total energies of the more stable staggered form of C₂H₆
and the eclipsed form is 2.90 kcal/mole. This may be
compared with the experimental rotation barrier of
2.93 kcal/mole. The most elaborate LCAO calculation
for ethane is the one recently published by Veillard. Using
a large Gaussian basis set and the program IBMOL, Veillard calculated a barrier of 3.65 kcal/mole
for the experimental geometry and a barrier of 3.07
cal/mole for the optimized geometry. The close agree­
ment obtained recently with the

\[ \text{SCF-Xα-SW} \]

satisfied by the statistical total energy and kinetic
energy for both the staggered and eclipsed conforma­
tions, indicating stable and metastable equilibrium,
respectively. Close agreement between the

\[ Xα \]

method, in only a few minutes of computer time, is
not fortuitous. The virial theorem is approximately
satisfied by the

\[ \text{SCF-Xα-SW} \]

was extended to bandgap phonons and in-band
phonons. Some of the

\[ \text{LCAO} \]

was established in the last decade. Originally it applied only
to guest localized phonons with energy well above the
fundamental host phonon band, but subsequently it
was extended to bandgap phonons and in-band
"resonance" phonons. Some of the "resonance phonons" are by implication pseudolocalized, that is,
characterized by a large amplitude at the guest site
and by small but finite amplitudes extended throughout
the host crystal. In contrast, a localized excitation has
not only a maximum amplitude at the guest site, but
also its amplitudes at host sites decay asymptotically with increased distance from the guest. In 1965
Dettman and Ludwig established the concept of a
rotational (librational) localized phonon in a molecular
lattice with the help of a model calculation on a
linear-chain doped molecular crystal. An important
result of their investigation was that localized as well
as pseudolocalized guest rotations are possible in the
frequency region of host translations (but not rotations). We present below an experimental verification
of this concept of localized and/or pseudolocalized
rotational phonons for two real, three-dimensional
systems and suggest that this phenomenon should be
quite general for chemically mixed molecular crystals.

A criterion for localization or pseudolocalization is

\[ \text{localized In-Band Rotational Phonons in Mixed Molecular Crystals: Electronic Spectra of Naphthalene Doped Biphenyl and Durene*} \]

Peter H. Chereau, Peter S. Friedman, and Raoul Kopelman
Department of Chemistry, The University of Michigan, Ann Arbor, Michigan 48104
(Received 23 December 1971)

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LETTERS TO THE EDITOR

Coherence Length in the Isotropic Phase of a Nematic Liquid Crystal:
$p$-Methoxybenzylidene $p$-n-Butylaniline

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(Received 24 January 1972)

In this Communication we report the results of an experimental study of the angular dependence of the intensity of light scattered by fluctuations of the order parameter $Q^1$ in the isotropic phase of a nematic liquid crystal, $p$-methoxybenzylidene $p$-n-butylaniline (MBBA). The intensity and spectrum of

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In this context we note that our observed guest frequencies of 12.5 and 17 cm$^{-1}$ (Figs. 1 and 2) are well below the lowest observed rotational lattice modes of the biphenyl and durene hosts, but well inside their translational manifolds as required by Dettman and Ludwig's model. Experiments have been performed on samples immersed in supercooled helium (1.8 K). The spectra were taken at a resolution of 0.5 cm$^{-1}$ on a Jarrell–Ash 1 m double grating monochromator (photographically and photoelectrically). The sample preparation will be discussed in full separately. We only point out here that the crystals were of good to perfect optical quality, that the data are reproducible and that the nominal guest concentrations of 0.5%–1% are really upper limits, due to segregation upon crystallization, etc.

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* Supported by NSF Grant GP-18718 and NIH Grant NS08116.
6 This is not the same "phonon" observed in emission experiments by us (unpublished) and earlier by R. M. Hochstrasser and G. J. Small, J. Chem. Phys. 48, 3612 (1968).
11 A. Hadni, Ibid., p. 31.
13 The spectrum of Fig. 1 was discussed in terms of localized guest rotations by P. S. Friedman and R. Kopelman, Molecular Structure and Spectroscopy Symposium, Ohio State University, Columbus, N. 2, 1969; U. S. 3, 1971. Figure 2 was discussed by P. K. Chereson and R. Kopelman, Ibid., U. S. 5, 1971. R. Ostertag and H. C. Wolf, Phys. Status Solidi 31, 139 (1969), could not satisfactorily explain anthracene doped naphthalene spectra in terms of host phonons and suggested the possibility of a local oscillator. G. J. Small, J. Chem. Phys. 52, 656 (1970), discussed pseudolocalized phonons in some doped molecular crystals and R. M. Hochstrasser and P. N. Prasad (private communication) have very recently discussed some conditions for host vs localized phonon side bands in mixed crystals.