowest optical mode at zone center in Fig. 1 has been observed experimentally,[4] as well as other optical modes calculated by the lattice theory.[5] As seen in Fig. 1 the lowest longitudinal acoustic branch does extrapolate linearly to zero frequency at zone center. The Brillouin observations in the gigahertz region fall on this branch. The heavy lines indicate the continuation of the compressional character of the phonons on the successive branches of the dispersion plot of Fig. 1. The experimental resolution is such that the splitting of the branches near the crossover cannot be seen. We note that a feature exists in the experimental data near the second from bottom optic-acoustic crossover that is consistent with the predicted region of crossover.

The value of the acoustic velocity from this calculation is 4.5 km/s. To compare with the Brillouin work in the gigahertz region, we changed the long-range water dielectric to 45 (from 9) and calculated an acoustic velocity of 3.1 km/s. This is about what would be expected for a helix unburdened by water of hydration, based on measurements by Lee *et al.*[6]

This work is supported by National Institutes of Health Grant No. GM 24443 and U.S. Office of Naval Research, Grants No. N00014-86-K-0252 and No. N00014-87-K-0162.

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Received 6 November 1987
PACS numbers: 87.15.−v, 25.40.Fq, 43.20.+g

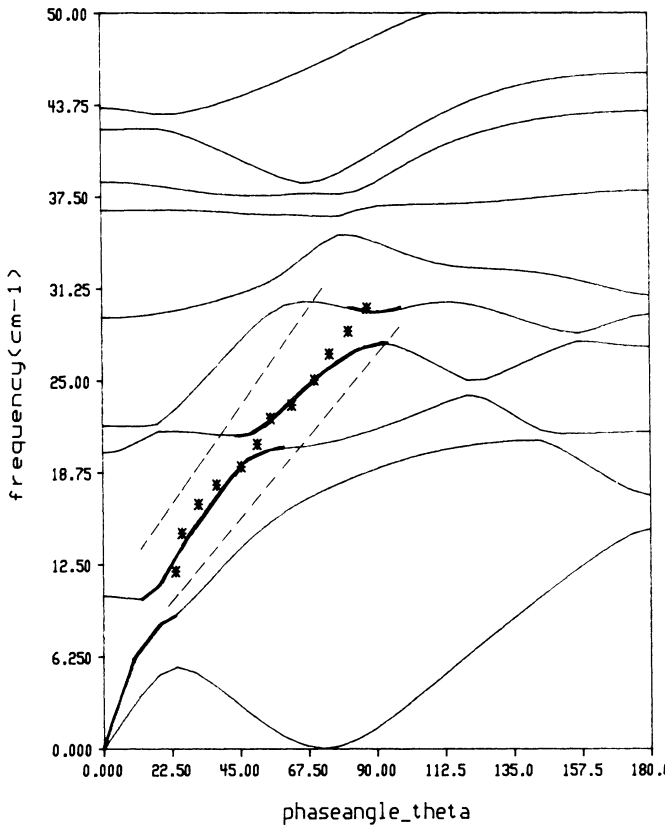

FIG. 1. The continuous lines are our helical lattice dispersion calculations of the phonon spectrum of DNA. The θ axis is displayed in degrees of phase shift from one unit cell of two DNA base pairs to the next. The central row of stars shows the reported frequencies from the neutron data and the outer rows of dashes show the reported FWHM line width. The heavy lines indicate the continuation of the compressional character of the phonons on the successive branches of the dispersion plot.

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