This Week's Citation Classic®

Diehl P, Khetrapal C L & Kellerhals H P. The N.M.R. spectrum of pyridine oriented in the nematic phase. *Molec. Phys.* 15:333-7, 1968.
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NMR spectra of molecules oriented in liquid crystals are much more informative than those in "isotropic" media and provide the only direct method for the precise determination of molecular geometries in the liquid phase. This work deals with the foundations of the interpretation of such spectra in multi-spin systems. [The *SCI*® indicates this paper has been cited in more than 115 publications.]

NMR of Molecules Oriented in Liquid Crystals

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The discovery that the NMR spectra of molecules oriented in the nematic phase of liquid crystals contain information on molecular geometries' has opened a new branch of research dealing with structure, conformation, and function of molecules. Though the potentials and the promises of the technique become apparent from the principles underlying the phenomena, the actual developments have some interesting episodes associated with them.

When I reached Basel, Switzerland, in September 1967, as a postdoctoral fellow on leave from the Tata Institute of Fundamental Research, Bombay, India, I was asked to start work in this new field. Though we realized that the future of NMR lay in this area, we were initially not enthusiastic because of difficulties[2] others in the field had experienced. Furthermore, our knowledge of the subject was close to nil. Not much literature was available. This was an advantage in that the entire sea was available to us for exploration. But, the disadvantage was that we might not believe our own observations. Nevertheless, we started the work and got encouraging results on the first day! Such a rapid and unexpected success resulted in heated arguments, discussions, and fights among us, and we did not talk to each other for the next two days! During these two days, both sides were busy in proving their points of view and, finally, a cool drink outside the campus in a cafeteria was considered essential to bring us together again! We were then convinced that our success was genuine, and we entered the field with full force.

Initially, we concentrated on the use of the technique for the determination of the structure and function of small molecules in order to understand the intricacies involved. Then, we went deeper to explore ways and means of making the method more versatile. In the meantime, several other active groups entered the field, and developments exploded.

One of the major difficulties experienced in this area was the rapid increase of the spectral complexity with the number of interacting nuclei. Consequently, developments in the area of the use of computers for interpreting such spectra and correlating the derived information with molecular structures[3] were considered essential.

This publication is the first such effort and hence has found widespread use by a large number of workers.[4] Subsequently, numerous developments to handle complex spectra have taken place.[5,6] Some of these advances involve the use of isotopically enriched species, multiple quantum spectroscopy.multipulse experiments, automatic analysis, variable and magic angle sample spinning, mixed solvents, and electric and high magnetic fields.

The current interest and future hopes for developments in the area of novel techniques as aids for the interpretation of the NMR spectra of strongly coupled, oriented systems suggest that only a small and humble beginning was made in the publication of this early paper.

1. **Saupe A & Englert G.** High-resolution nuclear magnetic resonance spectra of oriented molecules. *Phys. Rev. Lett.* 11:462-4, 1963. (Cited 190 times.)
2. **Buckingham A D & McLauchian K A**. *Progress in NMR spectroscopy.* (Emsley J W. Feeney J & Sutcliffe L H. eds.) Oxford. England: Pergamon Press, 1967. Vol. 2. (Cited 105 times.)
3. **Diehl P, Henrichs PM& Niederberger W.** A study of the molecular structure and of the barrier to methyl rotation in o-chjorotoluene partially oriented in the nematic phase. *Molec. Phys.* 20:139-45, 1971. (Cited 185 times.)
4. **Diehl P & Khetrapal C L**. NMR studies of molecules oriented in the nematic phase of liquid crystals. *NMR—Basic Princ. Prog.* 1:1-95, 1969. (Cited 190 times.) [See also: **Diehl P & Khetrapal C L.** Citation Classic. *Current Contents/Physical. Chemical & Earth Sciences* 23(43): 18. 24 October 1983. Reprinted in: *Contemporary classics in physical, chemical, and earth sciences.* (Thackray A, comp.) Philadelphia: IS1 Press. 1986. p. 269.]
5. **Khetrapal CL& Kunwar A C.** (Webb G A, ed.) *Nuclear magnetic resonance: oriented molecules.* London: Royal Society of Chemistry. 1982. Vol. 11. p. 248-63.
6. **Khetrapal C L, Weiss R G & Kunwar** A C. (Bahadur B. ed.) *Liquid crystals—applications and uses.* London: World Scientific, 1990. Vol. 2.

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