CC/NUMBER 51
DECEMBER 17, 1979

This Week's Citation Classic

Pawley G S. A model for the lattice dynamics of naphthalene and anthracene. *Phys. Stat. Sol.* **20**:347-60, 1967. [Department of Natural Philosophy, University of Edinburgh, Edinburgh, Scotland]

The theoretical and experimental work on the lattice dynamics of molecular crystals has grown over the years from these small beginnings to an international endeavour. [The *SCI*® indicates that this paper has been cited over 155 times since 1967.]

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October 1, 1979

"The field of molecular lattice dynamics is, at this moment, making major advances, and so I am particularly pleased that my paper has been chosen for this issue. In it was the first realistic calculation of the phonon spectra of typical molecular solids (naphthalene and anthracene), though this claim may well be made for the earlier work on hexamethylene-tetramine inspired by Bill Cochran, who was my supervisor at the time.[1]

"Many of those working in the field of lattice dynamics were content to study cubic crystals, and were perhaps a little wary of the oblique axes of the monoclinic system. I had enjoyed a thorough undergraduate course on crystallography at Cambridge and was undaunted by obliquity. By accident I had also studied organic chemistry and could accept the long names with equanimity, treating the exotic molecules as the humble rigid bodies of classical mechanics.

"Others may have been deterred by the lack of a thoroughly reliable intermolecular potential, especially in the long range attraction, but I followed the prophesy of Kit (A.I. Kitaigorodskii) that all potentials are much the same, and came up with a result which has recently been shown by experiment to be remarkably close to the truth.

"This experimental work has been blessed by fruitful and happy cooperation with scientists from Denmark, Russia, Poland, and Germany. I value such cooperation highest in my work, as this is our contribution to international understanding. Closely related work also involves co-workers from Canada, Finland, Yugoslavia, Italy, and France— may I thank my colleagues in this quasi-anonymous way?

"Further work on theoretical models is being retarded by a fixation of mine that all models should be based on an equilibrium structure. It is self-evident that a crystal is in equilibrium, but it is difficult to get a model to give equilibrium with the molecules at their known positions. In the cited paper the molecules were allowed to relax into an equilibrium configuration, whereupon all the calculated physical properties are true to the model. Nonequilibrium calculations, with their concomitant physical contradictions, leave me sceptical, but I am being persuaded that some form of compromise is necessary.

"Comparing the early calculations with recent measurements is satisfying indeed,[2] but I can rejoice that the old model is not fully adequate —experiments are now sufficiently sensitive that they demand a greater sophistication in the theory, and thereby ensure continued international cooperation for some time to come!"

1. **Cochran W & Pawley G S**. The theory of diffuse scattering of X-rays by a molecular crystal. *Proc. Roy. Soc. London A* **280**:1-22, 1964.
2. **Schmelzer U, Dorner B, Kalus I, Natkaniec I, Oslertag R, Pawley G S, Mackenzie G A, Sheka E F** & **Bokhenkov E L.** Pressure dependence of lattice frequencies of deuterated naphthalene at 100K. *Phys. Stat. Sol. B.* **91**.K27-9, 1979.